UNIVERSITÉ DE LORRAINE

École doctorale IAEM Lorraine

États fondamentaux dans l'approximation quasi-classique pour des modèles d'électrodynamique quantique non relativiste

THÈSE

présentée et soutenue publiquement le 12 Mai 2023

pour l'obtention du

Doctorat de l'Université de Lorraine

(mention Mathématiques)

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Remerciements

Mes premières pensées vont évidemment à mes directeurs de thèse : Jérémy Faupin et Sébastien Breteaux. Il serait difficile de leur faire honneur et de montrer en seulement quelques lignes à quel point je leur suis reconnaissant pour ces années. Merci à eux pour leur bienveillance, leur patience, leurs conseils avisés, leur soutien, leur sympathie, leur bonne humeur constante, et pour tout ce qu'ils m'ont apporté et appris durant cette thèse.

Merci à Nicolas pour tout, pour nos discussions et tes conseils, les conférences et les formations passées ensemble. Merci aussi à toutes ces personnes que j'ai pu rencontrer, qu'ils ou elles soient de Metz ou de Nancy, qu'ils ou elles soient doctorants ou personnels de l'université, un grand merci pour ces années.

Je remercie du fond du coeur ma famille et mes amis. Merci à mes parents qui n'ont jamais cessé de m'encourager depuis le début de mes études. Merci à Jason et à Jonathan pour tout, pour nos parties, nos appels, nos week-ends, nos délires, nos aventures ! Merci Claudine, pour votre soutien sans failles et vos conseils bienveillants.

Merci à toi Léa, pour ta force et ton soutien indéfectible qui me porte depuis toutes ces années, et pour le magnifique cadeau que tu t'apprêtes à nous faire au moment où j'écris ces lignes. Il me tarde de voir notre famille s'agrandir !

Table des matières

Introduction générale

1 Hamiltoniens de Pauli-Fierz

La théorie quantique des champs fournit un cadre théorique à l'étude de systèmes quantiques composés d'un nombre infini de particules. Parmi les quatre interactions fondamentales présentes dans la nature, trois (les interactions électromagnétiques, faibles et fortes) peuvent être décrites grâce à la théorie quantique des champs. L'interprétation commune est que les interactions fondamentales sont véhiculées par l'intermédiaire de quanta (particules du champ quantifié), les photons dans le cas de l'interaction électromagnétique, les bosons vecteurs intermédiaires dans le cas de l'interaction faible, et les gluons dans le cas de l'interaction forte.

Le cadre de cette thèse est *l'électrodynamique quantique non relativiste*. C'est une théorie quantique des champs de l'électromagnétisme qui décrit l'interaction des particules chargées pour des énergies basses. Plus particulièrement, dans cette thèse, on s'intéresse à un système composé d'une particule non relativiste (par exemple, un électron) interagissant avec un champ de bosons quantifié (par exemple, des photons). D'un point de vue mathématique, le formalisme adopté est celui de la seconde quantification. Les états du système sont des vecteurs de norme 1 dans un espace de Hilbert que l'on note $\mathcal{H}$, et qui est donné par le produit tensoriel suivant :

$$\mathcal{H} = \mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}},$$

où l'espace $\mathcal{H}_{\mathrm{el}}$ représente les états de la particule, tandis que $\mathcal{H}_{\mathrm{f}}$ représente les états du champ quantifié. Dans les travaux exposés dans cette thèse, l'espace $\mathcal{H}_{\mathrm{f}}$ décrit les états d'un champ de bosons scalaires ou bien du champ électromagnétique quantifié. L'espace $\mathcal{H}_{\mathrm{f}}$ est alors donné par l'espace de Fock symétrique associé à un espace de Hilbert $\mathfrak{h}$:

$$\mathcal{H}_{\mathrm{f}} := \mathfrak{F}_s(\mathfrak{h}) = \bigoplus_{n=0}^{\infty} \bigvee^{n} \mathfrak{h}, \quad \bigvee^{0} \mathfrak{h} = \mathbb{C}.$$

où $\mathfrak{h}$ est donné par l'espace $L^2(\mathbb{R}^3)$ dans le cas d'un champ *scalaire*, ou bien par l'espace $L^2(\mathbb{R}^3; \mathbb{C}^2)$ dans le cas du champ de photons transverses. L'énergie d'un tel système est associée à un opérateur auto-adjoint $\mathbb{H}$, agissant sur $\mathcal{H}$, appelé Hamiltonien de *Pauli-Fierz*, introduit par les auteurs éponymes dans l'article [104]. De façon générale, un Hamiltonien de Pauli-Fierz se présente sous la forme suivante

$$\mathbb{H} = H_{\text{el}} \otimes \mathbf{I}_{\text{f}} + \mathbf{I}_{\text{el}} \otimes \mathbb{H}_{\text{f}} + \mathbb{H}_{\text{int}}.$$

L'opérateur H_{el} représente l'énergie de la particule et $\mathbb{H}_{\text{f}}$ l'énergie du champ, tandis que l'opérateur $\mathbb{H}_{\text{int}}$ correspond à l'interaction entre les deux précédents systèmes cités. L'opérateur d'interaction est parfois considéré dépendant d'une constante de couplage g qui peut être traitée comme un petit paramètre. L'énergie du champ de bosons est donnée par la seconde quantification de l'opérateur de multiplication par la relation de dispersion du champ, notée ω :

$$\mathbb{H}_{\text{f}} := \mathrm{d}\Gamma(\omega),$$

(voir l'appendice 1.4.1 pour une définition précise des opérateurs second quantifiés). Notons que pour que ces modèles aient un sens mathématique rigoureux, il est souvent nécessaire d'introduire dans la partie décrivant l'interaction un paramètre supplémentaire et non-issu de la physique : une *troncature ultraviolette*. En effet, hormis dans quelques cas particuliers, pour que le modèle soit bien défini, l'interaction entre la particule non relativiste et les hautes énergies du champ doit être négligée (voir par exemple les livres [37, 105] de A. Das et M.E. Peskin et D.V. Schroeder pour plus de détails). Dans [102], E. Nelson a développé une procédure de renormalisation permettant de définir un modèle d'une particule non relativiste couplée linéairement à un champ de bosons scalaire dans la limite ultraviolette. Pour d'autres systèmes, la définition de modèles de Pauli-Fierz renormalisés dans la limite ultraviolette reste un problème ouvert important. Son étude fait aujourd'hui encore l'objet de recherches très actives. Citons notamment les articles récents de B. Alvarez et J. Møller [1], ou encore J. Lampart [81], qui proposent une renormalisation du modèle de départ afin de s'affranchir du paramètre ultraviolet.

L'image physique générale décrivant l'évolution asymptotique de systèmes représentés par un hamiltonien de Pauli-Fierz est la suivante : étant donné un état initial quelconque, le système, au bout d'un temps infini, retourne à l'équilibre en émettant des bosons qui se propagent à l'infini à vitesse constante. Afin de justifier ce phénomène, on s'intéresse notamment au spectre de l'opérateur $\mathbb{H}$. Une première propriété à laquelle on s'attend est l'existence d'un *état fondamental*, correspondant à l'état d'équilibre du système. Autrement dit, on s'attend à ce que l'infimum du spectre du Hamiltonien $\mathbb{H}$, appelé *énergie fondamentale*, soit une valeur propre.

De nombreuses difficultés bien connues apparaissent lorsqu'on essaye de démontrer cette propriété. En particulier, la théorie usuelle des perturbations de valeurs propres isolées n'est pas applicable. De plus, l'interaction n'est pas une perturbation relativement compacte du Hamiltonien libre ; même pour de petites valeurs de la constante de couplage, l'étude spectrale du Hamiltonien total reste délicate.

La théorie spectrale et de la diffusion des Hamiltoniens de Pauli-Fierz a fait l'objet de nombreuses études depuis la fin des années 90. Citons notamment les travaux fondateurs de V. Bach, J. Fröhlich et I.-M. Sigal [11, 12], J. Derezinski et C. Gérard [40, 53], ou encore M. Griesemer, E. Lieb et M. Loss [63]. En particulier, l'existence d'un état fondamental sans restriction sur la petitesse de la constante de couplage est démontrée dans ces articles, à la fois pour une particule non relativiste linéairement couplée à un champ scalaire [53] et pour le modèle standard de l'électrodynamique quantique non relativiste [63]. D'autres propriétés sont également établies, par exemple la complétude asymptotique des opérateurs d'ondes pour des modèles de champs massifs [40] ou l'existence de résonances issues des états excités non perturbés [11]. De nombreux auteurs depuis se sont penchés sur des questions liées. On peut citer, sans être exhaustif, les travaux suivants [6, 8, 10, 13, 16, 38, 46, 52, 62, 68, 71, 76, 87, 110, 111] ainsi que les références contenues dans ces articles.

2 États cohérents et énergie quasi-classique

Étant donné un opérateur auto-adjoint A, on note $\mathcal{Q}(A)$ son domaine de forme. Le calcul explicite de l'énergie fondamentale

$$\inf_{\Psi\in\mathcal{Q}(\mathbb{H}),\|\Psi\|=1} \langle \Psi, \mathbb{H}\,\Psi\rangle_{\mathcal{H}}$$

pour des Hamiltoniens de Pauli-Fierz est en général un problème difficile. Selon le modèle considéré, plusieurs techniques permettent d'en calculer un développement asymptotique pour un petit couplage. On peut citer entre autres les travaux de V. Bach, J. Fröhlich et I.-M. Sigal dans leurs articles [11, 12], M. Griesemer et D. Hasler dans [62] ou encore D. Hasler et I. Herbst dans l'article [71] où un développement est obtenu en utilisant un "groupe de renormalisation spectral".

D'autres techniques permettent d'obtenir un même type de résultat. On pourra consulter les articles de C. Hainzl [68], I. Catto et C. Hainzl [29], C. Hainzl, M. Hirokawa et H. Spohn [69], J.-M. Barbaroux, T. Chen, V. Vougalter et V. Vugalter [15, 16], J.-M. Barbaroux et S. Vugalter [17], qui traitent le problème à l'aide d'une procédure d'itération variationnelle, ou encore les articles de A. Pizzo [106], et V. Bach, J. Fröhlich et A. Pizzo [10] qui utilisent de l'analyse multi-échelle itérative.

Dans cette thèse, on s'intéresse à des approximations de l'énergie fondamentale en étudiant l'énergie du modèle lorsque le champ se trouve dans un état ayant une structure particulière. Mentionnons ici les articles de E. Lieb et M. Loss [87] et de V. Bach et A. Hach [13] qui considèrent l'infimum de la fonctionnelle d'énergie calculée sur des états produits,

$$\inf_{(u,\Psi)\in\mathcal{Q}(H_{\mathrm{el}})\times\mathcal{Q}(\mathbb{H}_{\mathrm{f}}),\|u\|=\|\Psi\|=1} \langle (u\otimes\Psi), \mathbb{H}(u\otimes\Psi)\rangle_{\mathcal{H}}$$

pour le modèle standard de l'électrodynamique quantique non relativiste invariant par translation. Il est montré dans [13, 87] que cette quantité diverge comme $\Lambda^{12/7}$ dans la limite ultraviolette. Dans [9], V. Bach, S. Breteaux et T. Tzaneteas, pour le même modèle et à impulsion totale fixée, montrent l'existence et l'unicité d'un minimiseur pour l'énergie lorsqu'on restreint Ψ à la classe des états quasi-libres purs. Ils obtiennent de plus un développement asymptotique du minimum de l'énergie associée pour un petit couplage, ainsi que les équations de Lagrange pour le minimiseur.

Ici nous considérons le champ lorsqu'il se trouve dans un *état cohérent*, qui correspond en quelque sorte à un état classique d'un système quantique. Plus précisément, les états cohérents correspondent à des états quantiques d'oscillateur harmonique quantique qui ressemblent à ceux d'un oscillateur harmonique classique. Visuellement, on peut imaginer une fonction d'onde, qui décrit les états quantiques du système, osciller de la même façon que l'oscillateur harmonique classique. On pourra consulter par exemple le livre de Y. Castin [28] pour une définition plus précise des états cohérents. On pourra aussi consulter les articles de K. Hepp [74], J. Ginibre et G. Velo [56], ainsi que celui de M. Lewin, P.T. Nam et B. Schlein [86] pour l'utilisation des états cohérents dans l'étude de la limite de champ moyen.

D'un point de vue mathématique, un état cohérent correspond à une fonction de Gauss que l'on aurait translatée dans l'espace des phases, c'est-à-dire en position puis en impulsion. L'état cohérent centré en (x_0, ξ_0) en dimension finie $d \in \mathbb{N}$ est alors donné par la fonction de norme 1 suivante :

$$\varphi_{(x_0,\xi_0)}(x) = \pi^{-d/4} e^{-i\xi_0(x-x_0/2)} e^{-(x-x_0)^2/2}, \quad \forall x \in \mathbb{R}^d.$$

Dans la représentation de Fock, un état cohérent d'un système quantique de dimension infinie est donné par un opérateur de Weyl agissant sur le vide Ω : On considère f dans $\mathfrak{h}$, l'état cohérent Ψ_f de paramètre f est :

$$\Psi_f := e^{i\Phi\left(\frac{\sqrt{2}}{i} f\right)}\Omega, \quad \|\Psi_f\| = 1,$$

où $\Phi(f) = a^*(f) + a(f)$ est l'opérateur de champ paramétré par f, et où a^* et a sont respectivement les opérateurs de *création* et d'*annihilation* dans l'espace de Fock $\mathfrak{F}_s(\mathfrak{h})$:

$$\begin{aligned} a^*(f)_{|\bigvee^n \mathfrak{h}} &= \sqrt{(n+1)}\; |f\rangle \bigvee \mathbf{I}_{\bigvee^n \mathfrak{h}}, \quad n \geq 0, \\ a(f)_{|\bigvee^n \mathfrak{h}} &= \sqrt{n}\; \langle f| \otimes \mathbf{I}_{\bigvee^{n-1} \mathfrak{h}}, \quad n > 0, \qquad a(h)_{|\mathbb{C}} = 0. \end{aligned}$$

La particularité des états cohérents vient du fait que ce sont des vecteurs propres de l'opérateur d'annihilation. Si on considère f et g deux fonctions dans $\mathfrak{h}$, alors :

$$a(g)\Psi_f = \langle g, f\rangle\, \Psi_f\,.$$

Notons que, généralement, l'interaction entre le champ quantifié et la particule non relativiste est donnée en fonction d'un opérateur de champ, tandis que l'énergie cinétique du champ est donnée par la seconde quantification de la relation de dispersion, et que cet opérateur peut aussi être exprimé en fonction des opérateurs de création et d'annihilation. Ainsi, lorsque l'énergie d'un champ quantifié est évaluée sur des états cohérents, cela revient en quelque sorte, à étudier les états classiques du champ. Plus rigoureusement, on ajoute une dépendance en un certain paramètre ε aux opérateurs de création et d'annihilation. On pose

$$a_\varepsilon^* = \sqrt{\varepsilon} a^*, \quad a_\varepsilon = \sqrt{\varepsilon} a\,,$$

et on considère l'opérateur Hamiltonien quasi-classique $\mathbb{H}_\varepsilon$ obtenu en remplaçant a^* et a par a_ε^* et a_ε respectivement. L'idée est alors d'étudier les propriétés dynamiques et spectrales de l'opérateur $\mathbb{H}_\varepsilon$ lorsque ε tend vers 0. En ce sens, les travaux récents de M. Falconi [45], Z. Ammari et M. Falconi [3], M. Correggi, M. Falconi et M. Olivieri [31, 33–35] (voir aussi des travaux antérieurs de J. Ginibre et G. Velo [57], J. Ginibre, F. Nironi et G. Velo [55], Z. Ammari et F. Nier [5], N. Leopold et P. Pickl [83], et les références contenues dans ces articles) montrent, entre autres, la propriété suivante

$$\inf_{\Psi \in \mathcal{Q}(\mathbb{H}), \|\Psi\|=1} \langle \Psi, \mathbb{H}_\varepsilon \Psi \rangle \underset{\varepsilon \to 0}{\longrightarrow} \inf_{(u,f) \in \mathcal{Q}(H_{\text{el}}) \times \mathfrak{h}, \|u\|=1} \mathcal{E}(u, f) \, ,$$

où $\mathcal{E}$ est la fonctionnelle d'énergie quasi-classique définie par :

$$\mathcal{E}(u, f) = \langle (u \otimes \Psi_f), \mathbb{H}(u \otimes \Psi_f) \rangle_{\mathcal{H}} \, ,$$

et où Ψ_f est un état cohérent de paramètre f. Cette thèse est dédiée à l'étude de la fonctionnelle $\mathcal{E}$, définie par l'expression précédente. Les principaux résultats de cette thèse sont les suivants : un premier résultat concerne le modèle spin-boson, pour lequel la particule non relativiste est décrite par un système de dimension finie et est couplée linéairement à un champ quantifié scalaire. On obtient pour ce modèle une expression explicite de l'énergie fondamentale quasi-classique et de l'ensemble des minimiseurs, pour toute valeur de la constante de couplage. On montre également que l'ensemble des minimiseurs est trivial si la constante de couplage est inférieure à une valeur critique. On considère ensuite des modèles physiquement plus réalistes pour lesquels la particule non relativiste est décrite par un opérateur de Schrödinger dans $L^2(\mathbb{R}^3)$. Dans le cas où le couplage entre la particule et le champ est linéaire en les opérateurs de création et d'annihilation (modèle de Nelson, modèle du Polaron), on montre l'existence et l'unicité d'un état fondamental quasi-classique associé à l'énergie $\mathcal{E}$, à symétrie de phase près. On suppose le potentiel extérieur le plus général possible et nous n'imposons pas de troncature ultraviolette dans la définition de la fonctionnelle d'énergie. Nous obtenons ensuite un développement asymptotique de l'énergie fondamentale quasi-classique lorsque le paramètre de couplage g tend vers 0. Enfin, en faisant dépendre l'énergie du paramètre ultraviolet Λ, on montre que les états fondamentaux, ainsi que les énergies fondamentales associées convergent dans la limite ultraviolette, c'est-à-dire lorsque Λ tend vers $+\infty$. Dans le cas du modèle standard de l'électrodynamique quantique non relativiste, sous des hypothèses similaires, on montre l'existence d'un état fondamental quasi-classique. Nous obtenons aussi un développement asymptotique lorsque g tend vers 0 et la convergence dans la limite ultraviolette de l'énergie fondamentale.

3 Présentation des résultats et organisation de la thèse

3.1 Modèle Spin-Boson

Le premier modèle considéré dans cette thèse est le modèle Spin-boson. Il s'agit d'un des modèles les plus simples (mais non trivial) représentant un système atomique à deux niveaux (par exemple, un qubit) et interagissant avec un champ de bosons scalaire. Sous des hypothèses génerales, même sans régularisation infrarouge, l'existence d'un état fondamental pour le modèle Spin-Boson est connue, on pourra consulter par exemple les travaux de M. Hübner et H. Spohn dans [77], D. Hasler et I. Herbst [72], D. Hasler, B. Hinrichs et O. Siebert [73], ainsi que ceux de A. Arai et M. Hirokawa qui obtiennent le résultat pour un modèle dit "généralisé" dans [6].

Dans le cas du modèle Spin-Boson, les états de la particule non relativiste sont associés à des vecteurs normalisés dans $\mathbb{C}^2$ et l'Hamiltonien décrivant son énergie se réduit à la troisième matrice de Pauli :

$$H_{\mathrm{el}} := \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Comme mentionné précédemment, l'énergie du champ est représentée par l'opérateur de seconde quantification $\mathbb{H}_{\mathrm{f}} := \mathrm{d}\Gamma(\omega)$ dans l'espace de Fock symétrique $\mathcal{H}_{\mathrm{f}} := \mathfrak{F}_s(L^2(\mathbb{R}^3))$ où $\omega : \mathbb{R}^3 \to \mathbb{R}_+$ est une fonction mesurable positive. L'exemple typique est la relation de dispersion relativiste $\omega(k) = \sqrt{k^2 + m^2}$ où $m \geq 0$ est la masse des particules du champ. L'interaction entre la particule non relativiste et le champ est associée à l'opérateur suivant :

$$\mathbb{H}_{\mathrm{int}} := g\,\sigma_1 \otimes \Phi(h), \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

où h est une fonction de carré intégrale.

Un calcul explicite (voir chapitre 1, section 1.1.1) permet de vérifier que l'énergie quasi-classique du système,

$$\mathcal{E}_1(u, f) = \langle (\zeta \otimes \Psi_f), \mathbb{H}(\zeta \otimes \Psi_f) \rangle_{\mathcal{H}}, \quad \zeta \in \mathbb{C}^2, f \in L^2(\mathbb{R}^3),$$

(où Ψ_f est l'état cohérent associé à f comme ci-dessus) est alors donnée par la formule :

$$\mathcal{E}_1(\zeta, f) = \langle \zeta, \sigma_3 \zeta \rangle_{\mathbb{C}^2} + \|\omega^{1/2} f\|_{L^2}^2 + 2g \langle \zeta, \sigma_1 \zeta \rangle_{\mathbb{C}^2} \mathfrak{Re} \int_{\mathbb{R}^3} f(k) h(k)\, \mathrm{d}k, \quad \zeta \in \mathbb{C}^2, f \in L^2(\mathbb{R}^3).$$

L'idée est alors de minimiser cette fonctionnelle dans un espace approprié en ζ et en f, sous la contrainte que ζ soit de norme 1. Pour que la fonctionnelle $\mathcal{E}_1$ soit bien définie, il est suffisant de supposer que (ζ, f) appartient au produit cartésien des deux espaces suivants

$$\mathfrak{Z} := \{\zeta \in \mathbb{C}^2,\ \|\zeta\|_{\mathbb{C}^2} = 1\}, \quad \mathcal{Z}_\omega := \{f : \mathbb{R}^3 \to \mathbb{C} \text{ mesurable} \mid \omega^{1/2} f \in L^2(\mathbb{R}^3, \mathrm{d}k)\},$$

(en particulier il n'est pas nécessaire que f appartienne à $L^2(\mathbb{R}^3)$) et que la fonction h vérifie l'hypothèse suivante :

Hypothèse 1. *h est une fonction mesurable et réelle, telle que $\omega^{-1/2} h$ est dans $L^2(\mathbb{R}^3)$.*

Afin de s'affranchir de la contrainte que ζ soit de norme 1 et de la symétrie de phase globale de ζ, on peut exprimer la fonctionnelle d'énergie $\mathcal{E}_1$ dans la représentation de Bloch :

$$\zeta = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{pmatrix}, \text{ où } \begin{cases} \theta \in [0, \pi], \\ \phi \in [0, 2\pi[, \end{cases} \quad \text{et } \|\zeta\|_{\mathbb{C}^2} = 1,$$

ce qui permet de seulement minimiser, sans contrainte, en les variables θ, ϕ et f. La fonctionnelle $\mathcal{E}$ possède néanmoins la propriété de symétrie suivante :

$$\mathcal{E}_1(\zeta, f) = \mathcal{E}_1(\sigma_3\zeta, -f), \quad \forall\zeta \in \mathbb{C}^2, \forall f \in L^2(\mathbb{R}^3).$$

On ne peut donc obtenir l'unicité d'un minimiseur que modulo cette symétrie. Le premier résultat obtenu dans cette thèse est le suivant :

Théorème 1. *On suppose que h vérifie l'hypothèse 1. Soit $g \geq 0$. Alors il existe un unique état fondamental quasi-classique $(\zeta_{\mathrm{gs}}, f_{\mathrm{gs}})$ dans $\mathfrak{Z} \times \mathcal{Z}_\omega$ tel que chacune des composantes de ζ_{gs} soient positives, et*

(i) Si $g^2\|\omega^{-1/2}h\|_{L^2}^2 \leq \frac{1}{2}$, alors

$$\zeta_{\mathrm{gs}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad f_{\mathrm{gs}} \equiv 0,$$

et l'ensemble des minimiseurs est :

$$\left\{(e^{i\phi}\zeta_{\mathrm{gs}}, f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\}.$$

De plus, l'énergie fondamentale quasi-classique est donnée par la formule

$$\min_{\zeta\in\mathfrak{Z},\, f\in\mathcal{Z}_\omega} \mathcal{E}_1(\zeta, f) = -1.$$

(ii) Si $g^2\|\omega^{-1/2}h\|_{L^2}^2 > \frac{1}{2}$, alors

$$\zeta_{\mathrm{gs}} = \frac{1}{2}\Big(\sqrt{2 - \frac{1}{g^2\|\omega^{-1/2}h\|_{L^2}^2}}, \sqrt{2 + \frac{1}{g^2\|\omega^{-1/2}h\|_{L^2}^2}}\Big),$$
$$f_{\mathrm{gs}} = -g\sqrt{1 - \frac{1}{4g^4\|\omega^{-1/2}h\|_{L^2}^4}}\,\omega^{-1}h,$$

et l'ensemble des minimiseurs est :

$$\left\{(e^{i\phi}\zeta_{\mathrm{gs}}, f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\} \cup \left\{(e^{i\phi}\sigma_z\zeta_{\mathrm{gs}}, -f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\}.$$

Dans ce cas, l'énergie fondamentale quasi-classique est donnée par la formule :

$$\min_{\zeta\in\mathfrak{Z},\, f\in\mathcal{Z}_\omega} \mathcal{E}_1(\zeta, f) = -g^2\|\omega^{-1/2}h\|_{L^2}^2 - \frac{1}{4g^2\|\omega^{-1/2}h\|_{L^2}^2}.$$

Démonstration. voir chapitre 1. □

Le phénomène que décrit ce théorème est le suivant : il existe un minimiseur pour toutes valeurs de g, mais celui-ci diffère selon le régime de couplage choisi. En effet, lorsque g est plus petite qu'une certaine constante dépendante de la quantité $\|\omega^{-1/2}h\|_{L^2}$, l'état fondamental quasi-classique coïncide avec l'état fondamental de l'Hamiltonien libre (c'est-à-dire lorsque l'interaction est enlevée de l'Hamiltonien total du système). Par contre, lorsque g est choisi strictement plus grand que cette constante, l'état fondamental possède une toute autre forme, dépendant de la symétrie citée plus tôt, et l'énergie associée est alors strictement plus petite que l'énergie fondamentale de l'Hamiltonien libre.

Dans une seconde partie, on s'intéresse à l'énergie fondamentale du modèle Spin-boson lorsque le champ se trouve dans une superposition de deux états cohérents. On considère α et β deux nombres complexes tels que $|\alpha|^2 + |\beta|^2 = 1$, f_1 et f_2 deux fonctions de carré intégrable. Un calcul direct donne :

$$\left\langle \left(\begin{pmatrix} 0 \\ \alpha \end{pmatrix} \otimes \Psi_{f_1} + \begin{pmatrix} \beta \\ 0 \end{pmatrix} \otimes \Psi_{f_2} \right), \mathbb{H}\left(\begin{pmatrix} 0 \\ \alpha \end{pmatrix} \otimes \Psi_{f_1} + \begin{pmatrix} \beta \\ 0 \end{pmatrix} \otimes \Psi_{f_2} \right) \right\rangle_{\mathcal{H}} = \mathcal{E}_2(\alpha, \beta, f_1, f_2),$$

où $\mathcal{E}_2$ est la fonctionnelle d'énergie définie par :

$$\begin{aligned}\mathcal{E}_2(\alpha, \beta, f_1, f_2) = |\alpha|^2 \left(\|\omega^{1/2} f_1\|_{L^2}^2 - 1\right) + |\beta|^2 \left(\|\omega^{1/2} f_2\|_{L^2}^2 + 1\right) \\ + 2g e^{-\|f_1 - f_2\|_{L^2}^2/4} \mathfrak{Re}\left(\bar{\alpha}\beta e^{-\frac{i}{2}\mathfrak{Im}\langle f_1, f_2\rangle_{L^2}} \left(\langle f_1, h\rangle_{L^2} + \langle h, f_2\rangle_{L^2} \right)\right).\end{aligned}$$

L'idée est de minimiser cette fonctionnelle dans un espace approprié. Ici, l'espace naturel est $\mathfrak{Z} \times (L^2 \cap \mathcal{Z}_\omega)^2$. D'une part, on suppose que la fonction h vérifie l'hypothèse suivante :

Hypothèse 2. *h est une fonction mesurable et réelle, telle que $\omega^{-1/2}h$ et $\omega^{-1}h$ sont dans $L^2(\mathbb{R}^3)$.*

Cela nous permet d'obtenir le théorème suivant, qui s'avère très utile pour montrer par la suite l'existence d'un état fondamental (voir chapitre 1 pour plus de détails) :

Théorème 2. *On suppose que la fonction h vérifie l'hypothèse 2, alors*

$$\inf_{(\alpha,\beta)\in\mathfrak{Z}, (f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2} \mathcal{E}_2(\alpha, \beta, f_1, f_2) \leq -1 - C_h g^2 + \underset{g\to 0}{\mathcal{O}}(g^3),$$

où $C_h > 0$ est une constante qui dépend de $\|\omega^{-1/2}h\|_{L^2}$ et $\|\omega^{-1}h\|_{L^2}$.

En particulier, pour g assez petit, on a

$$\inf_{(\alpha,\beta)\in\mathfrak{Z}, (f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2} \mathcal{E}_2(\alpha, \beta, f_1, f_2) < -1.$$

Afin d'obtenir l'existence d'un état fondamental pour la fonctionnelle d'énergie $\mathcal{E}_2$, on a besoin d'hypothèses supplémentaires sur la relation de dispersion ω et sur la fonction de couplage h :

Hypothèse 3. *Il existe $\Lambda > 0$ tel que :*

1. *La fonction h est définie avec une troncature ultraviolette, c'est-à-dire que :*

$$h = \mathbf{1}_{|k|\leq\Lambda} h.$$

2. *La relation de dispersion ω est telle que $\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda}$ et $\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}$ appartiennent à $L^\infty(\mathbb{R}^3)$.*

Théorème 3. *On suppose que la fonction h et la relation de dispersion ω vérifient les hypothèses 2 et 3. Alors il existe $g_0 > 0$ tel que, pour tout $0 \leq g < g_0$, la fonctionnelle $\mathcal{E}_2$ admet un état fondamental dans $\mathfrak{Z} \times (\mathcal{Z}_\omega \cap L^2)^2$.*

En particulier, le théorème 2 montre que, contrairement au cas de l'énergie quasi-classique (c'est-à-dire, avec un seul état cohérent), on obtient une énergie fondamentale plus petite que l'énergie triviale du vide Ω, et ce même pour une petite valeur de la constante de couplage.

3.2 Modèle d'une particule non relativiste couplée linéairement à un champ de bosons scalaire

Le chapitre 2 est dédié à l'étude de l'énergie quasi-classique d'une classe abstraite d'Hamiltoniens de Pauli-Fierz de couplage linéaire, couvrant par exemple le modèle de Nelson introduit par E. Nelson dans l'article [102], ou encore le modèle du Polaron de Fröhlich exposé par H. Fröhlich dans l'article [48]. On suppose la particule non relativiste (l'électron) soumise à un potentiel extérieur V, ses états quantiques sont considérés dans l'espace $L^2(\mathbb{R}^3)$. Son énergie est alors représentée par un opérateur de Schrödinger :

$$H_{\mathrm{el}} = H_V := -\Delta + V\,.$$

Nous marquons la dépendance en V de l'Hamiltonien électronique afin de pouvoir considérer un potentiel extérieur le plus général possible.

Comme dans la section précédente pour le modèle Spin-Boson, nous considérons un champ scalaire, $\mathcal{H}_{\mathrm{f}} = \mathfrak{F}_s(L^2(\mathbb{R}^3))$, avec une énergie donnée par $\mathbb{H}_{\mathrm{f}} = \mathrm{d}\Gamma(\omega)$ où $\omega : \mathbb{R}^3 \to \mathbb{R}_+$ est une fonction mesurable positive.

L'électron est supposé couplé linéairement avec le champ de bosons, c'est-à-dire que l'opérateur d'interaction est donné par :

$$\mathbb{H}_{\mathrm{int}} = g\sqrt{2}\Phi(h_x), \quad h_x(k) := v(k)e^{-ikx}, \quad \forall x \in \mathbb{R}^3,$$

où v est une fonction de couplage définie selon le modèle considéré et $g \in \mathbb{R}$. Par exemple, dans le cas du modèle de Nelson, on a

$$v(k) = \omega(k)^{-1/2}\chi(k),$$

où χ est une troncature ultraviolette et la relation de dispersion relativiste est donnée par

$$\omega(k) = \sqrt{k^2 + m^2}\,,$$

correspondant à un champ de photons de masse $m \geq 0$. Citons aussi le modèle du Polaron de Fröhlich [48], dans ce cas la fonction de couplage v et la relation de dispersion sont données par :

$$v(k) = |k|^{-1}, \quad \omega(k) = 1.$$

Soit u dans $\mathcal{Q}(H_V)$, le domaine de forme de l'Hamiltonien électronique, et soit f dans l'espace $\mathcal{Z}_\omega$, (cf section "Modèle Spin-Boson", page 6). En calculant l'énergie quasi-classique du système complet, on obtient une fonctionnelle d'énergie de Klein-Gordon-Schrödinger (voir chapitre 2 pour plus de détails) :

$$\mathcal{E}(u,f) := \int_{\mathbb{R}^3} |\vec{\nabla} u(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} V(x)|u(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} \omega(k)|f(k)|^2 \,\mathrm{d}k \\ + 2g\mathfrak{Re} \int_{\mathbb{R}^6} e^{ikx} v(k) f(k) |u(x)| \,\mathrm{d}k \,\mathrm{d}x,$$

où le dernier terme correspond au couplage. Notons que cette fonctionnelle est bien définie sans troncature ultraviolette (on peut prendre $\chi = 1$ dans la définition de v). Lorsqu'on tente de minimiser cette fonctionnelle, on remarque que la composante de champ f du potentiel minimiseur peut se réécrire comme une fonction de la composante électronique u. Le problème se réduit alors à la minimisation d'une fonctionnelle de *Hartree* donnée par :

$$J(u) := \langle u, H_V u \rangle_{L^2_x} - \int_{\mathbb{R}^3} (\bar{\mathcal{F}}(W) * |u|^2)(x)|u(x)|^2 \,\mathrm{d}x,$$

avec $W := g^2\omega^{-1}v^2$. Ici $\mathcal{F}$ désigne la transformée de Fourier agissant sur les distributions tempérées normalisée de telle façon que pour toute fonction f appartenant à l'espace de Schwartz $\mathcal{S}(\mathbb{R}^3)$,

$$\mathcal{F}(f)(x) = \int_{\mathbb{R}^3} e^{-ix\cdot\xi} f(\xi) \,\mathrm{d}\xi, \tag{1}$$

et la transformée de Fourier inverse est donnée par $\mathcal{F}^{-1}(f) = (2\pi)^{-3}\bar{\mathcal{F}}(f)$ avec :

$$\bar{\mathcal{F}}(f)(x) = \int_{\mathbb{R}^3} e^{ix\cdot\xi} f(\xi) \,\mathrm{d}\xi.$$

Sous les hypothèses ci-dessous, la fonctionnelle J est bien définie pour u dans l'espace suivant :

$$\mathcal{U} = \{u \in \mathcal{Q}(H_V) \mid \|u\|_{L^2} = 1\}.$$

La littérature concernant l'étude des minimiseurs de l'énergie de Hartree est très fournie, on pourra consulter [4, 7, 39, 49, 60, 67, 85, 91–93] ainsi que les références contenues dans ces articles . Dans cette thèse, les techniques utilisées pour montrer l'existence d'un minimiseur consistent à appliquer les arguments usuels du calcul des variations développés par P.-L. Lions dans [92, 93]. Une première nouveauté apportée par cette thèse vient des hypothèses générales considérées sur le potentiel V :

Hypothèse 4. *Il existe* $0 \leq a < 1$ *et* b *dans* $\mathbb{R}$ *tels que la partie négative de* V *satisfait*

$$V_- \leq -a\Delta + b\,,$$

au sens des formes quadratiques sur $H^1(\mathbb{R}^3)$*. De plus,* V *se décompose en* $V = V_1 + V_2$ *avec*

(i) $V_1 \in L^1_{\text{loc}}(\mathbb{R}^3;\mathbb{R}^+)$,

(ii) $V_2 \in L^{3/2}_{\text{loc}}(\mathbb{R}^3;\mathbb{R})$ *et* $\lim_{|x|\to\infty} V_2(x) = 0$,

(iii) $\mu_V < \mu_{V_1}$*, où* $\mu_V = \inf \sigma(H_V)$*,* $\mu_{V_1} = \inf \sigma(H_{V_1})$ *et où* $\sigma(H_V)$ *est le spectre de l'opérateur* H_V.

On considère ainsi un potentiel extérieur V qui pourrait se décomposer en deux parties, l'une serait par exemple un potentiel confinant, l'autre un potentiel extérieur de type Coulomb. L'item (iii) signifie que l'on suppose un gap entre l'énergie fondamentale de l'opérateur H_V et celle de H_{V_1}. C'est une hypothèse qui s'avère nécessaire pour prouver l'existence d'un minimiseur pour la fonctionnelle de Hartree J définie plus haut (voir chapitre 2). Comme mentionné précédemment, on n'impose pas de troncature ultraviolette dans la définition de l'énergie, ce qui présente une difficulté importante dans l'étude du problème de minimisation. Pour résoudre cette difficulté, l'idée est de décomposer la fonction de couplage W en deux parties, une régulière et une singulière, et de contrôler les cas critiques de la partie singulière par des estimations dans des espaces bien choisis. Pour p dans l'intervalle $[1, +\infty[$, on définit les espaces $L^{p,\infty}$ (ou L^p "faibles") par

$$L^{p,\infty}(\mathbb{R}^3) = \{f : \mathbb{R}^3 \to \mathbb{C} \text{ mesurable}, \ \|f\|_{L^{p,\infty}} = \sup_{t>0} \lambda(\{|f| > t\})^{\frac{1}{p}} t < \infty\}\,, \tag{2}$$

où λ est la mesure de Lebesgue. Ainsi, on suppose l'hypothèse suivante sur la fonction W :

Hypothèse 5. *La fonction* $W = g^2\omega^{-1}v^2$ *se décompose en* $W = W_1 + W_2$ *avec*

(i) $W_1 \in L^1(\mathbb{R}^3)$,

(ii) $W_2 \in L^{3,\infty}(\mathbb{R}^3)$.

Notons que cette hypothèse couvre le cas du modèle du Polaron [48], mais aussi du modèle de Nelson [102] sans troncature ultraviolette, avec $\chi = 1$ et $\omega(k) = \sqrt{k^2 + m^2}$ avec $m \geq 0$, pour un champ massif. Cette hypothèse nous permet d'obtenir l'existence d'un état fondamental quasi-classique pour la fonctionnelle d'énergie de Klein-Gordon-Schrödinger :

Théorème 4 (Existence d'un état fondamental)**.** *On suppose que* V *vérifie l'hypothèse 4 et que* W *satisfait l'hypothèse 5. Il existe une constante* $C_V > 0$ *telle que, si les décompositions* $V = V_1 + V_2$ *et* $W = W_1 + W_2$ *peuvent être choisies de sorte que*

$$\|W_1\|_{L^1} + C_V\|W_2\|_{L^{3,\infty}} \leq \delta(\mu_{V_1} - \mu_V)\,,$$

et

$$C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a),$$

pour des constantes universelles $C, \delta > 0$ et où a est donné dans l'hypothèse 4, alors la fonctionnelle d'énergie de Klein-Gordon-Schrödinger admet un minimiseur dans $\mathcal{U} \times \mathcal{Z}_\omega$.

Démonstration. Voir chapitre 2. □

Afin d'obtenir l'unicité, nous avons besoin de supposer une hypothèse supplémentaire sur le potentiel extérieur V :

Hypothèse 6. *L'énergie fondamentale μ_V de l'Hamiltonien électronique H_V est une valeur propre simple et isolée associée à un unique état fondamental positif u_V dans $L^2(\mathbb{R}^3; \mathbb{R}_+)$, tel que $\|u_V\|_{L^2} = 1$.*

Cela nous permet d'obtenir le théorème suivant :

Théorème 5 (Unicité d'un état fondamental)**.** *On suppose que V vérifie les hypothèses 4 et 6, et que W satisfait l'hypothèse 5. Il existe $\varepsilon_V > 0$ tel que, si*

$$\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V,$$

alors la fonctionnelle de Klein-Gordon-Schrödinger admet un unique minimiseur $(u_{\rm gs}, f_{\rm gs})$ dans $\mathcal{U} \times \mathcal{Z}_\omega$ tel que $\langle u_{\rm gs}, u_V\rangle_{L^2} > 0$.

Démonstration. voir chapitre 2. □

Une fois qu'on a montré l'existence et l'unicité d'un état fondamental quasi-classique, il est alors possible de calculer un développement asymptotique de l'énergie minimisée lorsque g tend vers 0. Cela permet alors de décomposer le terme d'ordre deux dans le développement de l'énergie fondamentale de l'Hamiltonien total en deux termes : un premier terme, quasi-classique, obtenu en minimisant la fonctionnelle d'énergie de Klein-Gordon-Schrödinger, et un second, assimilé aux états excités du système :

Théorème 6 (Comparaison avec l'énergie fondamentale de $\mathbb{H}$)**.** *On suppose que V vérifie les hypothèses 4 et 6, et que W satisfait l'hypothèse 5. On a*

$$\min_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}(u,f) = \mu_V - g^2 \int_{\mathbb{R}^3} \left(\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_V|^2\right)(x)\, |u_V(x)|^2 \,\mathrm{d}x + \mathcal{O}(g^4),$$

lorsque $g \to 0$.

Si on suppose que $W_2 = 0$ dans la décomposition de W, c'est-à-dire $W = g^2\omega^{-1}v^2$ appartient à $L^1(\mathbb{R}^3)$, alors on a

$$\begin{aligned}\inf \sigma(\mathbb{H}) &- \mathcal{E}(u_{\rm gs}, f_{\rm gs}) \\ &= -g^2 \int_{\mathbb{R}^3} v(k)^2 \left\langle u_V, e^{ikx}\Pi_V^\perp \big(H_V - \mu_V + \omega(k)\big)^{-1} \Pi_V^\perp e^{-ikx} u_V \right\rangle_{L^2_x} \mathrm{d}k + o(g^2)\,,\end{aligned}$$

lorsque $g \to 0$, où $\Pi_V^\perp = \mathbf{I}_{L^2} - |u_V\rangle\langle u_V|$ est la projection orthogonale sur l'espace $(\mathbb{C}u_V)^\perp$.

Démonstration. voir le chapitre 2. □

Supposons à présent que le couplage dépende d'un paramètre ultraviolet Λ, c'est-à-dire que l'on remplace v par $v_\Lambda := v\mathbf{1}_{|k|\leq\Lambda}$, et on note $\mathcal{E}_\Lambda$ la nouvelle énergie quasi-classique obtenue. Alors, on a convergence de l'énergie fondamentale quasi-classique dans la limite ultraviolette :

Théorème 7 (Limite ultraviolette des énergies fondamentales)**.** *On suppose que V vérifie l'hypothèse 4 et que W vérifie 5. Alors*

$$\inf_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}_\Lambda(u,f) \underset{\Lambda\to\infty}{\longrightarrow} \inf_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}(u,f).$$

Démonstration. voir chapitre 2 □

Sous les hypothèses assurant l'unicité de l'état fondamental, il est possible d'obtenir également la convergence pour les états fondamentaux quasi-classique associés :

Théorème 8 (Limite ultraviolette des états fondamentaux)**.** *On suppose que V vérifie les hypothèses 4 et 6 et que W satisfait l'hypothèse 5. Il existe $\varepsilon_V > 0$ tel que, si*

$$\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V,$$

alors pour tout $\Lambda > 0$, $\mathcal{E}_\Lambda$ et $\mathcal{E}$ ont un unique minimiseur $(u_{\Lambda,\mathrm{gs}}, f_{\Lambda,\mathrm{gs}})$ et $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ dans l'espace $\mathcal{U}\times\mathcal{Z}_\omega$, respectivement, tels que $\langle u_{\Lambda,\mathrm{gs}}, u_V\rangle_{L^2} > 0$ et $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2} > 0$. Ils vérifient

$$\left\|(u_{\Lambda,\mathrm{gs}}, f_{\Lambda,\mathrm{gs}}) - (u_{\mathrm{gs}}, f_{\mathrm{gs}})\right\|_{\mathcal{Q}(H_V)\times\mathcal{Z}_\omega} \underset{\Lambda\to\infty}{\longrightarrow} 0.$$

Démonstration. voir chapitre 2. □

3.3 Modèle Standard de l'électrodynamique quantique non relativiste

Dans le chapitre 3, on s'intéresse au modèle standard de l'électrodynamique quantique non relativiste avec spin, introduit par W. Pauli et M. Fierz dans [104], décrivant un système atomique couplé de façon minimale au champ électromagnétique quantifié et provenant de la quantification des équations de Maxwell. Comme dans la section précédente, l'espace de Hilbert pour l'électron est $\mathcal{H}_{\mathrm{el}} = L^2(\mathbb{R}^3)$. L'espace de Hilbert pour le champ de photons transverses est $\mathcal{H}_{\mathrm{f}} = \mathfrak{F}_s(L^2_\perp(\mathbb{R}^3;\mathbb{C}^3))$, où

$$L^2_\perp(\mathbb{R}^3;\mathbb{C}^3) = \{\vec{f}\in L^2(\mathbb{R}^3;\mathbb{C}^3) \mid \forall k\in\mathbb{R}^3, k\cdot\vec{f}(k) = 0\}.$$

L'Hamiltonien total est alors donné par :

$$\mathbb{H} = \Big(\vec{\sigma}\cdot\big(-i\vec{\nabla}_x - \vec{\mathbb{A}}_\chi(x)\big)\Big)^2 + V + \mathbb{H}_{\mathrm{f}}\,,$$

où $\vec{\sigma}$ est un vecteur dont les composantes sont données par les matrices de Pauli :

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

et où $\vec{\mathbb{A}}_\chi(x)$ est le vecteur potentiel associé au champ électromagnétique dans la jauge de Coulomb :

$$\vec{\mathbb{A}}_\chi(x) = g\sqrt{2} \sum_{\tau=1,2,3} \int_{\mathbb{R}^3} \frac{\chi(k)}{|k|^{\frac{1}{2}}} \vec{\varepsilon}_\tau(k) \big(e^{-ikx} a_\tau^*(k) + e^{ikx} a_\tau(k)\big) \, \mathrm{d}k.$$

La fonction χ est une troncature ultraviolette (nécessaire pour que l'Hamiltonien s'identifie à un opérateur auto-adjoint), g est un paramètre de couplage et les vecteurs $(\vec{\varepsilon}_\tau)_{\tau=1,2,3}$ sont des vecteurs de polarisation, avec $\varepsilon_3(k) = k/|k|$. Afin de calculer l'énergie quasi-classique associée, on considère u dans $L^2(\mathbb{R}^3)$, et f dans $L^2_\perp(\mathbb{R}^3; \mathbb{C}^3)$ et où u est de norme 1. On décompose $f = f_+ + f_-$, avec

$$f_+(k) = \frac{1}{2}\Big(f(k) + \overline{f(-k)}\Big), \quad \text{et} \quad f_-(k) = \frac{1}{2}\Big(f(k) - \overline{f(-k)}\Big).$$

Un calcul direct de l'énergie testée sur les états cohérents donne :

$$\langle (u \otimes \Psi_f), \mathbb{H}(u \otimes \Psi_f) \rangle = \mathcal{E}_{V,\chi}(u, \vec{A}_{f_+}) + 2g^2 \||k|^{-1/2}\chi(k)\|^2_{L^2} + \||k|^{1/2} f_-\|^2_{L^2},$$

où

$$\vec{A}_{f_+} := 2\mathcal{F}(|k|^{-1/2}\overline{f_+(k)}),$$

et $\mathcal{E}_{V,\chi}(u, \vec{A})$ est l'énergie de *Maxwell-Pauli* dans la jauge de Coulomb :

$$\mathcal{E}_{V,\chi}(u, \vec{A}) = \|\vec{\sigma} \cdot (-i\vec{\nabla} - g\hat{\chi} * \vec{A})u\|^2_{L^2} + \langle u, Vu \rangle_{L^2} + (32\pi^3)^{-1} \|\vec{A}\|^2_{\dot{H}^1}.$$

Comme dans la section précédente, $\mathcal{F}$ désigne la transformation de Fourier (voir l'équation (1)), et la constante $(32\pi^3)^{-1}$ vient de notre normalisation de la transformée de Fourier.

Les propriétés dynamiques des équations de Maxwell-Schrödinger ou Maxwell-Pauli ont beaucoup été étudiées ces dernières années, on peut citer par exemple les travaux fondateurs de K. Nakamitsu et M. Tsutsumi dans l'article [100] qui montrent l'existence d'une solution aux équations de Maxwell-Schrödinger, puis I. Bejenaru et D. Tataru qui traitent du caractère bien posé du problème dans l'article [18]. On peut citer également les travaux de V. Benci et D. Fortunato dans l'article [19] qui traitent de l'existence de solitons pour ces même équations. On peut citer aussi, sans être exhaustif, les travaux [30, 57, 66, 79, 94, 97, 101, 109, 112, 113] et les références contenues dans ces articles. Notons par ailleurs qu'il existe de nombreux autres problèmes de minimisation faisant intervenir les matrices de Pauli dans un cadre relativiste. Citons par exemple l'article [44] de M. Esteban et S. Rota Nodari dans lequel un modèle de nucléon dans la limite de champ moyen est étudié.

Minimiser l'énergie quasi-classique de l'Hamiltonien $\mathbb{H}$ revient alors à minimiser la fonctionnelle de Maxwell-Pauli $\mathcal{E}_{V,\chi}$. Mentionnons que lorsque le potentiel extérieur V et la fonction de troncature χ sont définis par des fonctions paires, la fonctionnelle d'énergie de Maxwell-Pauli est invariante par la symétrie de Kramers (voir par exemple l'article de M. Loss, T. Miyao et H. Spohn [96]), c'est-à-dire que

$$\mathcal{E}_{V,\chi}(\nu u, \vec{A}(-\cdot)) = \mathcal{E}_{V,\chi}(u, \vec{A}),$$

où $\nu u\,(x) = \sigma_2 \overline{u(-x)}$. On ne peut donc alors espérer l'unicité d'un minimiseur pour cette fonctionnelle que modulo cette symétrie. L'espace naturel de minimisation de l'énergie est l'espace $\mathcal{U} \times \mathcal{A}$ où $\mathcal{A}$ est l'espace correspondant au choix de la jauge de Coulomb :

$$\mathcal{A} := \{\vec{A} \in \dot{H}^1(\mathbb{R}^3;\mathbb{R}^3) \,|\, \vec{\nabla} \cdot \vec{A} = 0\}.$$

Rappelons que les espaces $L^{p,\infty}$ ont été introduits dans la section précédente (voir l'équation (2)). On suppose les hypothèses suivantes :

Hypothèse 7. *La troncature $\chi : \mathbb{R}^3 \to \mathbb{R}$ vérifie $\chi(-k) = \chi(k)$ pour tout k dans $\mathbb{R}^3$ et*

$$\frac{\chi}{|k|} \in L^2(\mathbb{R}^3) + L^{3,\infty}(\mathbb{R}^3)\,.$$

Notons que cette hypothèse couvre en particulier le cas d'une interaction sans troncature ultraviolette ($\chi = 1$) puisque si χ est bornée alors $\chi/|k|$ appartient à $L^{3,\infty}(\mathbb{R}^3)$. L'idée sous-jacente derrière cette hypothèse est la même que pour le modèle de la section précédente, à savoir retirer la troncature ultraviolette de l'énergie et contrôler la partie singulière de la fonction de couplage par des estimations dans les espaces de Lorentz. On suppose de plus des hypothèses générales sur le potentiel extérieur V :

Hypothèse 8. *On a $V(x) = V(-x)$ pour tout x dans $\mathbb{R}^3$ et il existe $a \geq 0$ et b dans $\mathbb{R}$ tels que*

$$V_- \leq a\sqrt{-\Delta} + b$$

au sens des formes quadratiques dans $H^{1/2}(\mathbb{R}^3)$. De plus, V se décompose en $V = V_1 + V_2$ avec

(i) $V_1 \in L^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^+)$,

(ii) $V_2 \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R})$ *et* $\lim_{|x|\to\infty} V_2(x) = 0$.

Cette hypothèse couvre le cas où V peut se décomposer comme la somme d'un potentiel confinant, c'est-à-dire que $V_1(x) \to \infty$ quand $|x| \to \infty$, et d'un potentiel de type Coulomb : $V_2(x) = -\alpha|x|^{-1}$, $\alpha > 0$. On obtient alors le résultat suivant :

Théorème 9 (Existence d'un état fondamental pour Maxwell-Pauli)**.** *On suppose que V vérifie l'hypothèse 8 et χ vérifie l'hypothèse 7.*

On suppose que les décompositions $V = V_1 + V_2$ et $\chi = \chi_1 + \chi_2$, avec $\chi_1/|k|$ appartenant à L^2 et $\chi_2/|k|$ appartenant à $L^{3,\infty}$, peuvent être choisies de sorte que

$$\inf \mathcal{E}_{V_1,\chi} > \inf \mathcal{E}_{V,\chi}\,, \quad \textit{et} \quad 32\pi^3 a C^2 g^2 \left\| \frac{\chi_2}{|k|} \right\|^2_{L^{3,\infty}} < 1,$$

où a est la constante apparaissant dans l'hypothèse 8 et C est une constante universelle. Alors, $\mathcal{E}_{V,\chi}$ admet un minimiseur dans $\mathcal{U} \times \mathcal{A}$.

Démonstration. voir chapitre 3. □

Notons que pour $|g|\,\|\chi_2/|k|\|_{L^{3,\infty}}$ supposée suffisamment petite, on a l'existence d'un état fondamental sans la présence d'une troncature ultraviolette dans l'interaction. En effet, le cas $\chi = 1$ est couvert par le théorème précédent, puisque la fonction $1/|k|$ est dans l'espace $L^{3,\infty}$. La symétrie de Kramers mentionnée précédemment implique que si $(u, \vec{A})$ est un minimiseur de la fonctionnelle d'énergie $\mathcal{E}_{V,\chi}$, et si V est paire alors $(\nu u, \vec{A}(-\cdot))$ en est un second, différent du premier, puisque νu et u sont orthogonaux. Nous conjecturons que, pour $g > 0$ suffisamment petit, $\mathcal{E}_{V,\chi}$ admet exactement deux minimiseurs, à symétrie de phase près par rapport à u. Enfin, remarquons que si on considère une particule sans spin à la place d'un électron, alors le théorème précédent devient trivial : l'inégalité diamagnétique montre que l'énergie $\mathcal{E}_{V,\chi}$ atteint son minimum pour $\vec{A} = 0$. Ainsi, dans le chapitre 3, nous montrons que dans le cas d'un électron de spin $\frac{1}{2}$, un minimiseur de l'énergie de Mawell-Pauli n'est pas trivial en général.

On suppose à présent que V vérifie l'hypothèse 6 donnée dans la section précédente. En supposant de plus que V et χ sont des fonctions radiales, on peut montrer le résultat d'approximation suivant :

Théorème 10. *On suppose que V vérifie les hypothèses 8 et 6, et χ vérifie l'hypothèse 7. On suppose de plus que V et χ sont des fonctions radiales et que la décomposition $V = V_1 + V_2$ peut être choisie de sorte que $\inf \mathcal{E}_{V_1,\chi} > \inf \mathcal{E}_{V,\chi}$. Il existe $\varepsilon_V > 0$ et $C_V > 0$ tels que si*

$$\mathbf{g}_\chi := |g| \left\| \frac{\chi}{|k|} \right\|_{L^2 + L^{3,\infty}} \le \varepsilon_V,$$

Alors

$$\left| \min \mathcal{E}_{V,\chi} - \mu_V - \frac{32\pi^3}{3} g^2 \int \left(\hat{\chi} * u_V^2 \right)^2 \right| \le C_V \mathbf{g}_\chi^4,$$

où $\hat{\chi}$ désigne la transformée de Fourier de χ. En particulier, si $\chi = 1$, alors

$$\left| \min \mathcal{E}_{V,\chi} - \mu_V - \frac{4(8\pi^3)^3}{3} g^2 \int u_V^4 \right| \le C_V \mathbf{g}_\chi^4.$$

Démonstration. voir chapitre 3. □

Le calcul d'un développement asymptotique pour $g \to 0$ dans le cas d'un potentiel et d'une fonction χ non radiaux reste ouvert (voir la section "Perspectives" ci-dessous). Supposons à présent que la troncature soit de la forme

$$\chi_\Lambda = \mathbf{1}_{|k|\leq\Lambda}\chi, \quad \Lambda > 0.$$

Alors, on obtient la convergence de l'énergie fondamentale quasi-classique dans la limite ultraviolette :

Théorème 11. *On suppose que V vérifie l'hypothèse 8 et χ vérifie l'hypothèse 7, avec $\chi_1/|k|$ appartenant à L^2 et $\chi_2/|k|$ appartenant à $L^{3,\infty}$. Supposons de plus que*

$$aC^2g^2\left\|\frac{\chi_2}{|k|}\right\|^2_{L^{3,\infty}} < (32\pi^3)^{-1}.$$

Alors

$$\inf \mathcal{E}_{V,\chi_\Lambda} \underset{\Lambda\to\infty}{\longrightarrow} \inf \mathcal{E}_{V,\chi}\,.$$

Démonstration. voir chapitre 3. □

Contrairement au modèle de couplage linéaire, nous n'avons pas démontré de résultat de convergence des états fondamentaux associés dans la limite ultraviolette, des détails sont donnés un peu plus bas dans la section "Perspectives".

3.4 Organisation de la thèse

Cette thèse se présente comme suit :

1. Le chapitre 1 contient les premiers résultats obtenus durant cette thèse, ainsi que leur démonstration. Une première partie présente la preuve du théorème 1, la minimisation de l'énergie quasi-classique du modèle Spin-Boson dans la représentation de Bloch, tandis qu'une seconde s'intéresse au cas où l'énergie est calculée sur une combinaison linéaire de deux états cohérents de paramètres distincts.
2. Le chapitre 2 contient l'article "Quasi-classical Ground States. I. Linearly Coupled Pauli-Fierz Hamiltonians" [26] où sont détaillés et démontrés les théorèmes 4 et 5 sur l'existence et l'unicité d'un état fondamental quasi-classique pour la fonctionnelle d'énergie de Klein-Gordon-Schrödinger pour un potentiel supposé le plus général possible. Un développement asymptotique de l'énergie minimale est calculé puis comparé au développement de l'énergie fondamentale du modèle (cf théorème 6). De plus, on démontre la convergence des états fondamentaux et énergies associés dans la limite ultraviolette présentée par les théorèmes 7 et 8.
3. Le chapitre 3 contient l'article "Quasi-classical Ground States. II. Standard Model of Non-relativistic QED" [27] où sont détaillés les résultats présentés précédemment sur l'énergie de Maxwell-Pauli. La preuve du théorème 9 sur l'existence d'un état fondamental quasi-classique dans le cas d'un potentiel aussi général que possible y est détaillée, ainsi que la preuve du théorème 10 où un développement asymptotique de l'énergie minimale lorsque le paramètre de couplage g tend vers 0, et le résultat de convergence dans la limite ultraviolette exposé dans le théorème 11.

3.5 Perspectives

Nous mentionnons ici brièvement quelques exemples de perspectives ou de questions qui restent ouvertes à l'issue de cette thèse.

Dans l'article [9], V. Bach, S. Breteaux et T. Tzaneteas traitent de façon similaire le cas du modèle standard de l'électrodynamique quantique non relativiste et sans potentiel extérieur, où ils étudient l'énergie de l'Hamiltonien testée sur des états quasi-libres. Ces états sont plus précis que les états cohérents, mais aussi plus délicats à manipuler. Il pourrait être envisageable d'appliquer les mêmes procédés sur une fonctionnelle d'énergie "quasi-libre" dans le cas où un potentiel est présent comme dans notre contexte. L'une des difficultés à surmonter viendrait du fait que dans ce cas, le modèle n'est plus invariant par translation.

Dans l'article [64], M. Griesemer et C. Tix étudient un modèle pseudo-relativiste sans potentiel extérieur et sans restriction de troncature ultraviolette ou infrarouge. Ils obtiennent ainsi un résultat d'instabilité, c'est-à-dire la non-existence d'un infimum pour l'énergie associée au modèle testée sur les états cohérents, si le nombre de particules pseudo-relativistes dépasse une certaine constante. Il serait alors intéressant d'appliquer les techniques utilisées dans cette thèse pour voir s'il est possible d'obtenir l'existence d'un minimiseur dans ce contexte pseudo-relativiste, dans un régime de stabilité et en présence d'un potentiel extérieur général.

À la fois pour les modèles d'un électron couplé linéairement à un champ scalaire et pour le modèle standard de l'électrodynamique quantique non relativiste, nous avons montré (voir les théorèmes 7 et 11) que si on introduit une troncature ultraviolette de paramètre Λ dans le modèle, les énergies fondamentales associées convergent dans la limite $\Lambda \to \infty$ vers l'énergie fondamentale du modèle sans troncature. Une question naturelle serait alors d'essayer d'établir la Γ-convergence des fonctionnelles d'énergie dans la limite ultraviolette. Dans la mesure où pour les modèles avec un couplage linéaire nous avons aussi un résultat de convergence des états fondamentaux (voir théorème 8), on peut s'attendre à ce que la question soit plus simple pour de tels modèles que pour le modèle standard de l'électrodynamique quantique non relativiste.

Comme mentionné précédemment, dans le cas du modèle standard, l'unicité d'un état fondamental quasi-classique ne peut être espérée qu'en tenant compte de la symétrie de Kramers et de la symétrie de phase. Il serait intéressant de réussir à démontrer cette propriété, puis d'étudier ensuite la convergence des états, à symétrie près, dans la limite ultraviolette.

Enfin, comme mentionné dans la section précédente, étendre le résultat du théorème 10 à des cas où le potentiel extérieur V et la fonction de troncature χ ne sont pas radiaux reste, à notre connaissance, une question ouverte. Comme on le verra dans la section correspondante, le problème dans le cas non radial vient du fait qu'un des termes d'ordre g^2 est "implicite", dans le sens où il dépend du choix d'un minimiseur de la fonctionnelle d'énergie. Il n'est pour l'instant pas clair comment s'affranchir de ce problème sans faire une hypothèse de radialité.

Chapitre 1

The Spin-Boson Model

1.1 Model and assumptions

Recall that in this chapter, the Hilbert space and Hamiltonian for the particle are given by

$$\mathcal{H}_{\mathrm{el}} := \mathbb{C}^2, \quad H_{\mathrm{el}} := \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.1}$$

Recall also that we suppose that the radiation field is a scalar, bosonic field with Hilbert space given by the symmetric Fock space

$$\mathcal{H}_{\mathrm{f}} := \mathfrak{F}_s(L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^{\infty} \bigvee^{n} L^2(\mathbb{R}^3). \tag{1.2}$$

The energy of the free field is associated to the second quantization of the multiplication operator by $\omega(k)$,

$$\mathbb{H}_{\mathrm{f}} := \mathrm{d}\Gamma(\omega(k)), \tag{1.3}$$

where $\omega : \mathbb{R}^3 \to \mathbb{R}_+$ is a non-negative measurable function. The coupling between the particle and the field is linear in the creation and annihilation operators, given by

$$\mathbb{H}_{\mathrm{int}} := g\, \sigma_1 \otimes \Phi(h), \quad \sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1.4}$$

where g in $\mathbb{R}$ is a coupling constant, $\Phi(h)$ denotes the field operator, and h is in $L^2(\mathbb{R}^3)$ such that $\omega^{-1/2}h$ belongs to $L^2(\mathbb{R}^3)$. It is not difficult to verify that the total Hamiltonian

$$\mathbb{H} = \sigma_3 \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathrm{d}\Gamma(\omega(k)) + g\, \sigma_1 \otimes \Phi(h) \tag{1.5}$$

is a semi-bounded self-adjoint operator with domain

$$\mathcal{D}(\mathbb{H}) = \mathcal{D}(\mathbb{H}_{\mathrm{free}}), \quad \mathbb{H}_{\mathrm{free}} = \sigma_3 \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathrm{d}\Gamma(\omega(k)). \tag{1.6}$$

See Appendix 1.4.2 for details. Note that in the sequel, we will drop the hypothesis that h is in $L^2(\mathbb{R}^3)$ in our study of the quasi-classical energy functional. Under general conditions on h and on ω (in particular for $\omega(k) = |k|$ and $h(k) = |k|^{-\mu}\chi(k), \mu > -1$ and χ an ultraviolet cutoff function), it has been proved that there exists a unique ground state for the operator $\mathbb{H}$ (see [61, 62, 71, 73] for instance) and that one has the following asymptotic expansion of the ground state energy in terms of the coupling parameter g

$$\inf \sigma(\mathbb{H}) = -1 - g^2 \int_{\mathbb{R}^3} \frac{|h(k)|^2}{\omega(k)+2}\, \mathrm{d}k + \underset{g\to 0}{o}(g^2), \tag{1.7}$$

where $\sigma(\mathbb{H})$ is the spectrum of the operator $\mathbb{H}$. It is important to note that, although we can not apply the usual eigenvalues perturbation theory, Eq. (1.7) is given by the usual Rayleigh-Schrödinger second order-term, even if $\inf \sigma(\mathbb{H})$ coincides with the infimum of the essential spectrum of the Hamiltonian $\mathbb{H}$. We mention that in [32], M. Correggi, M. Falconi and M. Merkli studied the dynamics of the Spin-Boson model the quasi-classical limit.

1.1.1 Quasi-classical energy

Our first interest here is to compute the energy of a product state of the form $\zeta \otimes \Psi_f$, where ζ is in $\mathbb{C}^2$ and Ψ_f is a coherent state of parameter f, and then minimize the energy obtained over ζ and f, with the constraint $\|\zeta\|_{\mathbb{C}^2} = 1$.

For f in $L^2(\mathbb{R}^3)$, the coherent state of parameter f is denoted by

$$\Psi_f := e^{i\Phi\left(\frac{\sqrt{2}}{i} f\right)}\Omega \in \mathcal{H}_{\mathrm{f}},$$

where Ω stands for the Fock vacuum. Let ζ be in $\mathbb{C}^2$ such that $\|\zeta\|_{\mathbb{C}^2} = 1$, and let f in $L^2(\mathbb{R}^3)$ be such that $\omega^{1/2} f$ belongs to $L^2(\mathbb{R}^3)$. We aim at studying the energy of the product state $\zeta \otimes \Psi_f$:

$$\langle (\zeta \otimes \Psi_f), \mathbb{H}(\zeta \otimes \Psi_f)\rangle_{\mathcal{H}} =: \mathcal{E}_1(\zeta, f), \tag{1.8}$$

where the energy functional $\mathcal{E}_1$ can be computed thanks to the properties of coherent states with respect to the field and second quantization operators (see Appendix 1.4.1 for details). This allows us to obtain

$$\mathcal{E}_1(\zeta, f) = \langle \zeta, \sigma_3 \zeta\rangle_{\mathbb{C}^2} + \|\omega^{1/2} f\|^2_{L^2} + 2g\,\langle \zeta, \sigma_1\zeta\rangle_{\mathbb{C}^2}\, \mathfrak{Re}\int_{\mathbb{R}^3} h(k) f(k)\mathrm{d}k. \tag{1.9}$$

We aim at proving the existence and uniqueness of a minimizer for this energy functional under suitable assumptions on the function h.

The natural energy space for $\mathcal{E}_1(\zeta, f)$ is $\mathfrak{Z} \times \mathcal{Z}_\omega$, where

$$\mathfrak{Z} := \{\zeta \in \mathbb{C}^2,\ \|\zeta\|_{\mathbb{C}^2} = 1\}, \quad \mathcal{Z}_\omega := \{f : \mathbb{R}^3 \to \mathbb{C} \text{ measurable} \mid \omega^{1/2} f \in L^2(\mathbb{R}^3, \mathrm{d}k)\}. \tag{1.10}$$

In order for the functional $\mathcal{E}_1$ to be well-defined, we require that the function h satisfies the following hypothesis :

Hypothesis 1.1.1. *The function h is measurable, real-valued and such that $\omega^{-1/2}h$ is in $L^2(\mathbb{R}^3)$.*

In particular, we relax the condition $h \in L^2(\mathbb{R}^3)$, necessary for the field operator $\Phi(h)$ appearing in the definition of $\mathbb{H}$ to be well-defined.

The functional $\mathcal{E}_1$ has the following symmetry property :

$$\mathcal{E}_1(\zeta, f) = \mathcal{E}_1(\sigma_3\zeta, -f)\,. \tag{1.11}$$

Hence, we can only hope for uniqueness of the minimizer modulo this symmetry and up to a phase for ζ.

1.1.2 Energy of the superposition of two quasi-classical states

In this part, we consider the energy of linear combination of vectors, which form a basis of $\mathbb{C}^2$, tensored with coherent states. Let (α, β) in $\mathbb{C}^2$ such that $|\alpha|^2 + |\beta|^2 = 1$, and let (f_1, f_2) be in $L^2(\mathbb{R}^3)^2$. The energy of the state $\left(\begin{smallmatrix}0\\ \alpha\end{smallmatrix}\right) \otimes \Psi_{f_1} + \left(\begin{smallmatrix}\beta\\ 0\end{smallmatrix}\right) \otimes \Psi_{f_2}$ is given by

$$\left\langle \left(\begin{pmatrix}0\\ \alpha\end{pmatrix} \otimes \Psi_{f_1} + \begin{pmatrix}\beta\\ 0\end{pmatrix} \otimes \Psi_{f_2} \right), \mathbb{H}\left(\begin{pmatrix}0\\ \alpha\end{pmatrix} \otimes \Psi_{f_1} + \begin{pmatrix}\beta\\ 0\end{pmatrix} \otimes \Psi_{f_2} \right) \right\rangle_{\mathcal{H}} = \mathcal{E}_2(\alpha, \beta, f_1, f_2), \tag{1.12}$$

where $\mathcal{E}_2$ is the energy functional given by

$$\begin{aligned} \mathcal{E}_2(\alpha, \beta, f_1, f_2) = {} & |\alpha|^2 \left(\|\omega^{1/2} f_1\|_{L^2}^2 - 1\right) + |\beta|^2 \left(\|\omega^{1/2} f_2\|_{L^2}^2 + 1\right) \\ & + 2g e^{-\|f_1 - f_2\|_{L^2}^2/4} \mathfrak{Re}\left(\bar{\alpha}\beta e^{-\frac{i}{2}\mathfrak{Im}\langle f_1, f_2\rangle_{L^2}} \left(\langle f_1, h\rangle_{L^2} + \langle h, f_2\rangle_{L^2} \right)\right). \end{aligned} \tag{1.13}$$

The natural energy space for this functional is $\mathfrak{Z} \times (L^2 \cap \mathcal{Z}_\omega)^2$.

As before, we aim at proving the existence and uniqueness of a minimizer for the energy functional. This functional also has a symmetry, defined by the relation :

$$\mathcal{E}_2(\alpha, \beta, f_1, f_2) = \mathcal{E}_2(\alpha, -\beta, -f_1, -f_2) = \mathcal{E}_2(-\alpha, \beta, -f_1, -f_2)\,. \tag{1.14}$$

So once more, we can only hope for uniqueness modulo this symmetry. Furthermore, in order to obtain the existence of a minimizer, we need assumptions on the coupling function h and on the dispersion relation ω (recall that ω is a non-negative measurable function). Our minimal assumptions will be

Hypothesis 1.1.2. *The function h is measurable and real-valued such that $\omega^{-1/2}h$ and $\omega^{-1}h$ are in $L^2(\mathbb{R}^3)$.*

In order to prove the existence of a ground state for $\mathcal{E}_2$, we will need the following further condition

Hypothesis 1.1.3. *There exists $\Lambda > 0$ such that*

1. *The coupling function h comes with an ultraviolet cutoff in the sense that*

$$h = \mathbf{1}_{|k|\leq\Lambda} h.$$

2. *The dispersion relation ω is such that $\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda}$ and $\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}$ belong to $L^\infty(\mathbb{R}^3)$.*

Remark 1.1.1. *Hypothesis 1.1.3 covers the "massive case", where the dispersion relation of the boson field is $\omega(k) = \sqrt{k^2 + m^2}$, with $m > 0$.*

1.1.3 Main results

We are now ready to state our main results. For convenience, we set

$$\mathbf{g}_{h,\frac{1}{2}} := 2g^2 \left\|\omega^{-1/2}h\right\|_{L^2}^2 . \tag{1.15}$$

Theorem 1.1.2 (Quasi-classical ground state energy)**.** *Suppose that the function h satisfies Hypothesis 1.1.1, and consider $g \geq 0$. Then $\mathcal{E}_1$ has a unique quasi-classical ground state $(\zeta_{\mathrm{gs}}, f_{\mathrm{gs}})$ in $\mathfrak{Z} \times \mathcal{Z}_\omega$ such that each component of ζ_{gs} is non-negative, and*

(i) if $\mathbf{g}_{h,\frac{1}{2}} \leq 1$, then

$$\zeta_{\mathrm{gs}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad f_{\mathrm{gs}} \equiv 0, \tag{1.16}$$

and the set of minimizers of $\mathcal{E}_1$ is

$$\left\{(e^{i\phi}\zeta_{\mathrm{gs}}, f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\}.$$

Moreover, the associated quasi-classical ground state energy is given by

$$\min_{\zeta\in\mathfrak{Z},\, f\in\mathcal{Z}_\omega} \mathcal{E}_1(\zeta, f) = -1. \tag{1.17}$$

(ii) if $\mathbf{g}_{h,\frac{1}{2}} > 1$, then

$$\zeta_{\mathrm{gs}} = \frac{1}{\sqrt{2}}\Big(\sqrt{1 - \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}}, \sqrt{1 + \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}}\Big), \quad f_{\mathrm{gs}} = -g\sqrt{1 - \frac{1}{\mathbf{g}_{h,\frac{1}{2}}^2}}\, \omega^{-1}h, \tag{1.18}$$

and the set of minimizers of $\mathcal{E}_1$ is

$$\left\{(e^{i\phi}\zeta_{\mathrm{gs}}, f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\} \cup \left\{(e^{i\phi}\sigma_z\zeta_{\mathrm{gs}}, -f_{\mathrm{gs}}) \mid \phi \in \mathbb{R}\right\}. \tag{1.19}$$

In this case, the associated quasi-classical ground state energy is

$$\min_{\zeta\in\mathfrak{Z},\, f\in\mathcal{Z}_\omega} \mathcal{E}_1(\zeta, f) = -\frac{1}{2}\big(\mathbf{g}_{h,\frac{1}{2}} + \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}\big). \tag{1.20}$$

Remark 1.1.3. *If $\mathbf{g}_{h,\frac{1}{2}} > 1$, since the space $\mathcal{Z}_\omega$ is not always contained in $L^2(\mathbb{R}^3)$, the field component f_{gs} of a minimizer $(\zeta_{\mathrm{gs}}, f_{\mathrm{gs}})$ of the functional energy $\mathcal{E}$ over $\mathfrak{Z} \times \mathcal{Z}_\omega$ may not belong to the original one-particle space $L^2(\mathbb{R}^3)$. In other terms, the coherent state $\Psi_{f_{\mathrm{gs}}}$ does not belong to the Fock space. If however $\omega^{-1}h$ belongs to the space $L^2(\mathbb{R}^3)$ (i.e. an infrared regularization is imposed), then f_{gs} is in $L^2(\mathbb{R}^3)$, and the coherent state $\Psi_{f_{\mathrm{gs}}}$ belongs to the symmetric Fock space $\mathfrak{F}_s(L^2(\mathbb{R}^3))$.*

Remark 1.1.4. *Since the function $\gamma : x \mapsto -\frac{1}{2}(x + \frac{1}{x})$ is non-increasing for x in $(1, +\infty)$, and since $\gamma(1) = -1$, we have*

$$\min_{\zeta\in\mathfrak{Z},\, f\in\mathcal{Z}_\omega} \mathcal{E}_1(\zeta, f) < -1,$$

for $\mathbf{g}_{h,\frac{1}{2}} > 1$.

Our next results concern the energy functional $\mathcal{E}_2$ introduced in Eq. (1.13) for the superposition of two quasi-classical states.

Proposition 1.1.5. *Suppose that the function h satisfies Hypothesis 1.1.2, then*

$$\inf_{(\alpha,\beta)\in\mathfrak{Z},(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2} \mathcal{E}_2(\alpha,\beta,f_1,f_2) \leq -1 - C_h g^2 + \underset{g\to 0}{\mathcal{O}}(g^3). \tag{1.21}$$

where $C_h > 0$ is a constant depending on the quantities $\|\omega^{-1/2}h\|_{L^2}$ and $\|\omega^{-1}h\|_{L^2}$.

In particular, for g small enough, we have

$$\inf_{(\alpha,\beta)\in\mathfrak{Z},(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2} \mathcal{E}_2(\alpha,\beta,f_1,f_2) < -1\,. \tag{1.22}$$

Remark 1.1.6. *The constant C_h introduced in Ineq. (1.21) can be computed explicitly. Indeed, we have*

$$C_h = \frac{\lambda_0\|\omega^{-1/2}h\|_{L^2}^4 e^{-\lambda_0\|\omega^{-1}h\|_{L^2}^2/2}}{2+\lambda_0\|\omega^{-1/2}h\|_{L^2}^2},$$

where $\lambda_0 > 0$ is a constant given by

$$\lambda_0 = \frac{-\|\omega^{-1}h\|_{L^2}^2 + \sqrt{\|\omega^{-1}h\|_{L^2}^4 + 4\|\omega^{-1/2}h\|_{L^2}^2\|\omega^{-1}h\|_{L^2}^2}}{\|\omega^{-1/2}h\|_{L^2}^2\|\omega^{-1}h\|_{L^2}^2}.$$

Theorem 1.1.7 (Existence of a ground state)**.** *Suppose that the coupling function h and the dispersion relation ω satisfy Hypotheses 1.1.2 and 1.1.3. Then there exists $g_0 > 0$ such that, for all $0 \leq g < g_0$, the functional $\mathcal{E}_2$ admits a minimizer in $\mathfrak{Z} \times (\mathcal{Z}_\omega \cap L^2)^2$.*

Remark 1.1.8. *Proposition 1.1.5 shows that, contrary to the case of one quasi-classical state (see Theorem 1.1.2), considering a superposition of two quasi-classical states leads to a ground state energy strictly smaller, for small $g > 0$, than the trivial energy of the vacuum.*

1.2 Proof of Theorem 1.1.2

The entire section is dedicated to the proof of Theorem 1.1.2. First, we prove the existence of a minimizer using coercivity and lower semi-continuity arguments. Then, we give equations to compute critical points of the energy, which are used to determine a minimizer and compute the associated ground state energy.

Let ζ in $\mathfrak{Z}$, and f in $\mathcal{Z}_\omega$. In order to deal with the constraint that $\|\zeta\|_{\mathbb{C}^2} = 1$, it is convenient to use the Bloch representation, which was introduced by Felix Bloch in [24]. Here we write

$$\zeta = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix}, \text{ where } \begin{cases} \theta \in [0,\pi], \\ \phi \in [0, 2\pi), \end{cases} \quad \text{so that } \|\zeta\|_{\mathbb{C}^2} = 1. \tag{1.23}$$

The energy functional then becomes

$$\mathcal{E}_1(\zeta, f) = \cos(\theta) + \|\omega^{1/2} f\|_{L^2}^2 + 2g\sin(\theta)\cos(\phi)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k =: \tilde{\mathcal{E}}_1(\theta, \phi, f). \quad (1.24)$$

Here, the symmetry of the energy functional is given by

$$\tilde{\mathcal{E}}_1(\theta, \phi, f) = \tilde{\mathcal{E}}_1(\theta, \phi + \pi, -f). \quad (1.25)$$

1.2.1 Coercivity and Existence of a minimizer

Lemma 1.2.1 below proves that the functional $\tilde{\mathcal{E}}_1$ is coercive, and this argument will be useful in the proof of Lemma 1.2.2 to show the existence of a minimizer for the energy.

Lemma 1.2.1 (Coercivity)**.** *Suppose the function h satisfies Hypothesis 1.1.1 and let $g \geq 0$. Then there exist $C_1 > 0$ and $C_2 > 0$ such that, for all f in $\mathcal{Z}_\omega$*

$$\tilde{\mathcal{E}}_1(\theta, \phi, f) \geq C_1 \left\|\omega^{1/2} f\right\|_{L^2}^2 - C_2, \quad (1.26)$$

uniformly in (θ, ϕ) in $[0, \pi] \times [0, 2\pi)$.

Proof. The energy can be written as follows

$$\tilde{\mathcal{E}}_1(\theta, \phi, f) = \cos(\theta) + \left\|\omega^{1/2} f\right\|_{L^2}^2 + 2g\sin(\theta)\cos(\phi)\mathfrak{Re}\left\langle \omega^{-1/2} h, \omega^{1/2} f\right\rangle_{L^2}. \quad (1.27)$$

Using the Cauchy-Schwarz inequality yields

$$\tilde{\mathcal{E}}_1(\theta, \phi, f) \geq -1 + \left\|\omega^{1/2} f\right\|_{L^2}^2 - 2g\left\|\omega^{-1/2} h\right\|_{L^2}\left\|\omega^{1/2} f\right\|_{L^2}. \quad (1.28)$$

We can introduce $\varepsilon > 0$ and use the standard Young inequality to obtain

$$\tilde{\mathcal{E}}_1(\theta, \phi, f) \geq -1 + \left\|\omega^{1/2} f\right\|_{L^2}^2 - g\Big(\varepsilon\left\|\omega^{1/2} f\right\|_{L^2}^2 + \frac{1}{\varepsilon}\left\|\omega^{-1/2} h\right\|_{L^2}^2\Big), \quad (1.29)$$

$$\geq (1 - g\varepsilon)\left\|\omega^{1/2} f\right\|_{L^2}^2 - 1 - \frac{g}{\varepsilon}\left\|\omega^{-1/2} h\right\|_{L^2}^2, \quad (1.30)$$

with $C_1 = 1 - g\varepsilon$ and $C_2 = 1 + \frac{g}{\varepsilon}\left\|\omega^{-1/2} h\right\|_{L^2}^2$, which yields the result for $g\varepsilon < 1$. □

Lemma 1.2.2 (Existence of a minimizer)**.** *Suppose the function h satisfies Hypothesis 1.1.1 and consider $g \geq 0$. Then, the functional energy $\tilde{\mathcal{E}}_1$ admits a minimizer in $[0, \pi] \times [0, 2\pi) \times \mathcal{Z}_\omega$.*

Proof. Let $((\theta_j, \phi_j, f_j))_{j\in\mathbb{N}}$ be a minimizing sequence for $\tilde{\mathcal{E}}_1$ in $[0, \pi] \times [0, 2\pi) \times \mathcal{Z}_\omega$. In particular, $(\tilde{\mathcal{E}}_1(\theta_j, \phi_j, f_j))_{j\in\mathbb{N}}$ is bounded and hence, by Lemma 1.2.1, $((\theta_j, \phi_j, f_j))_{j\in\mathbb{N}}$ is bounded in $[0, \pi] \times [0, 2\pi) \times \mathcal{Z}_\omega$. Thus, the sequence $((\theta_j, \phi_j, f_j))_{j\in\mathbb{N}}$ converges weakly to some limit $(\theta_\infty, \phi_\infty, f_\infty)$ in $[0,\pi] \times [0,2\pi] \times \mathcal{Z}_\omega$. In fact, the convergence is strong in the case of sequences $(\theta_j)_{j\in\mathbb{N}}$ and $(\phi_j)_{j\in\mathbb{N}}$ and for $g > 0$, we obviously have

$$\cos(\theta_j) + 2g\sin(\theta_j)\cos(\phi_j)\mathfrak{Re}\left\langle \omega^{-1/2}h, \omega^{1/2}f_j\right\rangle_{L^2} \underset{j\to\infty}{\longrightarrow} \cos(\theta_\infty) + 2g\sin(\theta_\infty)\cos(\phi_\infty)\mathfrak{Re}\left\langle \omega^{-1/2}h, \omega^{1/2}f_\infty\right\rangle_{L^2}. \quad (1.31)$$

Besides, using the lower semi-continuity property of the norm yields

$$\left\|\omega^{1/2}f_\infty\right\|_{L^2}^2 \leq \liminf_{j\to\infty}\left\|\omega^{1/2}f_j\right\|_{L^2}^2. \quad (1.32)$$

Finally, combining (1.31) and (1.32), we obtain

$$\tilde{\mathcal{E}}_1(\theta_\infty, \phi_\infty, f_\infty) \leq \liminf_{j\to\infty}\tilde{\mathcal{E}}_1(\theta_j, \phi_j, f_j). \quad (1.33)$$

Since $((\theta_j, \phi_j, f_j))_{j\in\mathbb{N}}$ is a minimizing sequence, we proved the existence of a minimizer. Note that if $\phi_\infty = 2\pi$, which means, in our case, in the closure of $[0,2\pi)$, then the minimizer that we are looking for is $(\theta_\infty, 0, f_\infty)$. □

1.2.2 Critical points of the energy

The result of Proposition 1.2.3 below provides equations satisfied by the critical points of the energy $\tilde{\mathcal{E}}_1$. Recall that $\mathbf{g}_{h,\frac{1}{2}}$ has been introduced in Eq. (1.15).

Proposition 1.2.3. *Suppose the function h satisfies Hypothesis 1.1.1, and consider $g \geq 0$. Then,*

(i) If $\mathbf{g}_{h,\frac{1}{2}} \leq 1$, then the set of the critical points of the functional $\tilde{\mathcal{E}}$ in $[0,\pi]\times[0,2\pi)\times\mathcal{Z}_\omega$ is

$$\mathcal{C}_0 := \{0,\pi\} \times [0,2\pi) \times \{0\}. \quad (1.34)$$

(ii) If $\mathbf{g}_{h,\frac{1}{2}} > 1$, then the set of critical points is

$$\mathcal{C}_0 \cup \{(\theta_c, 0, f_c), (\theta_c, \pi, -f_c\}, \quad (1.35)$$

where θ_c and f_c are given by

$$\theta_c = \arccos(-\frac{1}{\mathbf{g}_{h,\frac{1}{2}}}), \quad (1.36)$$

$$f_c = -g\omega^{-1}h\sqrt{1 - \frac{1}{\mathbf{g}_{h,\frac{1}{2}}^2}}. \quad (1.37)$$

Proof. A simple computation of the partial derivatives yields :

$$\partial_\theta \tilde{\mathcal{E}}_1(\theta,\phi,f) = -\sin(\theta) + 2g\cos(\theta)\cos(\phi)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k \quad \text{in } \mathbb{R}, \tag{1.38}$$

$$\partial_\phi \tilde{\mathcal{E}}_1(\theta,\phi,f) = -2g\sin(\theta)\sin(\phi)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k \quad \text{in } \mathbb{R}, \tag{1.39}$$

$$\partial_{\bar{f}} \tilde{\mathcal{E}}_1(\theta,\phi,f) = \omega f + g\sin(\theta)\cos(\phi)h \quad \text{in } \mathcal{Z}_\omega^*, \tag{1.40}$$

where the derivative $\partial_{\bar{f}}\tilde{\mathcal{E}}_1$ is taken in the sense of Frechet and where $\mathcal{Z}_\omega^*$ stands for the dual of $\mathcal{Z}_\omega$, namely

$$\mathcal{Z}_\omega^* := \{f : \mathbb{R}^3 \to \mathbb{C} \text{ measurable} \mid \omega^{-1/2} f \in L^2(\mathbb{R}^3, \mathrm{d}k)\}.$$

We are thus lead to solve the following system of equations

$$-\sin(\theta) + 2g\cos(\theta)\cos(\phi)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k = 0 \quad \text{in } \mathbb{R}, \tag{1.41}$$

$$-2g\sin(\theta)\sin(\phi)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k = 0 \quad \text{in } \mathbb{R}, \tag{1.42}$$

$$\omega f + g\sin(\theta)\cos(\phi)h = 0 \quad \text{in } \mathcal{Z}_\omega^* \tag{1.43}$$

Considering Eq. (1.42), it is easy to see that if $\theta \equiv 0[\pi]$, Eq. (1.43) gives $\omega^{1/2} f = 0$, and ϕ can be chosen arbitrarily in $[0, 2\pi)$.

Suppose now that $\theta \not\equiv 0[\pi]$. Then $\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k \neq 0$ by Eq. (1.41) and hence, Eq. (1.42) implies $\phi \equiv 0[\pi]$. Introducing $\phi = 0$ in Eq. (1.41) and Eq. (1.43) yields :

$$-\sin(\theta) + 2g\cos(\theta)\mathfrak{Re}\int_{\mathbb{R}^3} h(k)f(k)\,\mathrm{d}k = 0 \quad \text{in } \mathbb{R}, \tag{1.44}$$

$$\omega f + g\sin(\theta)h = 0 \quad \text{in } \mathcal{Z}_\omega^*. \tag{1.45}$$

Eq. (1.45) gives an explicit form of f in terms of θ and h :

$$f = -g\sin(\theta)\omega^{-1}h.$$

Inserting this expression in Eq. (1.44) yields :

$$-\sin(\theta) - \cos(\theta)\sin(\theta)\mathbf{g}_{h,\frac{1}{2}} = 0.$$

As θ is neither equal to 0 nor π, this yields :

$$\cos(\theta) = -\frac{1}{\mathbf{g}_{h,\frac{1}{2}}}, \tag{1.46}$$

which is possible if and only if :

$$\mathbf{g}_{h,\frac{1}{2}} > 1. \tag{1.47}$$

If this inequality is satisfied, we obtain Eq. (1.36). Then, by using the relations between the functions cos and sin, we obtain :

$$f = -g\sqrt{1 - \frac{1}{\mathbf{g}_{h,\frac{1}{2}}^2}}\,\omega^{-1}h. \tag{1.48}$$

Note that for the case $\phi = \pi$, the symmetry (1.25) implies that $(\theta, \pi, -f)$, where θ and f are given by equations (1.36) and (1.37), is also a critical point for the energy functional $\tilde{\mathcal{E}}_1$. This concludes the proof of Prop. 1.2.3. □

We are now ready to prove Theorem 1.1.2.

Proof of Theorem 1.1.2. Suppose that the function h satisfies Hypothesis 1.1.1, and let $g \geq 0$. Then, by Prop. 1.2.3, there exist (θ, ϕ, f) in $[0, \pi] \times [0, 2\pi) \times \mathcal{Z}_\omega$ a critical point of the functional $\tilde{\mathcal{E}}_1$. First, we assume that the following inequality holds :

$$\mathbf{g}_{h,\frac{1}{2}} \leq 1\,. \tag{1.49}$$

Then, by Prop. 1.2.3, we have θ equal to 0 or π, f equal to 0, and ϕ in $[0, 2\pi)$. Inserting these values in the energy yields :

$$\tilde{\mathcal{E}}_1(0, \phi, 0) = 1, \tag{1.50}$$

$$\tilde{\mathcal{E}}_1(\pi, \phi, 0) = -1. \tag{1.51}$$

Then, since we know that minimizers exist by Lemma 1.2.2, $(\pi, \phi, 0)$ are the only minimizers of $\tilde{\mathcal{E}}_1$, and we obtain Eq. (1.17). Since ζ is represented in its Bloch representation, a ground state $(\zeta_{\text{gs}}, f_{\text{gs}})$ of $\tilde{\mathcal{E}}_1$, up to phase symmetry with respect to ζ_{gs}, is then given by

$$\zeta_{\text{gs}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad f_{\text{gs}} \equiv 0.$$

Now, we assume that

$$\mathbf{g}_{h,\frac{1}{2}} > 1\,, \tag{1.52}$$

and we consider all critical points, in order to determine which ones are minimizers for the energy $\tilde{\mathcal{E}}_1$. As above, the critical points $(0, \phi, 0)$ and $(\pi, \phi, 0)$ satisfy Eq. (1.50) and Eq. (1.51), respectively. By Prop. 1.2.3, the other critical points are given by $(\theta_c, 0, f_c)$ and (θ_c, π, f_c) with θ_c given by Eq. (1.36) and f_c given by (1.37). A direct computation shows that the corresponding energy is

$$\tilde{\mathcal{E}}_1(\theta_c, 0, f_c) = \tilde{\mathcal{E}}_1(\theta_c, \pi, f_c) = -\frac{1}{2}\Big(\mathbf{g}_{h,\frac{1}{2}} + \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}\Big), \tag{1.53}$$

which is strictly less than -1 by Remark 1.1.4. Hence $(\theta_c, 0, f_c)$ and (θ_c, π, f_c) are global minimizers since we know from Lemma 1.2.2 that minimizers exist. Now, the relations between the functions cos and sin allow us to compute :

$$\cos(\theta/2) = \sqrt{\frac{1}{2} - \frac{1}{2\mathbf{g}_{h,\frac{1}{2}}}} = \frac{1}{\sqrt{2}}\sqrt{1 - \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}}, \tag{1.54}$$

$$\sin(\theta/2) = \sqrt{\frac{1}{2} + \frac{1}{2\mathbf{g}_{h,\frac{1}{2}}}} = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{1}{\mathbf{g}_{h,\frac{1}{2}}}}. \tag{1.55}$$

Since ζ is represented in its Bloch representation (see Eq. (1.23)), we obtain the Eq. (1.18). This conclude the proof. □

1.3 Superposition of two quasi-classical states

This section is dedicated to the proofs of the results concerning of the energy functional $\mathcal{E}_2$ introduced in Eq. (1.13) for the superposition of quasi-classical states. First, we prove Prop. 1.1.5 which provides an upper bound of the ground state energy and proves that it is lower than the ground state energy of the free Hamiltonian. Then, we prove Theorem 1.1.7 on the existence of a ground state for the energy functional $\mathcal{E}_2$. The strategy of the proof relies on the fact that we can reduce the problem to the minimization of a simpler functional. Indeed, as in the previous section, it is convenient to use the Bloch representation [24]. Here, we write $\alpha = \cos(\theta/2)$ and $\beta = e^{i\phi}\sin(\theta/2)$, with θ in $[0,\pi]$ and ϕ in $[0, 2\pi)$. The energy functional $\mathcal{E}_2$ then becomes

$$\begin{aligned}\mathcal{E}_2(\cos(\theta/2), e^{i\phi}\sin(\theta/2), f_1, f_2) &= \cos^2(\theta/2)\|\omega^{1/2}f_1\|_{L^2}^2 + \sin^2(\theta/2)\|\omega^{1/2}f_2\|_{L^2}^2 - \cos(\theta)\\ &+ ge^{-\frac{\|f_1-f_2\|_{L^2}^2}{4}}\sin(\theta)\mathfrak{Re}\left(e^{i\phi}e^{-\frac{i}{2}\mathfrak{Im}\langle f_1,f_2\rangle_{L^2}}\big(\langle f_1,h\rangle_{L^2} + \langle h,f_2\rangle_{L^2}\big)\right).\end{aligned}$$

In particular, we observe that

$$\begin{aligned}\mathcal{E}_2(\cos(\theta/2), e^{i\phi}\sin(\theta/2), f_1, f_2) &\geq \cos^2(\theta/2)\|\omega^{1/2}f_1\|_{L^2}^2 + \sin^2(\theta/2)\|\omega^{1/2}f_2\|_{L^2}^2\\ &\quad - \cos(\theta) - ge^{-\frac{\|f_1-f_2\|_{L^2}^2}{4}}\sin(\theta)\big|\langle f_1,h\rangle_{L^2} + \langle h,f_2\rangle_{L^2}\big|,\\ &= \mathcal{E}_2(\cos(\theta/2), e^{i\phi_0}\sin(\theta/2), f_1, f_2),\end{aligned}$$

with ϕ_0 suitably chosen (depending on f_1 and f_2).

This allows us to obtain

$$\inf_{(\alpha,\beta)\in\mathfrak{Z},(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2}\mathcal{E}_2(\alpha,\beta,f_1,f_2) = \inf_{\theta\in[0,\pi],(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2}\tilde{\mathcal{E}}_2(\theta,f_1,f_2),$$

where the functional $\tilde{\mathcal{E}}_2$ is given by

$$\begin{aligned}\tilde{\mathcal{E}}_2(\theta,f_1,f_2) &= \cos^2(\theta/2)\big(\|\omega^{1/2}f_1\|_{L^2}^2 - 1\big) + \sin^2(\theta/2)\big(\|\omega^{1/2}f_2\|_{L^2}^2 + 1\big)\\ &\quad - g\sin(\theta)e^{-\|f_1-f_2\|_{L^2}^2/4}\big|\langle f_1,h\rangle_{L^2} + \langle h,f_2\rangle_{L^2}\big|.\end{aligned} \tag{1.56}$$

Moreover, if we prove the existence of a minimizer for $\tilde{\mathcal{E}}_2$, we get the existence of a minimizer for the energy functional $\mathcal{E}_2$.

Proof of Proposition 1.1.5. Consider λ in $\mathbb{R}$, $0 \leq g \leq 1$ and θ in $[0,\pi]$. A direct computation gives

$$\tilde{\mathcal{E}}_2\big(g\theta, 0, \lambda\omega^{-1}h\big) = \sin^2(g\theta/2)\lambda^2\|\omega^{-1/2}h\|_{L^2}^2 - g\sin(g\theta)e^{-\lambda^2\|\omega^{-1}h\|_{L^2}^2/4}|\lambda|\|\omega^{-1/2}h\|_{L^2}^2 - \cos(g\theta). \quad (1.57)$$

Computing the second-order expansion in g yields

$$\begin{aligned}\tilde{\mathcal{E}}_2\big(g\theta, 0,\lambda\omega^{-1}h\big) &= \frac{g^2\theta^2}{4}\lambda^2\|\omega^{-1/2}h\|_{L^2}^2 - g^2\theta e^{-\lambda^2\|\omega^{-1}h\|_{L^2}^2/4}|\lambda|\|\omega^{-1/2}h\|_{L^2}^2 - 1 + \frac{g^2\theta^2}{2} + \underset{g\to 0}{\mathcal{O}}(g^3)\,,\\ &= -1 + g^2\Big(\big(\frac{1}{2} + \frac{\lambda^2}{4}\|\omega^{-1/2}h\|_{L^2}^2\big)\theta^2 - |\lambda|\|\omega^{-1/2}h\|_{L^2}^2 e^{-\lambda^2\|\omega^{-1}h\|_{L^2}^2/4}\theta\Big) + \underset{g\to 0}{\mathcal{O}}(g^3)\,.\end{aligned}$$

Computing the infimum on $[0,\pi]\times\mathbb{R}$ of the function defined by

$$F(\theta,\lambda) = \Big(\frac{1}{2} + \frac{\lambda^2}{4}\|\omega^{-1/2}h\|_{L^2}^2\Big)\theta^2 - |\lambda|\|\omega^{-1/2}h\|_{L^2}^2 e^{-\lambda^2\|\omega^{-1}h\|_{L^2}^2/4}\theta$$

yields Ineq. (1.21) and concludes the proof of Prop 1.1.5. □

Lemma 1.3.1 below states a useful inequality to prove the existence of a minimizer for the energy functional $\tilde{\mathcal{E}}_2$.

Lemma 1.3.1. *Suppose that the function h satisfies Hypothesis 1.1.2, and consider $g \geq 0$. Then, for all (θ, f_1, f_2) in $[0,\pi]\times(\mathcal{Z}_\omega\cap L^2)^2$, the following inequality holds*

$$\tilde{\mathcal{E}}_2(\theta, f_1, f_2) \geq \cos^2(\theta/2)\|\omega^{1/2}f_1\|_{L^2}^2(1 - g\|\omega^{-1/2}h\|_{L^2}) + \sin^2(\theta/2)\|\omega^{1/2}f_2\|_{L^2}^2(1 - g\|\omega^{-1/2}h\|_{L^2}) - \cos(\theta) - g\|\omega^{-1/2}h\|_{L^2}. \quad (1.58)$$

Proof. Using the Cauchy-Schwarz and standard Young inequalities allows us to obtain

$$\begin{aligned}&g\sin(\theta)e^{-\|f_1-f_2\|_{L^2}^2/4}\big|\,\langle f_1, h\rangle_{L^2} + \langle h, f_2\rangle_{L^2}\,\big|\\ &= 2g\sin(\theta/2)\cos(\theta/2)e^{-\|f_1-f_2\|_{L^2}^2/4}\big|\,\big\langle \omega^{1/2}f_1, \omega^{-1/2}h\big\rangle_{L^2} + \big\langle \omega^{-1/2}h, \omega^{1/2}f_2\big\rangle_{L^2}\,\big|\,,\\ &\leq 2g\big(\cos(\theta/2)\sin(\theta/2)\|\omega^{1/2}f_1\|_{L^2}\|\omega^{-1/2}h\|_{L^2} + \sin(\theta/2)\cos(\theta/2)\|\omega^{1/2}f_2\|_{L^2}\|\omega^{-1/2}h\|_{L^2}\big)\,,\\ &\leq g\|\omega^{-1/2}h\|_{L^2}\big(\cos^2(\theta/2)\|\omega^{1/2}f_1\|_{L^2}^2 + \sin^2(\theta/2)\|\omega^{1/2}f_2\|_{L^2}^2 + 1\big)\,,\end{aligned}$$

which yields the result. □

We are now ready to prove the existence of a ground state for the functional $\mathcal{E}_2$.

Proof of Theorem 1.1.7. The strategy relies on usual tools from the calculus of variations.

Let $((\theta_j, f_{1,j}, f_{2,j}))_{j\in\mathbb{N}}$ be a minimizing sequence for the functional $\tilde{\mathcal{E}}_2$. We aim to prove that this sequence is bounded in $[0,\pi]\times(\mathcal{Z}_\omega\cap L^2)^2$. Let us consider, for all j in $\mathbb{N}$

$$f_{1,j,\Lambda} := \mathbf{1}_{|k|\leq\Lambda}f_{1,j}\ ,\quad f_{2,j,\Lambda} := \mathbf{1}_{|k|\leq\Lambda}f_{2,j}\,. \quad (1.59)$$

Then, recalling that $h = \mathbf{1}_{|k|\leq\Lambda}h$ by Hypothesis 1.1.3, we have

$$\begin{aligned}\tilde{\mathcal{E}}_2(\theta_j, f_{1,j}, f_{2,j}) \geq \cos^2(\theta_j/2)\|\omega^{1/2}f_{1,j,\Lambda}\|_{L^2}^2 + \sin^2(\theta_j/2)\|\omega^{1/2}f_{2,j,\Lambda}\|_{L^2}^2 - \cos(\theta_j)\\ - g\sin(\theta_j)e^{-\|f_{1,j,\Lambda}-f_{2,j,\Lambda}\|_{L^2}^2/4}e^{-\|\mathbf{1}_{|k|\geq\Lambda}(f_{1,j}-f_{2,j})\|_{L^2}^2/4}\big|\langle f_{1,j,\Lambda}, h\rangle_{L^2} + \langle h, f_{2,j,\Lambda}\rangle_{L^2}\big|.\end{aligned}$$

Since $e^{-\|\mathbf{1}_{|k|\geq\Lambda}(f_{1,j}-f_{2,j})\|_{L^2}^2/4} \leq 1$, this yields

$$\tilde{\mathcal{E}}_2(\theta_j, f_{1,j}, f_{2,j}) \geq \tilde{\mathcal{E}}_2(\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}),$$

and hence $((\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}))_{j\in\mathbb{N}}$ is another minimizing sequence for the functional $\tilde{\mathcal{E}}_2$. By Lemma 1.3.1, the sequences $(\cos^2(\theta_j/2)\|\omega^{1/2}f_{1,j,\Lambda}\|_{L^2}^2)_{j\in\mathbb{N}}$ and $(\sin^2(\theta_j/2)\|\omega^{1/2}f_{2,j,\Lambda}\|_{L^2}^2)_{j\in\mathbb{N}}$ are bounded, since $g\|\omega^{-1/2}h\|_{L^2} < 1$.

Let us first assume by contradiction that

$$\delta := \limsup_{j\to\infty}\theta_j = \pi.$$

Then there exists a subsequence, that we still denote by $(\theta_j)_{j\in\mathbb{N}}$ for convenience, such that $\theta_j \underset{j\to\infty}{\longrightarrow} \pi$. In this case, $\cos(\theta_j) \underset{j\to\infty}{\longrightarrow} -1$ and we have

$$\tilde{\mathcal{E}}_2(\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}) \geq -g\|\omega^{-1/2}h\|_{L^2} - \cos(\theta_j),$$

this implies

$$\inf_{\theta\in[0,\pi],(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2}\tilde{\mathcal{E}}_2(\theta, f_1, f_2) \geq 1 - g\|\omega^{-1/2}h\|_{L^2},$$

which is a contradiction since we proved in Prop. 1.1.5 that $\inf\tilde{\mathcal{E}}_2 < -1$ and since we assumed that $g\|\omega^{1/2}h\|_{L^2} < 1$.

Then, we have

$$\delta = \limsup_{j\to\infty}\theta_j < \pi.$$

This gives the existence of a constant $C_\delta > 0$, such that

$$\cos^2(\theta_j/2) \geq C_\delta > 0,$$

uniformly in j. This yields

$$\tilde{\mathcal{E}}_2(\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}) \geq C_\delta\|\omega^{1/2}f_{1,j,\Lambda}\|_{L^2}^2 - g\|\omega^{-1/2}h\|_{L^2}^2 - 1,$$

which allows us to obtain that the sequence $(f_{1,j,\Lambda})_{j\in\mathbb{N}}$ is bounded in $\mathcal{Z}_\omega$. Now, let us assume by contradiction that the sequence $(f_{2,j,\Lambda})_{j\in\mathbb{N}}$ is not bounded in $\mathcal{Z}_\omega$. Then there exists a subsequence, that we still denote by $(f_{2,j,\Lambda})_{j\in\mathbb{N}}$ for convenience, such that the following limit holds

$$\|\omega^{1/2}f_{2,j,\Lambda}\|_{L^2} \underset{j\to\infty}{\longrightarrow} +\infty.$$

Using Hölder's inequality yields, since we assumed that $\|\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda}\|_{L^\infty} < \infty$ (see Hypothesis 1.1.3),

$$\|\omega^{1/2} f_{2,j,\Lambda}\|_{L^2} = \|\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda} f_{2,j,\Lambda}\|_{L^2} \leq \|\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda}\|_{L^\infty}\|f_{2,j,\Lambda}\|_{L^2},$$

which gives $\|f_{2,j,\Lambda}\|_{L^2} \underset{j\to\infty}{\longrightarrow} +\infty$ (note that $\|\omega^{1/2}\mathbf{1}_{|k|\leq\Lambda}\|_{L^\infty} \neq 0$ since $\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}$ is in L^∞ by Hypothesis 1.1.3). Furthermore, in the same way, we have

$$\|f_{1,j,\Lambda}\|_{L^2} = \|\omega^{-1/2}\omega^{1/2} f_{1,j,\Lambda}\|_{L^2} \leq \|\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}\|_{L^\infty}\|\omega^{1/2} f_{1,j,\Lambda}\|_{L^2}.$$

Therefore, since $\|\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}\|_{L^\infty}$ is bounded by assumption, and since we proved that the sequence $(f_{1,j,\Lambda})_{j\in\mathbb{N}}$ is bounded in $\mathcal{Z}_\omega$, $(f_{1,j,\Lambda})_{j\in\mathbb{N}}$ is also bounded in L^2. Hence the following limit holds

$$\|f_{1,j,\Lambda} - f_{2,j,\Lambda}\|_{L^2} \underset{j\to\infty}{\longrightarrow} +\infty\,.$$

Since

$$\tilde{\mathcal{E}}_2(\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}) \geq$$
$$-1-g e^{-\|f_{1,j,\Lambda}-f_{2,j,\Lambda}\|^2_{L^2}/4}\big(\cos^2(\theta_j/2)\|\omega^{1/2} f_{1,j,\Lambda}\|^2_{L^2}+\sin^2(\theta_j/2)\|\omega^{1/2} f_{2,j,\Lambda}\|^2_{L^2}-\|\omega^{-1/2}h\|^2_{L^2}\big),$$

since the sequences $(\cos^2(\theta/2)\|\omega^{1/2} f_{1,j,\Lambda}\|^2_{L^2})_{j\in\mathbb{N}}$ and $(\sin^2(\theta/2)\|\omega^{1/2} f_{2,j,\Lambda}\|^2_{L^2})_{j\in\mathbb{N}}$ are bounded, and since $e^{-\|f_{1,j,\Lambda}-f_{2,j,\Lambda}\|^2_{L^2}/4} \underset{j\to\infty}{\longrightarrow} 0$, we obtain

$$\inf_{\theta\in[0,\pi],(f_1,f_2)\in(\mathcal{Z}_\omega\cap L^2)^2} \tilde{\mathcal{E}}_2(\theta, f_1, f_2) \geq -1.$$

For g small enough, this contradicts Prop. 1.1.5. We conclude that the sequence $(f_{2,j,\Lambda})_{j\in\mathbb{N}}$ is bounded in $\mathcal{Z}_\omega$.

We have proven that $((\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}))_{j\in\mathbb{N}}$ is bounded in $[0,\pi]\times\mathcal{Z}_\omega^2$. Since $\omega^{-1/2}\mathbf{1}_{|k|\leq\Lambda}$ is in L^∞ by Hypothesis 1.1.3, $((\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}))_{j\in\mathbb{N}}$ is also bounded in $[0,\pi]\times(\mathcal{Z}_\omega\cap L^2)^2$. Therefore, the sequence $((\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}))_{j\in\mathbb{N}}$ converges weakly to some limit $(\theta_\infty, f_{1,\infty,\Lambda}, f_{2,\infty,\Lambda})$ in $[0,\pi]\times(\mathcal{Z}_\omega\cap L^2)^2$. Note that convergence is strong in the case of the sequence $(\theta_j)_{j\in\mathbb{N}}$. We have

$$\cos(\theta_j/2) \underset{j\to\infty}{\longrightarrow} \cos(\theta_\infty/2), \quad \sin(\theta_j/2) \underset{j\to\infty}{\longrightarrow} \sin(\theta_\infty/2),$$

and

$$\begin{aligned}\big|\,\langle f_{1,j,\Lambda}, h\rangle_{L^2} + \langle h, f_{2,j,\Lambda}\rangle_{L^2}\,\big| &= \big|\,\big\langle \omega^{1/2} f_{1,j,\Lambda}, \omega^{-1/2}h\big\rangle_{L^2} + \big\langle \omega^{-1/2}h, \omega^{1/2} f_{2,j,\Lambda}\big\rangle_{L^2}\,\big|\,,\\ &\underset{j\to\infty}{\longrightarrow} \big|\,\big\langle \omega^{1/2} f_{1,\infty,\Lambda},\ \omega^{-1/2}h\big\rangle_{L^2} + \big\langle \omega^{-1/2}h,\ \omega^{1/2} f_{2,\infty,\Lambda}\big\rangle_{L^2}\,\big|\,.\end{aligned}$$

Moreover, using the lower semi-continuity of the L^2-norm gives

$$\liminf_{j\to\infty} \|\omega^{1/2} f_{1,j,\Lambda}\|^2_{L^2} \geq \|\omega^{1/2} f_{1,\infty,\Lambda}\|^2_{L^2}\,,$$
$$\liminf_{j\to\infty} \|\omega^{1/2} f_{2,j,\Lambda}\|^2_{L^2} \geq \|\omega^{1/2} f_{2,\infty,\Lambda}\|^2_{L^2}\,,$$
$$\liminf_{j\to\infty} \big(-e^{-\|f_{1,j,\Lambda}-f_{2,j,\Lambda}\|^2_{L^2}/4}\big) \geq -e^{-\|f_{1,\infty,\Lambda}-f_{2,\infty,\Lambda}\|^2_{L^2}/4}.$$

Inserting this into the expression (1.56) of $\tilde{\mathcal{E}}_2$, we obtain

$$\tilde{\mathcal{E}}_2(\theta_\infty, f_{1,\infty,\Lambda}, f_{2,\infty,\Lambda}) \leq \liminf_{j\to\infty} \tilde{\mathcal{E}}_2(\theta_j, f_{1,j,\Lambda}, f_{2,j,\Lambda}) = \inf \tilde{\mathcal{E}}_2.$$

Therefore $(\theta_\infty, f_{1,\infty,\Lambda}, f_{2,\infty,\Lambda})$ is a minimizer for the energy functional $\tilde{\mathcal{E}}_2$. □

Remark 1.3.2. *Computing the Lagrange equations shows that a minimizer $(\theta_{\rm gs}, f_{1,\rm gs}, f_{2,\rm gs})$ of $\tilde{\mathcal{E}}_2$ satisfies*

$$\theta_{\rm gs} = \arctan\left(\frac{e^{-\|f_{1,\rm gs}-f_{2,\rm gs}\|^2_{L^2}/4}\mathfrak{Re}\big(\,\langle f_{1,\rm gs}, h\rangle_{L^2} + \langle h, f_{2,\rm gs}\rangle_{L^2}\,\big)}{\|\omega^{1/2}f_{2,\rm gs}\|^2_{L^2} - \|\omega^{1/2}f_{1,\rm gs}\|^2_{L^2} + 2} \right), \tag{1.60}$$

$$f_{1,\rm gs} = g\tan(\theta_{\rm gs}/2)e^{-\|f_{1,\rm gs}-f_{2,\rm gs}\|^2_{L^2}/4}(h - \frac{1}{2}(f_{1,\rm gs} - f_{2,\rm gs})\mathfrak{Re}\big(\,\langle f_{1,\rm gs}, h\rangle_{L^2} + \langle h, f_{2,\rm gs}\rangle_{L^2}\,\big)\omega^{-1}, \tag{1.61}$$

$$f_{2,\rm gs} = g\cot(\theta_{\rm gs}/2)e^{-\|f_{1,\rm gs}-f_{2,\rm gs}\|^2_{L^2}/4}(h - \frac{1}{2}(f_{2,\rm gs} - f_{1,\rm gs})\mathfrak{Re}\big(\,\langle f_{1,\rm gs}, h\rangle_{L^2} + \langle h, f_{2,\rm gs}\rangle_{L^2}\,\big)\omega^{-1}. \tag{1.62}$$

Computing then an asymptotic expansion for small g is possible. We conjecture that, under the assumption of Theorem 1.1.7, the upper bound computed in the right-hand-side of Ineq. (1.21) in Prop. 1.1.5 actually coincides with the second order expansion as $g \to 0$ of the ground state energy of $\tilde{\mathcal{E}}_2$.

1.4 Appendix : Fock space, Self-adjointness

1.4.1 Operators in Fock space

We recall in this section a few well-known properties of basic operators in Fock space. We do not specify their domains. For more details the reader may consult e.g. [21, 25, 107]. Recall that the symmetric Fock space $\mathfrak{F}_s(\mathfrak{h})$ over the one-particle space $\mathfrak{h} = L^2(\mathbb{R}^3)$ has been defined in (1.2). For h in $\mathfrak{h}$, the creation and annihilation operators $a^*(h)$ and $a(h)$ are defined as follows :

$$a^*(h)_{|\bigvee^n\mathfrak{h}} = \sqrt{(n+1)}\;|h\rangle \bigvee \mathbf{I}_{\bigvee^n\mathfrak{h}}, \quad n \geq 0,$$
$$a(h)_{|\bigvee^n\mathfrak{h}} = \sqrt{n}\;\langle h| \otimes \mathbf{I}_{\bigvee^{n-1}\mathfrak{h}}, \quad n > 0, \qquad a(h)_{|\mathbb{C}} = 0.$$

Formally, we also have

$$a(h) = \int_{\mathbb{R}^3} \overline{h(k)}a(k)\,\mathrm{d}k, \quad a^*(h) = \int_{\mathbb{R}^3} h(k)a^*(k)\,\mathrm{d}k,$$

where $a(k)$ and $a^*(k)$ are operator-valued distributions which satisfy the well-known canonical commutations relations

$$[a(k), a(k')] = [a^*(k), a^*(k')] = 0, \quad [a(k), a^*(k')] = \delta(k - k').$$

The field operator $\Phi(h)$ is defined by

$$\Phi(h) = (a(h) + a^*(h))/\sqrt{2}.$$

This operator identifies with an essentially self-adjoint operator, which allows us to define the Weyl operator :

$$W(h) = e^{i\Phi(h)}.$$

The Weyl operator satisfies the so-called Weyl relations :

$$W(h)^* = W(-h), \quad W(f+h) = e^{-\frac{i}{2}\mathfrak{Im}\langle f,h\rangle_{\mathfrak{h}}} W(f)W(h). \tag{1.63}$$

Let ω be a self-adjoint operator on $\mathfrak{h}$. The second quantization of ω is defined by

$$\mathrm{d}\Gamma(\omega)_{|\bigvee^n \mathfrak{h}} = \sum_{k=1}^{n} \mathbf{I}_{\bigvee^{k-1}\mathfrak{h}} \otimes \omega \otimes \mathbf{I}_{\bigvee^{n-k}\mathfrak{h}}.$$

Note that this operator can be expressed in terms of creation and annihilation operators :

$$\mathrm{d}\Gamma(\omega) = \int_{\mathbb{R}^3} \omega(k) a^*(k) a(k)\, \mathrm{d}k.$$

The coherent state of parameter f in $\mathfrak{h}$ is the vector in Fock space defined as

$$\Psi_f := e^{i\Phi\left(\frac{\sqrt{2}}{i} f\right)}\Omega = e^{-\frac{\|f\|_{\mathfrak{h}}^2}{2}} \sum_{n=0}^{\infty} \frac{f^{\otimes n}}{\sqrt{n!}},$$

where Ω stands for the Fock vacuum. Coherent states are eigenvectors of the annihilation operator in the sense that, for all f, h in $\mathfrak{h}$, we have

$$a(h)\Psi_f = \langle h, f\rangle_{\mathfrak{h}}\, \Psi_f.$$

This identity implies the following relations :

$$\langle \Psi_f, \Phi(h)\Psi_f\rangle_{\mathfrak{F}_s(\mathfrak{h})} = 2\mathfrak{Re}\, \langle h, f\rangle_{\mathfrak{h}}, \qquad \langle \Psi_f, \mathrm{d}\Gamma(\omega)\Psi_f\rangle_{\mathfrak{F}_s(\mathfrak{h})} = \langle f, \omega f\rangle_{\mathfrak{h}}.$$

Furthermore, considering coherent states with different parameters f and h in $\mathfrak{h}$ yields, using the Weyl relations (1.63) :

$$\langle \Psi_f, \Psi_h\rangle_{\mathfrak{F}_s(\mathfrak{h})} = e^{-\frac{\|f-h\|_{\mathfrak{h}}^2}{4}} e^{-\frac{i}{2}\mathfrak{Im}\langle f,h\rangle_{\mathfrak{h}}}.$$

These equalities were used to compute the energies (1.9) and (1.13) of product states of the form $u \otimes \Psi_f$.

1.4.2 Self-adjointness of the hamiltonian

Proposition 1.4.1. *Suppose h satisfies Hypothesis 1.1.1. Then $\mathbb{H}$ is a self-adjoint, semi-bounded operator with domain $\mathcal{D}(\mathbb{H}) = \mathcal{D}(\mathbb{H}_{\text{free}})$ for all g in $\mathbb{R}$.*

Proof. Let g in $\mathbb{R}$ and let ψ in $\mathfrak{F}_s(\mathfrak{h})$. We recall the well-known N_τ-estimates for the creation and annihilation operators :

$$\begin{aligned}\|a(h)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} &\leq \left\|\omega^{-1/2}h\right\|_{\mathfrak{h}} \left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|_{\mathfrak{F}_s(\mathfrak{h})} ,\\ \|a^*(h)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} &\leq \left\|\omega^{-1/2}h\right\|_{\mathfrak{h}} \left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|_{\mathfrak{F}_s(\mathfrak{h})} + \|h\|_{\mathfrak{h}} \|\psi\|_{\mathfrak{F}_s(\mathfrak{h})} .\end{aligned}$$

Here, these estimates hold since we assumed that the function $\omega^{-1/2}h$ is in $L^2(\mathbb{R}^3)$. Now, using the Cauchy-Schwarz inequality yields

$$\begin{aligned}\left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|^2_{\mathfrak{F}_s(\mathfrak{h})} &= \langle\psi, \mathrm{d}\Gamma(\omega)\psi\rangle_{\mathfrak{F}_s(\mathfrak{h})} ,\\ &\leq \|\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \|\mathrm{d}\Gamma(\omega)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq \frac{1}{2\varepsilon^2} \|\psi\|^2_{\mathfrak{F}_s(\mathfrak{h})} + \frac{\varepsilon^2}{2} \|\mathrm{d}\Gamma(\omega)\psi\|^2_{\mathfrak{F}_s(\mathfrak{h})} .\end{aligned}$$

Taking $\varepsilon > 0$ small enough allows us to conclude that there exist $a < 1$ and b in $\mathbb{R}$ such that, for all ψ in $\mathfrak{F}_s(\mathfrak{h})$, the following inequality holds

$$\|g\, \sigma_1 \otimes \Phi(h)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq a \|\mathbb{H}_{\text{free}}\psi\|_{\mathfrak{F}_s(\mathfrak{h})} + b \|\psi\|_{\mathfrak{F}_s(\mathfrak{h})} .$$

Therefore $g\sigma_1 \otimes \Phi(h)$ is relatively bounded with respect to $\mathbb{H}_{\text{free}}$ with relative bound less than 1. Applying the Kato-Rellich theorem then yields the result. □

Chapitre 2

Linearly Coupled Pauli-Fierz Hamiltonians

Abstract. We consider a spinless, non-relativistic particle bound by an external potential and linearly coupled to a quantized radiation field. The energy $\mathcal{E}(u,f)$ of product states of the form $u \otimes \Psi_f$, where u is a normalized state for the particle and Ψ_f is a coherent state in Fock space for the field, gives the energy of a Klein–Gordon–Schrödinger system. We minimize the functional $\mathcal{E}(u,f)$ on its natural energy space. We prove the existence and uniqueness of a ground state under general conditions on the coupling function. In particular, neither an ultraviolet cutoff nor an infrared cutoff is imposed. Our results establish the convergence in the ultraviolet limit of both the ground state and ground state energy of the Klein–Gordon–Schrödinger energy functional, and provide the second-order asymptotic expansion of the ground state energy at small coupling.

2.1 Introduction

We consider in this paper a non-relativistic, spinless quantum particle – say, an electron – in an external potential and coupled to a quantized, scalar radiation field. The Hilbert space for the total system is given by

$$\mathcal{H} := \mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}},$$

where $\mathcal{H}_{\mathrm{el}} = L^2(\mathbb{R}^3)$ is the Hilbert space for the electron and $\mathcal{H}_{\mathrm{f}}$ is the Hilbert space for the field, given as the symmetric Fock space over the one-particle Hilbert space $\mathfrak{h} = L^2(\mathbb{R}^3)$. The full Hamiltonian is a self-adjoint operator acting on $\mathcal{H}$, of the form

$$\mathbb{H} := H_V \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} + \mathbb{H}_{\mathrm{int}}, \tag{2.1}$$

where $H_V = -\Delta + V$ is the Hamiltonian for the non-relativistic particle in the external potential V, $\mathbb{H}_{\mathrm{f}}$ is the Hamiltonian for the free field, $\mathbf{I}_\sharp$ stands for the identity on $\mathcal{H}_\sharp$ and $\mathbb{H}_{\mathrm{int}}$ is the interaction Hamiltonian, acting on $\mathcal{H}$. Such operators are usually called *Pauli-Fierz*

Hamiltonians [104] in the literature. Their spectral theory has been thoroughly studied since the end of the nineties (see e.g. [110, 111] and references therein). In particular, concerning the existence of a ground state – namely the proof that the bottom of the spectrum of $\mathbb{H}$ is an eigenvalue – we refer, among others, to [40] for massive Pauli-Fierz Hamiltonians (i.e. Pauli-Fierz Hamiltonians with a massive field dispersion relation), [11, 12] for massless Pauli-Fierz Hamiltonians at small coupling and [53, 63] in the massless case without any restriction on the coupling strength. Expansions of the ground state energy of $\mathbb{H}$ for small coupling constants have also been obtained in [11, 12, 62, 71] using 'spectral renormalization', [16, 68] by an iterative variational procedure and [10] by iterative multiscale analysis.

We focus in this paper on the case of an electron *linearly coupled* to a scalar field. We consider an abstract class of linearly coupled Pauli-Fierz Hamiltonian that includes the *Nelson model* [102] and the *Fröhlich polaron model* [48]. For the Nelson model, in order for $\mathbb{H}$ to identify to a semi-bounded self-adjoint operator on $\mathcal{H}$, an ultraviolet cutoff must be imposed to the interaction Hamiltonian. The polaron model defines a self-adjoint operator even without an ultraviolet cutoff [65, 90]. The precise definition of the model we consider will be given in Section 2.1.1.

We aim at studying the energy of product states

$$\mathcal{E}(u,f) := \big\langle (u\otimes\Psi_f), \mathbb{H}(u\otimes\Psi_f)\big\rangle, \quad \|u\|_{\mathcal{H}_{\mathrm{el}}}=1, \quad \|\Psi_f\|_{\mathcal{H}_{\mathrm{f}}}=1, \tag{2.2}$$

assuming that the state of the quantized field, Ψ_f, is a *coherent state* parametrized by $f\in\mathfrak{h}$. The functional $\mathcal{E}(u,f)$ is sometimes called *quasi-classical energy.* Assuming indeed that the field degrees of freedom are 'almost classical', in the sense that the creation and annihilation operator a^*, a in $\mathcal{H}_{\mathrm{f}}$ are rescaled as $a^*_\varepsilon=\sqrt{\varepsilon}a^*$, $a_\varepsilon=\sqrt{\varepsilon}a$, see [5], one shows, under suitable assumptions, that the ground state energy of the rescaled Pauli-Fierz Hamiltonian $\mathbb{H}_\varepsilon$ converges, as $\varepsilon\to 0$, to the ground state energy of the quasi-classical energy functional (2.2), [31, 34, 35, 55]. In the case of the translation invariant Fröhlich polaron model (no external potential), a proper rescaling shows that the quasi-classical limit corresponds to the strong coupling limit of the original Hamiltonian $\mathbb{H}$, see e.g. [108].

As we recall below, the quasi-classical energy (2.2) coincides with the energy of a coupled *Klein–Gordon–Schrödinger* system. The variational and dynamical aspects of Klein–Gordon–Schrödinger systems in the quasi-classical limit have been studied in the recent mathematical literature (see [2–4, 31, 34, 35, 45]), as quasi-classical limits of Pauli-Fierz models. The strong coupling limit of the polaron model has also been studied in several contexts, especially in the case of translation invariant systems allowing one to study the effective mass of polarons, see [42, 90] for seminal results and [22, 43, 89, 99, 108] for more recent references ; see also [88] for another definition of the effective mass of the polaron in a slowly varying external potential and [47] for a polaron confined to a finite volume. In all these references, the existence of a ground state associated to the non-linear energy functional defined as in (2.2) constitute an essential ingredients of the analysis.

Our main concern in this paper is to prove the existence and study the properties of ground states of the quasi-classical Klein–Gordon–Schrödinger energy functional $\mathcal{E}(u,f)$, on its natural energy space and under general conditions on the external potential and the interaction term. We will recall that minimizing $\mathcal{E}(u,f)$ reduces to minimizing a Hartree (or Choquard-Pekar) energy functional. Existence, uniqueness and properties of ground states for these functionals have been studied by many authors. We refer to the seminal works [91] for the translation invariant model with a convolution potential given by the Coulomb potential, and [92, 93] in a more general setting, applying the concentration compactness method. See also [98] for a more recent extensive survey of the vast literature concerning Choquard type equations.

Our first main result in this paper provides the existence of a ground state for the quasi-classical energy functional $\mathcal{E}(u,f)$. We consider a wide class of external potentials and do not need to impose *neither an infrared nor an ultraviolet cutoff* into the interaction term of $\mathcal{E}(u,f)$.

Next, for small coupling, we verify that the ground state of $\mathcal{E}(u,f)$ is unique. In general, the field parameter f_{gs} of the ground state $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ does not necessarily belong to the orignal one-particle Hilbert space $\mathfrak{h}$. For massless fields, we will see that f_{gs} belongs to $\mathfrak{h}$ if and only if an infrared regularization is imposed. On the other hand, no ultraviolet cutoff is needed : Denoting by Λ the ultraviolet parameter associated to the ultraviolet cutoff introduced into the interaction Hamiltonian, our results show that both the ground states and ground state energies associated to (2.2) converge as $\Lambda \to \infty$.

We also study the difference between the ground state energy for the microscopic model and its quasi-classical counterpart,

$$\inf \sigma(\mathbb{H}) - \inf_{(u,f)} \mathcal{E}(u,f), \tag{2.3}$$

where $\sigma(\mathbb{H})$ stands for the spectrum of the Pauli-Fierz Hamiltonian $\mathbb{H}$. The expansion up to second order in the coupling constant of this expression reveals that the ground state energy $\inf \sigma(\mathbb{H})$ can be divided into two terms : a 'coherent term', given by $\inf_{(u,f)} \mathcal{E}(u,f)$, and a second term due to the contribution from the excited states of the electronic Hamiltonian.

As in previously cited references, our argument to prove the existence of a ground state relies on usual strategies from the calculus of variations. The main novelty comes from the possible absence of infrared and ultraviolet cutoffs in the interaction. This produces singular terms with a critical behavior in the energy functional that we handle using, in particular, suitable estimates in Lorentz spaces. The use of weak versions of Hölder and Young's inequalities in Lorentz spaces seems to be new in the present context. It constitutes one of the main technical tools in our argument.

The ultraviolet convergence of the ground state and the asymptotic expansion of (2.3) at small coupling also seem to be new. In order to establish them (as well as the uniqueness of the ground state), we project a non-linear eigenvalue equation associated to the minimization problem onto the vector space associated to the ground state of the electronic Hamiltonian and its orthogonal complement.

In a companion paper [27], we will study the Pauli-Fierz Hamiltonian of a non-relativistic particle with spin $\frac{1}{2}$ coupled to the quantized radiation field in the standard model of non-relativistic QED. In this case, the quasi-classical energy coincides with the energy of a coupled Maxwell–Pauli system. For the standard model of non-relativistic QED with a spinless electron in the translation invariant case, we mention the works [14, 87] about the Lieb-Loss model, related to ours, where the infimum of the energy functional

$$\mathfrak{E}(u,\Psi) := \big\langle (u\otimes\Psi), \mathbb{H}(u\otimes\Psi)\big\rangle, \quad \|u\|_{\mathcal{H}_{\mathrm{el}}} = 1, \quad \|\Psi\|_{\mathcal{H}_{\mathrm{f}}} = 1,$$

is considered. Here the expectation is taken over general product states, i.e. the field is not supposed to be in a coherent state as in our case. It is then proven that $\inf \mathfrak{E}(u,\Psi)$ diverges as $\Lambda^{12/7}$ in the ultraviolet limit, where Λ stands for the ultraviolet parameter. On the contrary, our results show that, if the field is restricted to coherent states, then the ground state energy converges in the ultraviolet limit $\Lambda \to \infty$, a ground state exists for all $0 \le \Lambda \le \infty$ and an asymptotic expansion of the ground state energy at second order in the coupling constant can be computed uniformly in Λ. Our results hold both for linearly coupling models (this is the content of the present paper) and for the standard model of non-relativistic QED (up to a trivial renormalization in Λ, see the companion paper [27]).

In the remainder of this section, we begin by introducing in Section 2.1.1 the abstract class of Hamiltonians we consider and our main hypotheses. Next, in Section 2.1.2, we state our main results.

Notations. We recall that for $1 \le p < \infty$, the Lorentz spaces (or weak L^p spaces) $L^{p,\infty}(\mathbb{R}^3)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^3 \to \mathbb{C}$ such that

$$\|f\|_{L^{p,\infty}} := \sup_{t>0} \lambda\big(\{|f| > t\}\big)^{\frac{1}{p}}\, t \tag{2.4}$$

is finite, where λ denotes Lebesgue's measure.

The usual Fourier transform acting on tempered distribution is denoted by $\mathcal{F}$ with inverse $(2\pi)^{-3}\bar{\mathcal{F}}$. (We use the normalization $\mathcal{F}(f)(x) = \int_{\mathbb{R}^3} e^{-ix\cdot\xi} f(\xi)\,\mathrm{d}\xi$ for f in $L^1(\mathbb{R}^3)$, and hence $\bar{\mathcal{F}}(f)(x) = \int_{\mathbb{R}^3} e^{ix\cdot\xi} f(\xi)\,\mathrm{d}\xi$. This normalization is not the standard one but it is convenient in our context.) Throughout the paper, we use the following convention. Let f, g be functions associated to tempered distributions. Assume that $\mathcal{F}(g)$ identifies with a function such that $f\mathcal{F}(g)$ can be associated to a tempered distribution. We write

$$\mathcal{F}(f) * g := (2\pi)^{-3}\mathcal{F}(f\bar{\mathcal{F}}(g)). \tag{2.5}$$

This convention extends the well-known equality which holds e.g. if f and g are in L^1 or f is in L^2 and g in L^1.

In several places, we will use localization functions in $C_0^\infty(\mathbb{R}^3)$ denoted by η and such that $0 \le \eta \le 1$, $\eta(x) = 1$ if $|x| \le 1$ and $\eta(x) = 0$ if $|x| \ge 2$. We define the non-negative function $\tilde{\eta}$ by

$$\eta^2 + \tilde{\eta}^2 = 1,$$

and for all $R > 0$, we set

$$\eta_R(x) := \eta(x/R) \quad \text{and} \quad \tilde{\eta}_R(x) := \tilde{\eta}(x/R). \tag{2.6}$$

If $\mathcal{H}_1$, $\mathcal{H}_2$ are two Hilbert spaces, $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ stands for the set of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. Given a linear operator A on a Hilbert space $\mathcal{H}$, we denote by $\mathcal{D}(A)$ its domain and $\mathcal{Q}(A)$ its form domain.

2.1.1 Model and assumptions

Before defining the abstract class of linearly coupled Pauli-Fierz Hamiltonians we consider, we introduce our conditions on the electronic Hamiltonian H_V.

The electronic Hamiltonian

We suppose that the non-relativistic particle is spinless and bound by an external potential. The Hilbert space and Hamiltonian for the particle are given by

$$\mathcal{H}_{\text{el}} := L^2(\mathbb{R}^3), \quad H_V = -\Delta + V(x), \tag{2.7}$$

where $V : \mathbb{R}^3 \to \mathbb{R}$ is a real potential. We display the dependence on V since one of our main hypotheses (see Hypothesis 2.1.1) assumes the existence of a decomposition $V = V_1 + V_2$ such that $V_1 \geq 0$, V_2 vanishes at ∞ and there is a gap between the ground state energies of H_V and H_{V_1}.

The main examples we have in mind are confining potentials, $V(x) \to \infty$ as $|x| \to \infty$, and Coulomb-type potentials, $V(x) = -c|x|^{-1}$ with $c > 0$. We introduce general hypotheses on V that are fulfilled by a large class of potentials, including the two preceding examples. As we will see below, some of our main results have interesting consequences in special cases, especially when V is confining.

We set

$$\mu_V := \inf \sigma(H_V),$$

and likewise if V is replaced by another potential. For $U : \mathbb{R}^3 \to \mathbb{R}$, we denote by

$$U_+ := \max(U, 0), \quad U_- := \max(-U, 0),$$

the positive and negative parts of U, respectively, so that $U = U_+ - U_-$.

We make the following hypothesis.

Hypothesis 2.1.1 (Conditions on V)**.** *There exist $0 \leq a < 1$ and b in $\mathbb{R}$ such that the negative part of V satisfies*

$$V_- \leq -a\Delta + b\,,$$

in the sense of quadratic forms on $H^1(\mathbb{R}^3)$. Moreover, V decomposes as $V = V_1 + V_2$ with

(i) $V_1 \in L^1_{\text{loc}}(\mathbb{R}^3; \mathbb{R}^+)$,

(ii) $V_2 \in L^{3/2}_{\text{loc}}(\mathbb{R}^3; \mathbb{R})$ *and* $\lim_{|x|\to\infty} V_2(x) = 0$,

(iii) $\mu_V < \mu_{V_1}$.

We have the following accompanying remarks (we refer to Section 2.2.1 for justifications). Since $V_+ \geq 0$, $H_{V_+} = -\Delta + V_+$ identifies with a non-negative self-adjoint operator on $L^2(\mathbb{R}^3)$ with form domain

$$\mathcal{Q}(H_{V_+}) = \mathcal{Q}(-\Delta) \cap \mathcal{Q}(V_+) = \Big\{ u \in H^1(\mathbb{R}^3) \mid \int_{\mathbb{R}^3} V_+(x)|u(x)|^2 \,\mathrm{d}x < +\infty \Big\}.$$

Moreover, it follows from our hypotheses that H_V identifies with a semi-bounded self-adjoint operator with form domain

$$\mathcal{Q}_V := \mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1}),$$

and that $\mathcal{Q}_V$ is a Hilbert space for the norm

$$\|u\|^2_{\mathcal{Q}_V} := \|u\|^2_{H^1} + \left\|(V_+)^{\frac{1}{2}} u\right\|^2_{L^2}. \tag{2.8}$$

In particular, μ_V and μ_{V_1} are well-defined. We will most of the time consider a state u in

$$\mathcal{U} := \{u \in \mathcal{Q}_V \mid \|u\|_{L^2} = 1\}. \tag{2.9}$$

In order to obtain uniqueness of minimizers, we require that the Schrödinger Hamiltonian H_V has a unique ground state. By Perron-Froebenius arguments, it is well-known that, under suitable conditions on V, if μ_V is an eigenvalue of H_V then it is simple and there exists a corresponding strictly positive eigenstate (see e.g. [107, Theorems XIII.46 and XIII.48]). We make the following related hypothesis.

Hypothesis 2.1.2 (Ground state of H_V)**.** *The ground state energy μ_V of the particle Hamiltonian H_V is a simple isolated eigenvalue associated to a unique positive ground state u_V in $L^2(\mathbb{R}^3;\mathbb{R}_+)$, such that $\|u_V\|_{L^2} = 1$.*

The orthogonal projection onto the vector space spanned by u_V is denoted by Π_V. We also set $\Pi_V^\perp := \mathbf{I} - \Pi_V$.

Linearly coupled Pauli-Fierz Hamiltonians

We suppose that the radiation field is a scalar, bosonic field with Hilbert space given by the symmetric Fock space

$$\mathcal{H}_{\mathrm{f}} := \mathfrak{F}_s(L^2(\mathbb{R}^3)) = \bigoplus_{n=0}^{\infty} \bigvee^n L^2(\mathbb{R}^3). \tag{2.10}$$

In the momentum representation, the free field Hamiltonian is the second quantization of the multiplication operator by $\omega(k)$,

$$\mathbb{H}_{\mathrm{f}} := \mathrm{d}\Gamma(\omega(k)), \tag{2.11}$$

where $\omega : \mathbb{R}^3 \to \mathbb{R}_+$ is a non-negative measurable function. See Appendix 2.4 for the precise definition of second quantized operators. The coupling between the electron and the field is linear in the creation and annihilation operators, given by

$$\mathbb{H}_{\mathrm{int}} := g\sqrt{2}\Phi(h_x), \tag{2.12}$$

where g in $\mathbb{R}$ is a coupling constant, $\Phi(h)$, for h in $L^2(\mathbb{R}^3)$, denotes the field operator (see Appendix 2.4 for the definitions of the field, creation and annihilation operators), and

$$h_x(k) := v(k)e^{-ikx}, \tag{2.13}$$

for all x in $\mathbb{R}^3$, where $v : \mathbb{R}^3 \to \mathbb{R}$ is a coupling function.

This framework covers several models of interest :

- The Nelson model [102], with the relativistic dispersion relation $\omega(k) := \sqrt{k^2+m^2}$ corresponding to a field of mass $m \geq 0$, and the coupling function $v(k) = \omega(k)^{-\frac{1}{2}}\chi(k)$ with v in $L^2(\mathbb{R}^3)$. Here, in particular, χ incorporates an ultraviolet cutoff. Moreover, without infrared regularization, $\chi = 1$ near $k = 0$, while if an infrared regularization is imposed, one assumes that $\chi(0) = 0$.
- The Fröhlich polaron model [48], with $\omega(k) = 1$ and $v(k) = |k|^{-1}$.
- The phonon Hamiltonian of solid state physic (see e.g. [80]), with a bounded dispersion relation $\omega : \mathbb{R}^3 \to \mathbb{R}$ such that $\omega(k) \sim c|k|$ near $k = 0$ in the case of acoustic phonons, or $0 < c_1 \leq \omega(k) \leq c_2$ in the case of optical phonons. Here c, c_1, c_2 are positive constants. Moreover, $v(k) = |k|^{\frac{1}{2}}\chi(k)$, with v in $L^2(\mathbb{R}^3)$ and $\chi = 1$ near $k = 0$.

Assuming that V satisfies Hypothesis 2.1.1 and that

$$\int_{\mathbb{R}^3} \frac{v^2}{\omega} < \infty, \tag{2.14}$$

it is not difficult to verify that, for all values of the coupling constant g, the total Hamiltonian

$$\mathbb{H} = H_V \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} + g\sqrt{2}\Phi(h_x), \tag{2.15}$$

is a semi-bounded self-adjoint operator with form domain

$$\mathcal{Q}(\mathbb{H}) = \mathcal{Q}(\mathbb{H}_{\mathrm{free}}), \quad \mathbb{H}_{\mathrm{free}} := H_V \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}}. \tag{2.16}$$

See Appendix 2.4 for details. The domains of $\mathbb{H}$ and $\mathbb{H}_{\mathrm{free}}$ in fact also coincide in this case. Note that the condition (2.14) is satisfied in the case of the Nelson model and the phonon model, but not for the polaron model. In the latter case, one can still prove that $\mathbb{H}$ identifies with a self-adjoint operator with form domain $\mathcal{Q}(\mathbb{H}) = \mathcal{Q}(\mathbb{H}_{\mathrm{free}})$, see [65].

Klein–Gordon–Schrödinger energy

For f in $L^2(\mathbb{R}^3)$, the coherent state of parameter f is denoted by

$$\Psi_f := e^{i\Phi(\frac{\sqrt{2}}{i}f)}\Omega \in \mathcal{H}_{\mathrm{f}}, \tag{2.17}$$

where Ω stands for the Fock vacuum. Let u in $\mathcal{U}$ and let f in $L^2(\mathbb{R}^3)$ be such that $\omega^{1/2}f$ belongs to $L^2(\mathbb{R}^3)$. A simple computation shows that the energy of the product state $u \otimes \Psi_f$ is given by

$$\big\langle (u \otimes \Psi_f), \mathbb{H}(u \otimes \Psi_f)\big\rangle_{\mathcal{H}} = \mathcal{E}(u, f) \tag{2.18}$$

(see Appendix 2.4) where

$$\mathcal{E}(u,f) := \int_{\mathbb{R}^3} |\vec{\nabla} u(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} V(x)|u(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} \omega(k)|f(k)|^2 \,\mathrm{d}k$$
$$+ 2g\,\mathfrak{Re} \int_{\mathbb{R}^6} e^{ikx} v(k) f(k) |u(x)|^2 \,\mathrm{d}x\,\mathrm{d}k\,. \tag{2.19}$$

Hence we obtain the energy of a coupled Klein–Gordon–Schrödinger system, the coupling being given by the last term in (2.19).

We aim at proving the existence and uniqueness of a minimizer for the energy functional $\mathcal{E}$, under suitable assumptions on ω and v. The natural energy space for $\mathcal{E}(u, f)$ is the space $\mathcal{U} \times \mathcal{Z}_\omega$ where

$$\mathcal{Z}_\omega := \left\{ f : \mathbb{R}^3 \to \mathbb{C} \text{ measurable} \mid \omega^{1/2} f \in L^2(\mathbb{R}^3, \mathrm{d}k) \right\}.$$

We make the following hypothesis on v which, combined with Hypothesis 2.1.1, ensures that $\mathcal{E}$ is well-defined on $\mathcal{U} \times \mathcal{Z}_\omega$ (see Proposition 2.3.1 and Lemma 2.5.1 below). Recall also that v is real-valued and ω is supposed to be a non-negative measurable function.

Hypothesis 2.1.3 (Condition on v)**.** *The map $W := g^2\omega^{-1}v^2$ decomposes as $W = W_1 + W_2$ with*

(i) $W_1 \in L^1(\mathbb{R}^3)$,

(ii) $W_2 \in L^{3,\infty}(\mathbb{R}^3)$.

It should be noted that this hypothesis covers all the examples previously mentioned (the Nelson, polaron and phonons Hamiltonians). Indeed, Hypothesis 2.1.3 is satisfied if one assumes that $\omega^{-1}v^2$ belongs to $L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and that

$$|\omega^{-1}(k)v^2(k)| \le C_1|k|^{-3+\varepsilon}\mathbb{1}_{|k|\le 1} + C_2|k|^{-1}\mathbb{1}_{|k|\ge 1}, \quad \varepsilon > 0,$$

for some positive constants C_1, C_2. This follows from the facts that $|k|^{-3+\varepsilon}\mathbb{1}_{|k|\le 1}$ is in $L^1(\mathbb{R}^3)$ while $|k|^{-1}\mathbb{1}_{|k|\ge 1}$ is in $L^{3,\infty}(\mathbb{R}^3)$. We emphasize in particular that, for the Nelson model, no infrared regularization is required and the ultraviolet cutoff can be removed, taking $v(k) = |k|^{-1/2}$ and $\omega(k) = \sqrt{k^2 + m^2}$, $m \ge 0$.

2.1.2 Main results

We are now ready to state our main results. For clarity we decompose the presentation into a few subsections.

Infrared problem for Klein–Gordon–Schrödinger

We begin with a relatively simple property, which we refer to as the 'infrared problem', keeping the usual terminology from QED. Since, in general, $\mathcal{Z}_\omega$ is not contained in $L^2(\mathbb{R}^3)$, the field component f_{gs} of a minimizer $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ of the Klein–Gordon–Schrödinger energy functional over $\mathcal{U} \times \mathcal{Z}_\omega$ may not belong to the original one-particle Hilbert space $\mathfrak{h} = L^2(\mathbb{R}^3)$. This formally corresponds to the fact that the coherent state $\Psi_{f_{\mathrm{gs}}}$ does not belong to Fock space. On the other hand, if f_{gs} belongs to $L^2(\mathbb{R}^3)$, then, using in addition that u_{gs} belongs to $\mathcal{Q}_V$ and f_{gs} to $\mathcal{Z}_\omega$, one easily verifies that $u_{\mathrm{gs}} \otimes \Psi_{f_{\mathrm{gs}}}$ belongs to $\mathcal{Q}(\mathbb{H})$, so that the Pauli-Fierz energy (2.18) in the state $u_{\mathrm{gs}} \otimes \Psi_{f_{\mathrm{gs}}}$ is well-defined.

The next proposition provides both a necessary and a sufficient condition ensuring that f_{gs} belongs to $L^2(\mathbb{R}^3)$.

Proposition 2.1.1. *Suppose that V satisfies Hypothesis 2.1.1 and W satisfies Hypothesis 2.1.3. If $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ is a minimizer of the Klein–Gordon–Schrödinger energy functional over $\mathcal{U} \times \mathcal{Z}_\omega$, then*

$$\frac{v}{\omega}\mathbb{1}_{|k|\leq 1} + \frac{v}{|k|\omega}\mathbb{1}_{|k|\geq 1} \in L^2(\mathbb{R}^3) \implies f_{\mathrm{gs}} \in L^2(\mathbb{R}^3) \implies \frac{v}{\omega}\mathbb{1}_{|k|\leq 1} \in L^2(\mathbb{R}^3).$$

Considering the massless Nelson model where $\omega(k) = |k|$ and $v(k) = |k|^{-1/2}\chi(k)$, the previous conditions reduce to

$$k \mapsto |k|^{-5/2}\chi(k)\mathbb{1}_{|k|\geq 1} \in L^2(\mathbb{R}^3) \quad \text{and} \quad k \mapsto |k|^{-3/2}\chi(k)\mathbb{1}_{|k|\leq 1} \in L^2(\mathbb{R}^3).$$

Thus, in order to have that f_{gs} belongs to $L^2(\mathbb{R}^3)$, it is necessary to impose an infrared regularization, but no ultraviolet regularization is needed. Note that the presence of an infrared regularization is also necessary to have the existence of a ground state for the massless Nelson Hamiltonian [41, 54, 95], while it is well-known that the Nelson Hamiltonian is renormalizable in the ultraviolet limit [102].

For the Fröhlich polaron model, we have $\omega = 1$, hence $\mathcal{Z}_\omega = L^2(\mathbb{R}^3)$ and the previous proposition is trivial.

Existence of a ground state

One of our main results is the following theorem which provides the existence of a ground state for the Klein–Gordon–Schrödinger energy functional under our general assumptions on V and W.

Theorem 2.1.2 (Existence of a ground state)**.** *Suppose that V satisfies Hypothesis 2.1.1 and W satisfies Hypothesis 2.1.3. There exists $C_V > 0$ such that, if the decompositions $V = V_1 + V_2$ and $W = W_1 + W_2$ as in Hypotheses 2.1.1 and 2.1.3, respectively, can be chosen such that*

$$\|W_1\|_{L^1} + C_V\|W_2\|_{L^{3,\infty}} \leq \delta(\mu_{V_1} - \mu_V) \tag{2.20}$$

and

$$C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a), \tag{2.21}$$

for some universal constants $C, \delta > 0$ and where a is given by Hypothesis 2.1.1, then the Klein–Gordon–Schrödinger energy functional (2.19) has a minimizer over $\mathcal{U} \times \mathcal{Z}_\omega$.

We have the following accompanying remarks concerning the smallness conditions (2.20) and (2.21).

Remark 2.1.3. *The smallness condition (2.21) only concerns the term W_2 in $L^{3,\infty}$ of W, not the term W_1 in L^1. Moreover, in the case of a confining potential, $V(x) \to \infty$ as $|x| \to \infty$, the condition (2.20) is automatically satisfied provided one suitably chooses the potential V_1, see Lemma 2.2.2. This implies that if V is confining and $W_2 = 0$, then a minimizer exists for any g in $\mathbb{R}$. In fact, for the special case of a confining potential, one* *can prove the existence of a minimizer by simpler arguments than those we use in the proof of Theorem 2.1.2, since in this case the relative compactness of minimizing sequences can easily be deduced from the confining assumption.*

Remark 2.1.4. *Our assumptions cover the critical case $\bar{\mathcal{F}}(W)(x) = g^2|x|^{-2}$ of the Hartree equation (2.22) (taking $W(k) = cg^2|k|^{-1}$ in $L^{3,\infty}(\mathbb{R}^3)$), which has been studied e.g. in [39, 67]. In particular, with $\bar{\mathcal{F}}(W)(x) = g^2|x|^{-2}$, it has been proven in [39, 67] that the Hartree energy has no minimizer for g larger than some critical value g^*. Hence the smallness condition (2.21) in Theorem 2.1.2 cannot be removed.*

The proof of Theorem 2.1.2 follows from observing that (u, f) is a minimizer for the Klein–Gordon–Schrödinger energy functional (2.19) if and only if it is of the form (u, f_u) where the field parameter satisfies $f_u = -g\omega^{-1}v\mathcal{F}(|u|^2)$ and where u minimizes the *Hartree energy*

$$J(u) = \langle u, H_V u\rangle_{L^2_x} - \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W) * |u|^2\big)(x)|u(x)|^2 \,\mathrm{d}x, \quad u \in \mathcal{U}. \tag{2.22}$$

Our strategy then rests on usual arguments from the calculus of variations [92, 93]. As mentioned in the introduction, the existence of minimizers for the Hartree (or Choquard-Pekar) energy has been studied by many authors in different contexts (see in particular [4, 7, 39, 49, 60, 67, 85, 91–93], see also [98] for a detailed survey of results). We are not aware, however, of a result giving the existence of a minimizer under our general conditions on V and W. The main difficulties come from the fact that we consider external potentials with possibly both a confining and a negative part, the latter vanishing at infinity, and, more importantly, that our assumptions on the convolution term in the Hartree energy (2.22) concerns the Fourier transform of the usual pair potential, with possibly a critical behavior corresponding to the term W_2 in $L^{3,\infty}$. Such critical terms are due to the fact that we do not impose an ultraviolet cutoff into the interaction. To handle them, we have to rely on suitable estimates in Lorentz spaces whose use, to our knowledge, seems to be new in the context of minimizing the Hartree energy functional. For completeness, we provide a complete proof of the existence of a minimizer for (2.22) under our conditions in Appendix 2.5.

We mention that the minimization problem for $\mathcal{E}(u, f)$ has been studied in the recent paper [4], in the particular case of the massive Nelson model with V confining, the dispersion relation $\omega(k) = \sqrt{k^2 + m^2}$ and $v(k) = \omega(k)^{-1/2}\chi(k)$ with χ a smooth compactly supported function. Our results cover this particular case.

Uniqueness of the ground state and expansion of the ground state energy at small coupling

Our next concern is the question of the uniqueness of the ground state for the Klein–Gordon–Schrödinger energy functional. To establish it, we need to strengthen our assumptions, assuming that the electronic Hamiltonian H_V has a unique ground state as stated in Hypothesis 2.1.2 and that the coupling is sufficiently small. Of course, uniqueness of a minimizer for $\mathcal{E}(u,f)$ only holds up to a phase, since $\mathcal{E}(u,f) = \mathcal{E}(e^{i\theta}u,f)$ for any θ in $\mathbb{R}$.

Theorem 2.1.5 (Uniqueness of the ground state)**.** *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V > 0$ such that, if*

$$\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V,$$

then the Klein–Gordon–Schrödinger energy functional (2.19) has a unique minimizer $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ in $\mathcal{U} \times \mathcal{Z}_\omega$ such that $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2} > 0$.

Under the conditions of the previous theorem, recalling that $W = g^2\omega^{-1}v^2$, we can now compute the asymptotic expansion of the ground state energy as the coupling constant g goes to 0.

Proposition 2.1.6 (Expansion of the ground state energy at small coupling)**.** *Under the conditions of Theorem 2.1.5, we have*

$$\min_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}(u,f) = \mu_V - g^2 \int_{\mathbb{R}^3} \left(\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_V|^2\right)(x)\, |u_V(x)|^2 \,\mathrm{d}x + \mathcal{O}(g^4), \tag{2.23}$$

as $g \to 0$.

To obtain uniqueness of the minimizer, as well as the expansion (2.23), we use that any minimizer of (2.22) is a non-linear Hartree eigenstate and project the non-linear eigenvalue equation to the vector space spanned by the electronic ground state u_V and its orthogonal complement.

As mentioned above, in the case where $W_2 = 0$, i.e. $W = g^2\omega^{-1}v^2$ is in $L^1(\mathbb{R}^3)$, the Hamiltonian $\mathbb{H}$ in (2.15) identifies with a semi-bounded self-adjoint operator. Hence we can compare the ground state energy of $\mathbb{H}$ with its quasi-classical counterpart :

Proposition 2.1.7 (Comparison with the ground state energy of $\mathbb{H}$)**.** *Under the conditions of Theorem 2.1.5, with W in $L^1(\mathbb{R}^3)$, we have*

$$\begin{aligned}\inf\sigma(\mathbb{H}) &- \mathcal{E}(u_{\mathrm{gs}}, f_{\mathrm{gs}}) \\ &= -g^2 \int_{\mathbb{R}^3} v(k)^2 \left\langle u_V, e^{ikx}\Pi_V^\perp \left(H_V - \mu_V + \omega(k)\right)^{-1} \Pi_V^\perp e^{-ikx} u_V\right\rangle_{L^2_x} \mathrm{d}k + o(g^2)\,,\end{aligned}$$

as $g \to 0$.

The term of order g^2 of the asymptotic expansion given by Proposition 2.1.7 can be rewritten as

$$\begin{aligned}\inf\sigma(\mathbb{H}) &- \mathcal{E}(u_{\mathrm{gs}}, f_{\mathrm{gs}}) \\ &= -g^2 \left\langle u_V \otimes \Omega, a(h_x)(\Pi_V^\perp \otimes \mathbf{I}_{\mathrm{f}})\left(\mathbb{H}_{\mathrm{free}} - \mu_V\right)^{-1}(\Pi_V^\perp \otimes \mathbf{I}_{\mathrm{f}})a^*(h_x) u_V \otimes \Omega\right\rangle + o(g^2)\,.\end{aligned}$$

It should be compared with the term of order g^2 in the asymptotic expansion (2.23) of the quasi-classical ground state energy $\mathcal{E}(u_{\mathrm{gs}}, f_{\mathrm{gs}})$, which is given by

$$\begin{aligned} &- g^2 \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_V|^2\big)(x)\, |u_V(x)|^2 \,\mathrm{d}x \\ &= -g^2 \left\langle u_V \otimes \Omega, a(h_x)(\Pi_V \otimes \Pi_\Omega^\perp)\big(\mathbb{H}_{\mathrm{free}} - \mu_V\big)^{-1}(\Pi_V \otimes \Pi_\Omega^\perp)a^*(h_x)u_V \otimes \Omega\right\rangle, \qquad (2.24) \end{aligned}$$

where Π_Ω is the projection onto the Fock vacuum and $\Pi_\Omega^\perp := \mathbf{I} - \Pi_\Omega$. Hence we see that, at second order in the coupling constant, the ground state energy of $\mathbb{H}$ can be divided into two terms : a 'coherent' term which is independent of the excited electronic eigenstates, and a 'non-coherent' term which sums the contributions from these excited states. In particular, defining $\delta_V := \mathrm{dist}(\mu_V, \sigma(H_V)\backslash\{\mu_V\})$ the distance between μ_V and the rest of the spectrum of H_V, we deduce from the previous expressions that if δ_V is large, then the non-coherent term is small and hence the coherent term becomes a good approximation to the ground state energy of $\mathbb{H}$.

Remark 2.1.8. *Under the conditions of Proposition 2.1.7 and assuming in addition that* $\frac{v}{\omega}\mathbb{1}_{|k|\le 1} + \frac{v}{|k|\omega}\mathbb{1}_{|k|\ge 1}$ *belongs to* $L^2(\mathbb{R}^3)$ *(so that* f_{gs} *is in* L^2 *by Proposition 2.1.1 and hence the coherent state in Fock space* $\Psi_{f_{\mathrm{gs}}}$ *(see (2.17)) is well-defined), one can also choose a ground state* Ψ_{gs} *of* $\mathbb{H}$ *such that*

$$\big\|\Psi_{\mathrm{gs}} - u_{\mathrm{gs}} \otimes \Psi_{f_{\mathrm{gs}}}\big\|_{\mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}}} = \mathcal{O}(g). \qquad (2.25)$$

Note that the existence of a ground state for $\mathbb{H}$ *under these conditions follows from [53]. The estimate (2.25) is then a direct consequence of our proofs of Theorem 2.1.5 and Propositions 2.1.6–2.1.7 together with [11], since [11] shows that*

$$\big\|\Psi_{\mathrm{gs}} - u_V \otimes \Omega\big\|_{\mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}}} = \mathcal{O}(g),$$

for a suitably constructed ground state Ψ_{gs}*, while our argument will show that*

$$\|u_{\mathrm{gs}} - u_V\|_{\mathcal{H}_{\mathrm{el}}} = \mathcal{O}(g^2), \quad \|f_{\mathrm{gs}}\|_{L^2} = \mathcal{O}(g),$$

see Section 2.3.4.

Ultraviolet limit

We suppose here that the coupling function is cut-off in the ultraviolet, i.e. that it is of the form $v_\Lambda = v\mathbb{1}_{|k|\le\Lambda}$ for some ultraviolet parameter $0 < \Lambda < \infty$. We are interested in the ultraviolet limit $\Lambda \to \infty$. We write

$$W_\Lambda := g^2\omega^{-1}v_\Lambda = W\mathbb{1}_{|k|\le\Lambda},$$

and note that if W satisfies Hypothesis 2.1.3, then for all $\Lambda > 0$, W_Λ is in L^1 (this follows from the weak Hölder inequality, see (2.37) below). The fact that W_Λ belongs to L^1 in turn ensures that the Pauli-Fierz Hamiltonian

$$\mathbb{H}_\Lambda := H_V \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} + g\Phi(h_{\Lambda,x}), \quad h_{\Lambda,x}(k) := v_\Lambda(k)e^{-ikx},$$

identifies to a self-adjoint operator (see Appendix 2.4).

Let $\mathcal{E}_\Lambda$ be the Klein–Gordon–Schrödinger energy functional with an ultraviolet cutoff, i.e. $\mathcal{E}_\Lambda$ is given by (2.19) with v_Λ instead of v. The next proposition establishes the convergence of the ground state energies in the ultraviolet limit. Note that the assumptions are rather weak. In particular they do not necessarily imply the existence of a ground state for $\mathcal{E}$ and $\mathcal{E}_\Lambda$.

Proposition 2.1.9 (Ultraviolet limit of the ground state energies)**.** *Suppose that V satisfies Hypothesis 2.1.1 and that W satisfies Hypothesis 2.1.3. Then*

$$\inf_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}_\Lambda(u,f) \underset{\Lambda\to\infty}{\longrightarrow} \inf_{(u,f)\in\mathcal{U}\times\mathcal{Z}_\omega} \mathcal{E}(u,f).$$

Under conditions ensuring that $\mathcal{E}_\Lambda$ and $\mathcal{E}$ have unique minimizers, we can also establish the convergence of the ground states of $\mathcal{E}_\Lambda$ to the ground state of $\mathcal{E}$, as $\Lambda\to\infty$.

Proposition 2.1.10 (Ultraviolet limit of the ground states)**.** *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V>0$ such that, if*

$$\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V,$$

then for all $\Lambda>0$, $\mathcal{E}_\Lambda$ and $\mathcal{E}$ have unique minimizers $(u_{\Lambda,\mathrm{gs}}, f_{\Lambda,\mathrm{gs}})$ and $(u_{\mathrm{gs}}, f_{\mathrm{gs}})$ in $\mathcal{U}\times\mathcal{Z}_\omega$, respectively, such that $\langle u_{\Lambda,\mathrm{gs}}, u_V\rangle_{L^2}>0$ and $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2}>0$. They satisfy

$$\big\|(u_{\Lambda,\mathrm{gs}}, f_{\Lambda,\mathrm{gs}}) - (u_{\mathrm{gs}}, f_{\mathrm{gs}})\big\|_{\mathcal{Q}_V\times\mathcal{Z}_\omega} \underset{\Lambda\to\infty}{\longrightarrow} 0.$$

The proofs of Propositions 2.1.9 and 2.1.10 are not straightforward. The main difficulty comes from the fact that, in general, W_Λ does *not* converge to W in $L^1+L^{3,\infty}$. To circumvent this difficulty, we use a convergence property in a weaker sense, based on a suitable application of Lebesgue's dominated convergence theorem.

2.1.3 Organisation of the paper

Our paper is essentially self-contained. It is organized as follows. Section 2.2 is a preliminary section containing several technical estimates that we subsequently use in Section 2.3 to establish our main results. In Appendix 2.4, we recall the definitions of standard objects related to second quantization as well as the self-adjointness of the Pauli-Fierz Hamiltonian $\mathbb{H}$. Appendix 2.5 contains a proof of the existence of a minimizer for the Hartree energy functional under our conditions.

Acknowledgements. The research of S.B. was partly done during a CNRS sabbatical semester.

2.2 Preliminaries

In this preliminary section, we gather several technical estimates that are useful for our concern. The first subsection mainly concerns the electronic Hamiltonian H_V. In a second subsection, we prove some functional estimates in Lorentz spaces that are used in Section 2.3 in a crucial way to control the interactions terms of the Klein–Gordon–Schrödinger energy functional.

2.2.1 Estimates on the electronic part

Recall that our assumptions on the external potential V of the electronic Hamiltonian $H_V = -\Delta + V$ have been introduced in Section 2.1.1. We begin with a few remarks showing that H_V is well-defined and that its form domain satisfies $\mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1})$, with V_1 as in Hypothesis 2.1.1.

First, V_- is form bounded with respect to $-\Delta$ with a relative bound less than 1, by Hypothesis 2.1.1. Thus V_- is also form bounded with respect to H_{V_+} with a relative bound less than 1, and hence the KLMN Theorem (see e.g. [107, Theorem X.17]) implies that H_V identifies with a semi-bounded self-adjoint operator with form domain $\mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+})$.

Next, Hypothesis 2.1.1(ii) implies that V_2 is relatively form bounded with respect to $-\Delta$ with relative bound 0. Indeed, for R large enough, we have $V_2 \mathbb{1}_{|x|\geq R} \in L^\infty(\mathbb{R}^3)$ since $V_2(x) \to 0$ as $|x| \to \infty$, while $V_2 \mathbb{1}_{|x|\leq R} \in L^{3/2}(B_R)$ with $B_R := \{x \in \mathbb{R}^3 \,|\, |x| \leq R\}$, since $V_2 \in L^{3/2}_{\text{loc}}(\mathbb{R}^3)$. Therefore $V_2 \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and hence we can apply [107, Theorem X.19] to deduce that V_2 is infinitesimally form-bounded with respect to $-\Delta$. In turn, since $V_+ - V_1 = V_2 + V_-$ is form bounded with respect to $-\Delta$, it is not difficult to verify that $\mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1})$.

Recall the notation $\mathcal{Q}_V = \mathcal{Q}(H_V)$. We begin with the following easy lemma.

Lemma 2.2.1. *Suppose that V satisfies Hypothesis 2.1.1. Then, for all u in $\mathcal{Q}_V$,*

$$\|u\|^2_{\dot{H}^1} \leq \frac{1}{1-a}\big(\langle u, H_V u\rangle + b\|u\|^2_{L^2}\big). \tag{2.26}$$

Proof. The positivity of V_+ and the bound on V_- from Hypothesis 2.1.1 yield, for u in $\mathcal{Q}_V$,

$$\langle u, H_V u\rangle \geq \|u\|^2_{\dot{H}^1} - \langle u, V_- u\rangle \geq \|u\|^2_{\dot{H}^1} - a\langle u, -\Delta u\rangle - b\|u\|^2_{L^2} = (1-a)\|u\|^2_{\dot{H}^1} - b\|u\|^2_{L^2},$$

which proves the result. □

The next lemma shows that, for confining potentials V, the gap $\mu_{V_1} - \mu_V$ can be made as large as we want, provided that the potential V_1 is suitably chosen.

Lemma 2.2.2. *Suppose that $V = V_+ - V_-$ is such that*

(i) $V_+ \in L^1_{\text{loc}}(\mathbb{R}^3)$,

(ii) $V_- \in L^{3/2}_{\text{loc}}(\mathbb{R}^3)$,

(iii) $V(x) \to \infty$ *as* $|x| \to \infty$.

Then, for all $C > 0$*, there exist a decomposition* $V = V_{1,C} + V_{2,C}$ *as in Hypothesis 2.1.1 such that, moreover,*

$$\mu_{V_{1,C}} - \mu_V \geq C.$$

Proof. Recall that the localizations functions η_R, $\tilde{\eta}_R$ have been defined in (2.6). Let $C > 0$. We set

$$V_{1,C} = V_+ + 2C\eta_R^2, \quad V_{2,C} = -V_- - 2C\eta_R^2.$$

Observe that $V_{1,C} + V_{2,C} = V_+ - V_- = V$. Moreover, since $V(x) \to \infty$ as $|x| \to \infty$, we have that $V_-(x) = 0$ for $|x|$ large enough. Hence, since in addition η_R^2 is smooth and compactly supported, one sees that the decomposition $V = V_{1,C} + V_{2,C}$ satisfies the conditions of Hypothesis 2.1.1 for any R.

Now we verify that $\mu_{V_{1,C}} - \mu_V > C$ for suitably chosen R. Using the IMS localization formula (see e.g. [36]), we write

$$\begin{aligned}\mu_{V_{1,C}} &= \inf_{u \in \mathcal{U}} \Big(\langle (\eta_R^2 + \tilde{\eta}_R^2) u, (-\Delta + V_+) u \rangle + 2C \|\eta_R u\|_{L^2}^2 \Big) \\ &= \inf_{u \in \mathcal{U}} \Big(\langle \eta_R u, (-\Delta + V_+) \eta_R u \rangle + \langle \tilde{\eta}_R u, (-\Delta + V_+) \tilde{\eta}_R u \rangle + o(R^0) + 2C \|\eta_R u\|_{L^2}^2 \Big),\end{aligned}$$

since $|\vec{\nabla}\eta_R|^2 + |\vec{\nabla}\tilde{\eta}_R|^2 = o(R^0)$, $R \to \infty$. Next, using that $-\Delta \geq 0$ and that $\mathrm{supp}(\tilde{\eta}_R) \subset B(0,R)^c$, we estimate

$$\mu_{V_{1,C}} \geq \inf_{u \in \mathcal{U}} \Big(\big(\mu_{V_+} + 2C\big) \|\eta_R u\|_{L^2}^2 + \Big(\inf_{x \in B(0,R)^c} V_+(x) \Big) \|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0) \Big).$$

Since $V_+(x) \to \infty$ as $|x| \to \infty$, there exists $R_0 > 0$ such that for $R \geq R_0$,

$$\inf_{x \in B(0,R)^c} V_+(x) \geq \mu_{V_+} + 2C.$$

Therefore, for $R \geq R_0$, we obtain

$$\mu_{V_{1,C}} \geq \inf_{u \in \mathcal{U}} \Big(\big(\mu_{V_+} + 2C\big) \big(\|\eta_R u\|_{L^2}^2 + \|\tilde{\eta}_R u\|_{L^2}^2 \big) + o(R^0) \Big) = \mu_{V_+} + 2C + o(R^0). \qquad (2.27)$$

On the other hand, since $V_- \geq 0$, we have that

$$\mu_{V_+} \geq \inf_{u \in \mathcal{U}} \langle u, (-\Delta + V_+ - V_-) u \rangle = \mu_V. \qquad (2.28)$$

Combining (2.27) and (2.28) gives

$$\mu_{V_{1,C}} \geq \mu_V + 2C + o(R^0).$$

Fixing R large enough, we deduce that $\mu_{V_{1,C}} - \mu_V > C$, which proves the lemma. □

To conclude this section, we give a lemma which is useful to prove the existence of minimizers for the energy functional studied in Section 2.3.

Lemma 2.2.3. *Suppose that V satisfies Hypothesis 2.1.1. Let $(u_j)_{j\in\mathbb{N}}$ be a bounded sequence in $H^1(\mathbb{R}^3)$ which converges weakly to u_∞ in $H^1(\mathbb{R}^3)$, and strongly in $L^2(\mathbb{R}^3)$. Then*

$$\langle u_\infty, (-\Delta + V)u_\infty\rangle \leq \liminf_{j\to\infty} \langle u_j, (-\Delta + V)u_j\rangle \,.$$

Proof. We consider each term of

$$\langle u, -\Delta u\rangle + \langle u, V_1 u\rangle + \langle u, V_2 u\rangle \tag{2.29}$$

separately.

The first one is handled using the lower semi-continuity of $\|\cdot\|_{L^2}$. Indeed, as $u_j \to u_\infty$ weakly in $H^1(\mathbb{R}^3)$, it follows that $\nabla u_j \to \nabla u_\infty$ weakly in $L^2(\mathbb{R}^3)$ and hence

$$\langle u_\infty, -\Delta u_\infty\rangle = \|\nabla u_\infty\|_{L^2}^2 \leq \liminf_{j\to\infty} \|\nabla u_j\|_{L^2}^2 = \liminf_{j\to\infty} \langle u_j, -\Delta u_j\rangle. \tag{2.30}$$

For the second term of (2.29), we use Fatou's Lemma, which gives, since $V_1 \geq 0$,

$$\langle u_\infty, V_1 u_\infty\rangle \leq \liminf_{j\to\infty} \langle u_j, V_1 u_j\rangle. \tag{2.31}$$

As for the third term in (2.29), we claim that

$$\langle u_\infty, V_2 u_\infty\rangle = \lim_{j\to\infty} \langle u_j, V_2 u_j\rangle, \tag{2.32}$$

for some suitable subsequence that we keep denoting by $(u_j)_{j\in\mathbb{N}}$. Indeed, let $\varepsilon > 0$. We have that $\|\mathbb{1}_{|x|>R_0} V_2\|_\infty \leq \varepsilon$ for R_0 large enough, since $V_2(x) \to 0$ as $|x| \to \infty$. Therefore, for all j in $\mathbb{N}$,

$$\langle u_j, \mathbb{1}_{|x|>R_0} V_2 u_j\rangle \leq \varepsilon, \quad \langle u_\infty, \mathbb{1}_{|x|>R_0} V_2 u_\infty\rangle \leq \varepsilon. \tag{2.33}$$

Next, we approximate $\mathbb{1}_{|x|\leq R_0} V_2$ by a more regular function. More precisely, since $\mathbb{1}_{|x|\leq R_0} V_2$ lies in $L^{3/2}(\mathbb{R}^3)$, one can find $V_{2,\varepsilon}$ in $C_0^\infty(\mathbb{R}^3)$ such that

$$\big\|\mathbb{1}_{|x|\leq R_0} V_2 - V_{2,\varepsilon}\big\|_{L^{3/2}} \leq \varepsilon.$$

Hölder's inequality together with Sobolev's embedding $H^1(\mathbb{R}^3) \subset L^6(\mathbb{R}^3)$ then yield

$$\begin{aligned}\big|\langle u_j, \mathbb{1}_{|x|\leq R_0} V_2 u_j\rangle - \langle u_j, \mathbb{1}_{|x|\leq R_0} V_{2,\varepsilon} u_j\rangle\big| &\leq \big\|\mathbb{1}_{|x|\leq R_0} V_2 - V_{2,\varepsilon}\big\|_{L^{3/2}} \|u_j\|_{L^6}^2 \\ &\lesssim \varepsilon \|u_j\|_{H^1}^2 \lesssim \varepsilon,\end{aligned} \tag{2.34}$$

since we assumed that $(u_j)_{j\in\mathbb{N}}$ is bounded in $H^1(\mathbb{R}^3)$. Likewise,

$$\big|\langle u_\infty, \mathbb{1}_{|x|\leq R_0} V_2 u_\infty\rangle - \langle u_\infty, \mathbb{1}_{|x|\leq R_0} V_{2,\varepsilon} u_\infty\rangle\big| \lesssim \varepsilon. \tag{2.35}$$

Now, since $\mathbb{1}_{|x|\leq R_0} u_j \to \mathbb{1}_{|x|\leq R_0} u_\infty$ strongly in $L^2(\mathbb{R}^3)$, and since $V_{2,\varepsilon}$ is bounded, we deduce that

$$\langle u_\infty, \mathbb{1}_{|x|\leq R_0} V_{2,\varepsilon} u_\infty\rangle = \lim_{j\to\infty} \langle u_j, \mathbb{1}_{|x|\leq R_0} V_{2,\varepsilon} u_j\rangle. \tag{2.36}$$

Combining (2.33), (2.34), (2.35) and (2.36), we obtain (2.32). □

2.2.2 Some functional inequalities in Lorentz spaces

In the proof of our main results, we will use in a crucial way some functional inequalities in Lorentz spaces that we present in this section. For $1 \le p < \infty$, the Lorentz spaces $L^{p,\infty} = L^{p,\infty}(\mathbb{R}^d)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that (2.4) holds.

More generally, for $1 \le p < \infty$ and $1 \le q \le \infty$, the Lorentz spaces $L^{p,q} = L^{p,q}(\mathbb{R}^d)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that the quasi-norm

$$\|f\|_{L^{p,q}} := p^{1/q} \|\lambda(\{|f| > t\})^{1/p}\, t\|_{L^q((0,\infty),\mathrm{d}t/t)}$$

is finite.

For $1 \le p < \infty$ and $1 \le q_1 \le q_2 \le \infty$, the continuous embedding $L^{p,q_1} \subseteq L^{p,q_2}$ holds. Moreover $L^{p,p}$ identifies with L^p. We will use the following generalizations of Hölder and Young's inequality in Lorentz spaces, see [23, 82, 103, 114] or [58, Exercise 1.4.19].

For $1 \le p_1, p_2 < \infty$, $1 \le q_1, q_2 \le \infty$, Hölder's inequality states that

$$\|f_1 f_2\|_{L^{p,q}} \lesssim \|f_1\|_{L^{p_1,q_1}} \|f_2\|_{L^{p_2,q_2}}, \qquad \frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}, \quad \frac{1}{q} = \frac{1}{q_1} + \frac{1}{q_2}, \tag{2.37}$$

whenever the right hand side is finite.

Young's inequality states that, for $1 < p, p_1, p_2 < \infty$, $1 \le q_1, q_2 \le \infty$,

$$\|f_1 * f_2\|_{L^{p,q}} \lesssim \|f_1\|_{L^{p_1,q_1}} \|f_2\|_{L^{p_2,q_2}}, \qquad 1 + \frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}, \quad \frac{1}{q} = \frac{1}{q_1} + \frac{1}{q_2}, \tag{2.38}$$

and for $1 < p < \infty$, $1 \le q \le \infty$,

$$\|f_1 * f_2\|_{L^\infty} \lesssim \|f_1\|_{L^{p,q}} \|f_2\|_{L^{p',q'}}, \qquad \frac{1}{p} + \frac{1}{p'} = 1, \quad \frac{1}{q} + \frac{1}{q'} = 1. \tag{2.39}$$

We have the following estimates that are used several times in Section 2.3. The first one is an obvious application of the usual Hölder and Young inequalities. The second and third ones are close to the Hardy-Littlewood-Sobolev inequality but cannot be directly deduced from it. Recall the convention (2.5) on the Fourier transform.

Lemma 2.2.4.

(i) Let $u_1, u_2 \in L^2$ and $W \in L^1$. Then,

$$\left\|\bar{\mathcal{F}}(W) * (u_1 u_2)\right\|_{L^\infty} \lesssim \|W\|_{L^1} \|u_1\|_{L^2} \|u_2\|_{L^2}. \tag{2.40}$$

(ii) Let $u_1, u_2 \in \dot{H}^1$ and $W \in L^{3,\infty}$. Then $W\mathcal{F}(u_1 u_2) \in L^1$ and

$$\left\|\bar{\mathcal{F}}(W) * (u_1 u_2)\right\|_{L^\infty} \lesssim \|W\|_{L^{3,\infty}} \|u_1\|_{\dot{H}^1} \|u_2\|_{\dot{H}^1}. \tag{2.41}$$

(iii) Let $u_1 \in L^2$, $u_2, u_3 \in \dot{H}^1$ and $W \in L^{3,\infty}$. Then $W\mathcal{F}(u_1 u_2) \in L^{3/2,\infty}$ and

$$\left\|\big(\bar{\mathcal{F}}(W) * (u_1 u_2)\big) u_3\right\|_{L^2} \lesssim \|W\|_{L^{3,\infty}} \|u_1\|_{L^2} \|u_2\|_{\dot{H}^1} \|u_3\|_{\dot{H}^1}. \tag{2.42}$$

Proof. To simplify formulas below, we write $w = \bar{\mathcal{F}}(W)$.

(i) directly follows from the Hölder and Young inequalities :

$$\big\|w * (u_1 u_2)\big\|_{L^\infty} \lesssim \|w\|_{L^\infty} \big\|u_1 u_2\big\|_{L^1} \lesssim \|w\|_{L^\infty} \|u_1\|_{L^2} \|u_2\|_{L^2},$$

which yields (2.40) using $\|w\|_{L^\infty} \lesssim \|W\|_{L^1}$.

To prove (ii), we use first the Hölder inequality in Lorentz spaces (2.37),

$$\big\|w * (u_1 u_2)\big\|_{L^\infty} \lesssim \big\|W\,\mathcal{F}(u_1 u_2)\big\|_{L^1} \lesssim \|W\|_{L^{3,\infty}} \big\|\mathcal{F}(u_1 u_2)\big\|_{L^{3/2,1}},$$

and then both the Young (2.38) and Hölder (2.37) inequalities in Lorentz spaces

$$\begin{aligned}\big\|\mathcal{F}(u_1 u_2)\big\|_{L^{3/2,1}} &\lesssim \big\|\mathcal{F}(u_1) * \mathcal{F}(u_2)\big\|_{L^{3/2,1}} \lesssim \big\|\mathcal{F}(u_1)\big\|_{L^{6/5,2}} \big\|\mathcal{F}(u_2)\big\|_{L^{6/5,2}} \\ &\lesssim \big\||k|^{-1}\big\|^2_{L^{3,\infty}} \big\||k|\mathcal{F}(u_1)\big\|_{L^{2,2}} \big\||k|\mathcal{F}(u_2)\big\|_{L^{2,2}} \lesssim \|u_1\|_{\dot{H}^1} \|u_2\|_{\dot{H}^1}.\end{aligned}$$

To prove (iii), we use first the Young inequality in Lorentz spaces (2.38),

$$\big\|(w * (u_1 u_2)) u_3\big\|_{L^2} \lesssim \big\|(W\mathcal{F}(u_1 u_2)) * \mathcal{F}(u_3)\big\|_{L^2} \lesssim \big\|W\mathcal{F}(u_1 u_2)\big\|_{L^{3/2,\infty}} \big\|\mathcal{F}(u_3)\big\|_{L^{6/5,2}}.$$

The term with u_3 is controlled with the Hölder inequality in Lorentz spaces (2.37),

$$\big\|\mathcal{F}(u_3)\big\|_{L^{6/5,2}} \lesssim \||k|^{-1}\|_{L^{3,\infty}} \big\||k|\mathcal{F}(u_3)\big\|_{L^{2,2}} \lesssim \|u_3\|_{\dot{H}^1}.$$

The term with u_1 and u_2 is estimated using the Hölder inequality in Lorentz spaces (2.37) first, followed by the Young inequality in Lorentz spaces (2.38),

$$\big\|W\mathcal{F}(u_1 u_2)\big\|_{L^{3/2,\infty}} \lesssim \|W\|_{L^{3,\infty}} \big\|\mathcal{F}(u_1) * \mathcal{F}(u_2)\big\|_{L^{3,\infty}} \lesssim \|W\|_{L^{3,\infty}} \big\|\mathcal{F}(u_1)\big\|_{L^{2,\infty}} \big\|\mathcal{F}(u_2)\big\|_{L^{6/5,\infty}}.$$

The term $\|\mathcal{F}(u_2)\|_{L^{6/5,\infty}} \lesssim \|\mathcal{F}(u_2)\|_{L^{6/5,2}}$ is estimated in the same way as $\|\mathcal{F}(u_3)\|_{L^{6/5,2}}$, while

$$\big\|\mathcal{F}(u_1)\big\|_{L^{2,\infty}} \lesssim \big\|\mathcal{F}(u_1)\big\|_{L^{2,2}} \lesssim \|u_1\|_{L^2}.$$

This proves the lemma. □

2.3 Proof of the main results

In this section, we prove the results stated in Section 2.1.2. We begin with reducing the problem of the minimization of the Klein–Gordon–Schrödinger energy functional to the problem of the minimization of a well-chosen Hartree functional in Section 2.3.1. We prove the existence and uniqueness of a minimizer in Sections 2.3.2 and 2.3.3, respectively. In Section 2.3.4, we derive the asymptotic expansion of the ground state energy at small coupling. Finally, in Section 2.3.5 we prove the convergence of the ground state and ground state energy in the ultraviolet limit.

Throughout this section, C_V stands for a positive constant depending on V which may vary from line to line.

2.3.1 The Hartree energy functional

Recall that the Klein–Gordon–Schrödinger energy functional $\mathcal{E}(u,f)$ has been defined in (2.19). The next proposition shows that the minimization problem for $\mathcal{E}$ reduces to the minimization problem for the Hartree energy.

Proposition 2.3.1. *Suppose that V satisfies Hypothesis 2.1.1 and W satisfies Hypothesis 2.1.3. We have*

$$\inf_{u\in\mathcal{U}, f\in\mathcal{Z}_\omega} \mathcal{E}(u,f) = \inf_{u\in\mathcal{U}} J(u), \tag{2.43}$$

where

$$\begin{aligned} J(u) &:= \langle u, H_V\, u\rangle - \big\| W^{\frac12}\mathcal{F}(|u|^2)\big\|_{L^2}^2 \\ &= \langle u, H_V\, u\rangle - \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}\,(W) * |u|^2\big)(x)\ |u(x)|^2\,\mathrm{d}x = \mathcal{E}(u,f_u)\,, \end{aligned} \tag{2.44}$$

and

$$f_u := -g\omega^{-1} v\mathcal{F}(|u|^2)\,. \tag{2.45}$$

Moreover $u \mapsto (u, f_u)$ is a bijection between the minimizers of J and those of $\mathcal{E}$.

Proof. The Klein–Gordon–Schrödinger energy functional can be written under the form

$$\begin{aligned} \mathcal{E}(u,f) &= \langle u, H_V u\rangle + \big\langle \omega^{\frac12} f, \omega^{\frac12} f\big\rangle + 2g\,\mathfrak{Re}\big\langle \omega^{-\frac12} v\mathcal{F}(|u|^2), \omega^{\frac12} f\big\rangle \\ &= \langle u, H_V u\rangle + \big\|\omega^{\frac12} f + g\omega^{-\frac12} v\mathcal{F}(|u|^2)\big\|_{L^2}^2 - g^2\big\|\omega^{-\frac12} v\mathcal{F}(|u|^2)\big\|_{L^2}^2. \end{aligned} \tag{2.46}$$

Note that $\omega^{1/2} f$ belongs to L^2 since f is in $\mathcal{Z}_\omega$. Moreover, $\omega^{-\frac12} v\mathcal{F}(|u|^2)$ belongs to L^2 since

$$\begin{aligned} g^2\big\|\omega^{-\frac12} v\mathcal{F}(|u|^2)\big\|_{L^2}^2 &= \big\| W \big|\mathcal{F}(|u|^2)\big|^2\big\|_{L^1} \\ &\le \|W_1\|_{L^1} \|\mathcal{F}(|u|^2)\|_{L^\infty}^2 + \|W_2 \mathcal{F}(|u|^2)\|_{L^1} \|\mathcal{F}(|u|^2)\|_{L^\infty} \\ &\lesssim \|W_1\|_{L^1} \|u\|_{L^2}^4 + \|W_2\|_{L^{3,\infty}} \|u\|_{\dot H^1}^2 \|u\|_{L^2}^2 < \infty, \end{aligned}$$

where we used Lemma 2.2.4 in the second inequality. Eq. (2.46) then implies that

$$\mathcal{E}(u,f_u) = \langle u, H_V u\rangle - g^2\big\|\omega^{-\frac12} v\mathcal{F}(|u|^2)\big\|_{L^2}^2 = \min_{f\in\mathcal{Z}_\omega} \mathcal{E}(u,f)\,,$$

and f_u is the unique minimizer of $\mathcal{E}(u,f)$ at fixed u. By our convention (2.5) on the Fourier transform, the energy $\mathcal{E}(u,f_u)$ can be rewritten as the Hartree energy (2.44), which yields the result. ☐

We now establish Proposition 2.1.1 which gives necessary conditions and sufficient conditions so that $f_{\rm gs}$ belongs to $L^2(\mathbb{R}^3)$, where $(u_{\rm gs}, f_{\rm gs})$ a minimizer of the Klein–Gordon–Schrödinger energy functional $\mathcal{E}(u,f)$.

Proof of Proposition 2.1.1. By Proposition 2.3.1, any minimizer $(u_{\rm gs}, f_{\rm gs})$ of the Klein–Gordon–Schrödinger energy functional over $\mathcal{U} \times \mathcal{Z}_\omega$ satisfies the relation (2.45) :

$$\forall k \in \mathbb{R}^3, \quad f_{\rm gs}(k) = -g\omega^{-1}(k)v(k)\mathcal{F}(|u_{\rm gs}|^2)(k). \tag{2.47}$$

Since $u_{\rm gs}$ is in $H^1(\mathbb{R}^3)$, we have, for all k in $\mathbb{R}^3$,

$$\left|\mathcal{F}(|u_{\rm gs}|^2)(k)\right| \lesssim \min(1, |k|^{-1}).$$

Moreover, since $\mathcal{F}(|u_{\rm gs}|^2)$ is continuous at $k = 0$ and $\mathcal{F}(|u_{\rm gs}|^2)(0) = 1$, we have

$$\frac{1}{2} \le \left|\mathcal{F}(|u_{\rm gs}|^2)(k)\right| \le \frac{3}{2},$$

in a neighborhood of $k = 0$. Hence we see that sufficient conditions ensuring that $f_{\rm gs}$ belongs to $L^2(\mathbb{R}^3)$ are

$$k \mapsto \frac{v(k)}{|k|\omega(k)}\mathbb{1}_{|k|\ge 1} \in L^2(\mathbb{R}^3) \quad \text{and} \quad k \mapsto \frac{v(k)}{\omega(k)}\mathbb{1}_{|k|\le 1} \in L^2(\mathbb{R}^3),$$

while a necessary condition is

$$k \mapsto \frac{v(k)}{\omega(k)}\mathbb{1}_{|k|\le 1} \in L^2(\mathbb{R}^3).$$

This establishes Proposition 2.1.1. □

In the remainder of this section, we study the Hartree energy functional (2.44). By Proposition 2.3.1, the results that we prove for the Hartree energy directly imply the corresponding results for the Klein–Gordon–Schrödinger energy.

2.3.2 Existence of a minimizer

The next proposition gives the existence of a minimizer for the Hartree energy (2.44). It implies Theorem 2.1.2 from the introduction.

Proposition 2.3.2. *Suppose that V satisfies Hypothesis 2.1.1 and W satisfies Hypothesis 2.1.3. There exists $C_V > 0$ such that, if the decompositions of V and W of the form $V = V_1 + V_2$, $W = W_1 + W_2$ in Hypotheses 2.1.1 and 2.1.3, respectively, can be chosen such that*

$$\|W_1\|_{L^1} + C_V\|W_2\|_{L^{3,\infty}} \le \delta(\mu_{V_1} - \mu_V) \tag{2.48}$$

and

$$C\|W_2\|_{L^{3,\infty}} \le \frac{1}{2}(1-a), \tag{2.49}$$

then the Hartree energy functional (2.44) has a minimizer. Here C and δ are universal constants and a is given by Hypothesis 2.1.1.

As mentioned in the introduction, the existence of a minimizer for the Hartree energy has been proven under various conditions in different contexts, but we are not aware of a reference giving the result under our assumptions. We detail the proof of Proposition 2.3.2 in Appendix 2.5.

Remark 2.3.3. *Writing the Hartree energy in its usual form*

$$J(u) = \langle u, H_V\, u\rangle - \int_{\mathbb{R}^3} (w * |u|^2)(x)\; |u(x)|^2 \,\mathrm{d}x, \tag{2.50}$$

we have in our context $w = \bar{\mathcal{F}}(W)$ (in the sense of distributions) and it is thus natural to make an assumption on the Fourier transform of the convolution potential w. In other contexts, however, it might be more natural to make hypotheses on w rather than on its Fourier transform. It is straightforward to verify that our proof adapts to the conditions

$$\begin{aligned} &w = w_1 + w_2 \in L^\infty(\mathbb{R}^3) + L^{3/2,\infty}(\mathbb{R}^3), \\ &\|w_1\|_{L^\infty} + C_V \|w_2\|_{L^{3/2,\infty}} \le \delta(\mu_{V_1} - \mu_V), \quad C\|w_2\|_{L^{3/2,\infty}} \le \frac{1}{2}(1-a). \end{aligned}$$

It suffices to use, instead of (2.40)–(2.41), the inequalities

$$\begin{aligned} \left\|(w * |u_1|^2)|u_2|^2\right\|_{L^1} &\lesssim \|w\|_{L^\infty} \|u_1\|_{L^2}^2 \|u_2\|_{L^2}^2\,, \\ \left\|(w * |u_1|^2)|u_2|^2\right\|_{L^1} &\lesssim \|w\|_{L^{3/2,\infty}} \|u_1\|_{\dot{H}^1}^2 \|u_2\|_{L^2}^2\,, \end{aligned}$$

that can be proven using the weak Hölder and Young inequalities (2.37)–(2.39).

Remark 2.3.4. *As in Remark 2.1.3, in the case of a confining external potential V, one can always find a decomposition $V = V_1 + V_2$ such that (2.48) holds, by Lemma 2.2.2. Hence a minimizer exists in this case without any restriction on the size of $\|W_1\|_{L^1}$.*

2.3.3 Uniqueness of the minimizer

Now that we have the existence of a minimizer for the Hartree energy functional J, we prove the uniqueness of the minimizer. The next proposition implies Theorem 2.1.5 from the introduction.

Proposition 2.3.5. *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V > 0$ such that, if*

$$\|W\|_{L^1 + L^{3,\infty}} \le \varepsilon_V,$$

then J has a unique minimizer u_{gs} in $\mathcal{U}$ such that $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2} > 0$.

To prove Proposition 2.3.5 we use the following decomposition :

$$L^2(\mathbb{R}^3) = \mathbb{C}u_V \oplus (\mathbb{C}u_V)^\perp,$$

where u_V is the ground state of H_V as in Hypothesis 2.1.2, and we write $u = \alpha u_V + \varphi$, with the normalization condition $|\alpha|^2 + \|\varphi\|_{L^2}^2 = 1$. The Hartree ground state energy is denoted by

$$E_V := \inf_{u \in \mathcal{U}} J(u).$$

We display the dependence on V since the existence of a gap, $E_V < E_{V_1}$, is an important step in our proof of the existence of a minimizer in Appendix 2.5.

Our proof of Proposition 2.3.5 relies on the following two lemmata. For $\lambda \in \mathbb{R}$, we set the resolvent $R_\lambda := (H_V - \lambda)^{-1}$ (defined, a priori, as an unbounded operator on $\mathrm{Ran}(\mathbf{1}_{\{\lambda\}}(H_V))^\perp$). We also recall that $\Pi_V^\perp := \mathbf{I} - |u_V\rangle\langle u_V|$.

Lemma 2.3.6. *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V > 0$ such that, if*

$$\|W\|_{L^1 + L^{3,\infty}} \leq \varepsilon_V,$$

then for all global minimizer u in $\mathcal{U}$ of J such that $u = \alpha u_V + \varphi$, with α in $\mathbb{C}$, φ in $\mathcal{Q}_V$, and $u_V \perp \varphi$ in L^2, we have

$$\varphi = 2R_{\lambda_V}\Pi_V^\perp(\bar{\mathcal{F}}(W) * |u|^2)u, \quad \lambda_V := E_V - \big\langle u, (\bar{\mathcal{F}}(W) * |u|^2)u\big\rangle. \tag{2.51}$$

Proof. We first recall that if u is a minimizer of J, then u is a non-linear Hartree eigenstate,

$$\big(H_V - 2\bar{\mathcal{F}}(W) * |u|^2\big)u = \lambda_V u \quad \text{in } \mathcal{Q}_V^*, \tag{2.52}$$

where $\mathcal{Q}_V^*$ is the topological dual of $\mathcal{Q}_V$ and λ_V is defined by (2.51). Here H_V should be understood as an operator in $\mathcal{L}(\mathcal{Q}_V, \mathcal{Q}_V^*)$. Eq. (2.52) can be proven by using that, for all t in $\mathbb{C}$ and all $u^\perp \in \mathcal{U}$ such that $u \perp u^\perp$ in L^2, we have

$$J\big((1 + |t|^2)^{-\frac{1}{2}}(u + tu^\perp)\big) \geq E_V.$$

Computing the term of order 1 in t in the asymptotic expansion of the previous expression as $t \to 0$ shows that

$$\big\langle u^\perp, \big(H_V - 2\bar{\mathcal{F}}(W) * |u|^2\big)u\big\rangle = 0,$$

for all $u^\perp \in \mathcal{U}$ such that $u \perp u^\perp$ in L^2. Hence (2.52) holds for some $\lambda_V \in \mathbb{C}$. Since $J(u) = E_V$, we obtain that λ_V is given by (2.51).

Now, applying $\Pi_V^\perp$ to (2.52) gives

$$(H_V - \lambda_V)\Pi_V^\perp u = 2\Pi_V^\perp\big(\bar{\mathcal{F}}(W) * |u|^2\big)u. \tag{2.53}$$

Let $\delta_V := \mathrm{dist}(\mu_V, \sigma(H_V) \setminus \{\mu_V\})$ be the distance from μ_V to the rest of the spectrum of H_V. Recall that Hypothesis 2.1.2 implies that $\delta_V > 0$. Using perturbative arguments, it is not difficult to verify that

$$E_V \leq \mu_V + \frac{1}{2}\delta_V, \tag{2.54}$$

provided that $\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V$, for some $\varepsilon_V > 0$ small enough (see (2.84) in Appendix 2.5 for a precise justification). Moreover, since

$$\left\langle u, (\bar{\mathcal{F}}(W) * |u|^2)u \right\rangle = \left\| W^{\frac{1}{2}} \mathcal{F}(|u|^2) \right\|_{L^2}^2 \geq 0\,,$$

we also have $\lambda_V \leq E_V$, and hence

$$\lambda_V \leq \mu_V + \frac{1}{2}\delta_V\,. \tag{2.55}$$

Therefore the operator

$$(H_V - \lambda_V)\Pi_V^\perp \in \mathcal{L}(\mathcal{Q}_V, \mathcal{Q}_V^*)$$

is bounded invertible with inverse $R_{\lambda_V}\Pi_V^\perp \in \mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$. Since $\varphi = \Pi_V^\perp u$, (2.53) then implies (2.51). ☐

In the following lemma, given u_1, u_2 two minimizers of J, we decompose as before, for $j = 1, 2$, $u_j = \alpha_j u_V + \varphi_j$, with $\alpha_j = \langle u_j, u_V\rangle > 0$, $\varphi_j \in \mathcal{Q}_V$ and $u_V \perp \varphi_j$ in L^2.

Lemma 2.3.7. *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V > 0$ such that, if*

$$\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V,$$

then for all global minimizers u_1, u_2 in $\mathcal{U}$ of J, we have

$$\|\varphi_1 - \varphi_2\|_{\mathcal{Q}_V} \leq C_V \|W\|_{L^1+L^{3,\infty}} \left(\|u_1\|_{H^1}^2 + \|u_2\|_{H^1}^2\right)^2 \|u_1 - u_2\|_{L^2}. \tag{2.56}$$

Proof. Let λ_1, λ_2 be defined as in Lemma 2.3.6, namely $\lambda_j = E_V - \langle u_j, (\bar{\mathcal{F}}(W) * |u_j|^2)u_j\rangle$. By Lemma 2.3.6 and the triangle inequality, we have

$$\|\varphi_1 - \varphi_2\|_{\mathcal{Q}_V} \leq S_1 + S_2,$$

where

$$\begin{aligned} S_1 &:= 2\left\|\left(R_{\lambda_1}\Pi_V^\perp - R_{\lambda_2}\Pi_V^\perp\right)(\bar{\mathcal{F}}(W) * |u_1|^2)u_1\right\|_{\mathcal{Q}_V}, \\ S_2 &:= 2\left\|R_{\lambda_2}\Pi_V^\perp\left((\bar{\mathcal{F}}(W) * |u_1|^2)u_1 - (\bar{\mathcal{F}}(W) * |u_2|^2)u_2\right)\right\|_{\mathcal{Q}_V}. \end{aligned}$$

We first estimate the second term. From (2.55) we deduce that $R_{\lambda_2}\Pi_V^\perp \in \mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$ and

$$\left\|R_{\lambda_2}\Pi_V^\perp\right\|_{\mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)} \leq 4\delta_V^{-1}. \tag{2.57}$$

Hence we can estimate

$$\begin{aligned} S_2 &\leq 8\delta_V^{-1} \left\|(\bar{\mathcal{F}}(W) * |u_1|^2)u_1 - (\bar{\mathcal{F}}(W) * |u_2|^2)u_2\right\|_{\mathcal{Q}_V^*} \\ &\leq 8\delta_V^{-1} \left\|(\bar{\mathcal{F}}(W) * |u_1|^2)u_1 - (\bar{\mathcal{F}}(W) * |u_2|^2)u_2\right\|_{L^2}\,, \end{aligned}$$

since $L^2 \subset \mathcal{Q}_V^*$. We obtain from the triangle inequality that

$$\begin{aligned} S_2 \leq\ & 8\delta_V^{-1} \left\| \left(\bar{\mathcal{F}}(W) * [(\bar{u}_1 - \bar{u}_2)u_1]\right)u_1 \right\|_{L^2} \\ & + 8\delta_V^{-1} \left\| \left(\bar{\mathcal{F}}(W) * [\bar{u}_2(u_1 - u_2)]\right)u_1 \right\|_{L^2} \\ & + 8\delta_V^{-1} \left\| \left(\bar{\mathcal{F}}(W) * |u_2|^2\right)(u_1 - u_2) \right\|_{L^2}, \end{aligned}$$

and hence Lemma 2.2.4 yields

$$S_2 \leq C_V \|W\|_{L^1+L^{3,\infty}} \left(\|u_1\|_{H^1}^2 + \|u_2\|_{H^1}^2\right) \|u_1 - u_2\|_{L^2}. \tag{2.58}$$

Now we estimate S_1. It follows from the resolvent equation that

$$S_1 \leq 2|\lambda_1 - \lambda_2| \left\| \left(R_{\lambda_1}\Pi_V^\perp R_{\lambda_2}\Pi_V^\perp\right)(\bar{\mathcal{F}}(W) * |u_1|^2)u_1 \right\|_{\mathcal{Q}_V}.$$

Using (2.57) twice, first for R_{λ_2} and next for R_{λ_1} (using also that $\mathcal{Q}_V \subset \mathcal{Q}_V^*$ in the latter case), and then appying Lemma 2.2.4, we obtain

$$S_1 \leq C_V \|W\|_{L^1+L^{3,\infty}} \|u_1\|_{H^1}^2 |\lambda_1 - \lambda_2|. \tag{2.59}$$

Since $\lambda_j = E_V - \langle u_j, (\mathcal{F}(W) * |u_j|^2)u_j \rangle$ and $\|u_j\|_{L^2} = 1$, we can estimate, by the triangle inequality,

$$|\lambda_1 - \lambda_2| \leq \|u_1 - u_2\|_{L^2} \left\| (\bar{\mathcal{F}}(W) * |u_1|^2)u_1 \right\|_{L^2} + \left\| (\bar{\mathcal{F}}(W) * |u_1|^2)u_1 - (\bar{\mathcal{F}}(W) * |u_2|^2)u_2 \right\|_{L^2}.$$

Using Lemma 2.2.4 to bound the first term, and the same argument we used to prove (2.58) for the second one, we obtain

$$|\lambda_1 - \lambda_2| \leq C_V \|W\|_{L^1+L^{3,\infty}} \left(\|u_1\|_{H^1}^2 + \|u_2\|_{H^1}^2\right) \|u_1 - u_2\|_{L^2}. \tag{2.60}$$

Putting together (2.59) and (2.60) yields

$$S_1 \leq C_V \|W\|_{L^1+L^{3,\infty}}^2 \|u_1\|_{H^1}^2 \left(\|u_1\|_{H^1}^2 + \|u_2\|_{H^1}^2\right) \|u_1 - u_2\|_{L^2}. \tag{2.61}$$

Using $\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V$ and combining (2.61) and (2.58), we obtain (2.56). Since the role of φ_1 and φ_2 in the left-hand-side of (2.56) is symmetric, this concludes the proof. □

We are now ready to prove the uniqueness of a minimizer for the Hartree energy (2.44).

Proof of Proposition 2.3.5. By Proposition 2.3.2, we know that the Hartree functional energy J has a minimizer for $\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V$ with ε_V small enough. Let u_1, u_2 be two minimizers of J. We use the same notations as in the previous proof, decomposing $u_j = \alpha_j u_V + \varphi_j$. Since $\alpha_j = \langle u_j, u_V \rangle > 0$, in order to verify that $u_1 = u_2$, it suffices to prove that $\varphi_1 = \varphi_2$.

To this end, we first show that $\|u_j\|_{\dot{H}^1}^2$ is bounded by C_V and next apply Lemma 2.3.7. We can write

$$\|u_j\|_{\dot{H}^1}^2 \leq \langle u_j, H_{V_+}u_j \rangle = J(u_j) + \langle u_j, V_- u_j \rangle - \left\langle u_j, (\bar{\mathcal{F}}(W) * |u_j|^2)u_j \right\rangle.$$

We have $J(u_j) = E_V$ since u_j is a minimizer, $\langle u_j, V_- u_j\rangle \le a\|u_j\|^2_{\dot H^1} + b$ with $a < 1$ by Hypothesis 2.1.1 and $|\langle u_j, (\bar{\mathcal{F}}(W) * |u_j|^2)u_j\rangle| \le C\|W\|_{L^1+L^{3,\infty}}\|u_j\|^2_{H^1}$ for some universal constant C by Lemma 2.2.4. Therefore

$$\|u_j\|^2_{H^1} \le 1 + \frac{1}{1 - a - C\|W\|_{L^1+L^{3,\infty}}}\big(E_V + b + C\|W\|_{L^1+L^{3,\infty}}\big).$$

Hence, since in addition, by (2.54), $E_V \le \mu_V + \frac{1}{2}\delta_V$ for $\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V$ with ε_V small enough, we deduce that $\|u_j\|^2_{H^1} \le C_V$. Lemma 2.3.7 then implies that

$$\|\varphi_1 - \varphi_2\|_{\mathcal{Q}_V} \le C_V\|W\|_{L^1+L^{3,\infty}}\|u_1 - u_2\|_{L^2}. \tag{2.62}$$

Now we have

$$\|u_1 - u_2\|^2_{L^2} = |\alpha_1 - \alpha_2|^2 + \|\varphi_1 - \varphi_2\|^2_{L^2}. \tag{2.63}$$

To conclude the proof, we show that $|\alpha_1 - \alpha_2|$ can be controlled by $\|\varphi_1 - \varphi_2\|^2_{L^2}$. Lemma 2.3.6 and the arguments used in the proof of Lemma 2.3.7 ensure that $\|\varphi_j\|_{L^2} \le \frac{1}{2}$. Indeed,

$$\begin{aligned}
\|\varphi_j\|_{L^2} \le \|\varphi_j\|_{\mathcal{Q}_V} &= 2\big\|R_{\lambda_j}\Pi_V^\perp(\bar{\mathcal{F}}(W) * |u_j|^2)u_j\big\|_{\mathcal{Q}_V} \\
&\le C_V\big\|(\bar{\mathcal{F}}(W) * |u_j|^2)u_j\big\|_{\mathcal{Q}_V^*} \\
&\le C_V\big\|(\bar{\mathcal{F}}(W) * |u_j|^2)u_j\big\|_{L^2} \\
&\le C_V\|W\|_{L^1+L^{3,\infty}}\|u_j\|^2_{H^1} \\
&\le C_V\|W\|_{L^1+L^{3,\infty}},
\end{aligned}$$

where in the last inequality we used in addition that $\|u_j\|^2_{\dot H^1} \le C_V$. Therefore $\|\varphi_j\|_{L^2} \le \frac{1}{2}$ for $\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V$ with ε_V small enough and we can thus estimate

$$\begin{aligned}
|\alpha_1 - \alpha_2| &= \Big|\big(1 - \|\varphi_1\|^2_{L^2}\big)^{1/2} - \big(1 - \|\varphi_2\|^2_{L^2}\big)^{1/2}\Big| \\
&= \left|\frac{\|\varphi_2\|_{L^2} + \|\varphi_1\|_{L^2}}{\big(1 - \|\varphi_1\|^2_{L^2}\big)^{1/2} + \big(1 - \|\varphi_2\|^2_{L^2}\big)^{1/2}}\right| \big|\|\varphi_2\|_{L^2} - \|\varphi_1\|_{L^2}\big| \\
&\le C\,\|\varphi_1 - \varphi_2\|_{L^2}\,.
\end{aligned} \tag{2.64}$$

Inserting this into (2.62)–(2.63) and using that $\|\varphi_1 - \varphi_2\|^2_{L^2} \le \|\varphi_1 - \varphi_2\|^2_{\mathcal{Q}_V}$, we finally conclude that

$$\|\varphi_1 - \varphi_2\|_{\mathcal{Q}_V} \le C_V\|W\|_{L^1+L^{3,\infty}}\|\varphi_1 - \varphi_2\|_{\mathcal{Q}_V}.$$

For $\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V$ with ε_V small enough, this implies that $\varphi_1 = \varphi_2$, which concludes the proof of the proposition. □

2.3.4 Expansion of the ground state energy for small coupling constants

Assuming that V satisfies Hypotheses 2.1.1 and 2.1.2 and that $W = g^2\omega^{-1}v^2$ satisfies Hypothesis 2.1.3, it follows from Proposition 2.3.5 that J has a unique ground state in $\mathcal{U}$, denoted by u_{gs}, such that $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2} > 0$. The next proposition provides the asymptotic expansion of the Hartree ground state energy (or equivalently the Klein–Gordon–Schrödinger ground state energy) stated in Proposition 2.1.6.

Proposition 2.3.8. *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that $W = g^2\omega^{-1}v^2$ satisfies Hypothesis 2.1.3. Then, as $g \to 0$,*

$$E_V = J(u_{\mathrm{gs}}) = \mu_V - g^2 \int \left(\bar{\mathcal{F}}\left(\omega^{-1}v^2\right) * |u_V|^2\right)(x)\, |u_V(x)|^2\, \mathrm{d}x + \mathcal{O}(g^4).$$

Proof. As in Lemma 2.3.6, we decompose the Hartree ground state $u_{\mathrm{gs}} = \alpha_{\mathrm{gs}} u_V + \varphi_{\mathrm{gs}}$, with α_{gs} in $\mathbb{C}$, φ_{gs} in $\mathcal{Q}_V$ and $u_V \perp \varphi_{\mathrm{gs}}$ in L^2. By Lemma 2.3.6, we have

$$\begin{aligned}\|\varphi_{\mathrm{gs}}\|_{\mathcal{Q}_V} &= 2g^2 \left\| R_{\lambda_V} \Pi_V^{\perp} (\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_{\mathrm{gs}}|^2) u_{\mathrm{gs}} \right\|_{\mathcal{Q}_V} \\ &\le C_V g^2 \left\| (\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_{\mathrm{gs}}|^2) u_{\mathrm{gs}} \right\|_{\mathcal{Q}_V^*} \\ &\le C_V g^2 \left\| (\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_{\mathrm{gs}}|^2) u_{\mathrm{gs}} \right\|_{L^2} = \mathcal{O}(g^2),\end{aligned}$$

the last equality being a consequence of Lemma 2.2.4. Similarly, using that $R_{\lambda_V} = (H_V - \lambda_V)^{-1}$, we can estimate

$$\begin{aligned}|\langle \varphi_{\mathrm{gs}}, H_V \varphi_{\mathrm{gs}}\rangle| &\le |\lambda_V| \|\varphi_{\mathrm{gs}}\|_{L^2}^2 + g^4 \left| \left\langle \Pi_V^{\perp} (\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_{\mathrm{gs}}|^2) u_{\mathrm{gs}}, R_{\lambda_V} \Pi_V^{\perp} (\bar{\mathcal{F}}(\omega^{-1}v^2) * |u_{\mathrm{gs}}|^2) u_{\mathrm{gs}} \right\rangle \right| \\ &= \mathcal{O}(g^4). \end{aligned} \tag{2.65}$$

Here we used (2.55) which shows that $|\lambda_V|$ is bounded by C_V and that $R_{\lambda_V}\Pi_V^{\perp} \in \mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$. Besides, since $|\alpha_{\mathrm{gs}}|^2 = 1 - \|\varphi_{\mathrm{gs}}\|_{L^2}^2$, we have

$$|\alpha_{\mathrm{gs}}| = 1 + \mathcal{O}(g^4). \tag{2.66}$$

We can then compute

$$\begin{aligned} J(u_{\mathrm{gs}}) &= \langle \alpha_{\mathrm{gs}} u_V + \varphi_{\mathrm{gs}}, H_V(\alpha_{\mathrm{gs}} u_V + \varphi_{\mathrm{gs}})\rangle_{L^2} \\ &\quad - g^2 \int \bar{\mathcal{F}}(\omega^{-1}v^2) * |\alpha_{\mathrm{gs}} u_V + \varphi_{\mathrm{gs}}|^2 (x)\, |\alpha_{\mathrm{gs}} u_V(x) + \varphi_{\mathrm{gs}}(x)|^2\, \mathrm{d}x \\ &= |\alpha_{\mathrm{gs}}|^2 \mu_V + \langle \varphi_{\mathrm{gs}}, H_V \varphi_{\mathrm{gs}}\rangle_{L^2} \\ &\quad - g^2 |\alpha_{\mathrm{gs}}|^4 \int \bar{\mathcal{F}}(\omega^{-1}v^2) * |u_V|^2 (x)\, |u_V(x)|^2\, \mathrm{d}x + \mathcal{O}(g^4), \end{aligned}$$

where in the second equality we used that $H_V u_V = \mu_V u_V$, $u_V \perp \varphi_{\mathrm{gs}}$ in L^2, and Lemma 2.2.4 in order to obtain the expansion of the convolution term. Inserting (2.65) and (2.66) into the last equality concludes the proof of the proposition. □

We conclude this section with the proof of Proposition 2.1.7 which provides the difference, at second order in the coupling constant, between the ground state energy of the Pauli-Fierz Hamiltonian $\mathbb{H}$ and the ground state energy of the Klein–Gordon–Schrödinger energy functional.

Proof of Proposition 2.1.7. Under the conditions of Proposition 2.1.7, using perturbative methods developed in the literature to study ground states of Pauli-Fierz Hamiltonians (see e.g. [10, 12, 62, 68, 71, 110]), it is not difficult to verify that the second-order asymptotic expansion of $\inf\sigma(\mathbb{H})$ is given by

$$\begin{aligned}&\inf\sigma(\mathbb{H})\\ &= \mu_V - g^2\Big\langle u_V\otimes\Omega, a(h_x)(\Pi_V\otimes\Pi_\Omega)^\perp\big(\mathbb{H}_{\mathrm{free}}-\mu_V\big)^{-1}(\Pi_V\otimes\Pi_\Omega)^\perp a^*(h_x)u_V\otimes\Omega\Big\rangle + o(g^2)\,,\end{aligned}$$

where we recall that Π_V stands for the orthogonal projection onto the ground state u_V of H_V, Π_Ω stands for the orthogonal projection onto the Fock vacuum Ω, and $(\Pi_V\otimes\Pi_\Omega)^\perp = \mathbf{I}-\Pi_\Omega$. Moreover, $\mathbb{H}_{\mathrm{free}} = H_V\otimes\mathbf{I}_{\mathrm{f}}+\mathbf{I}_{\mathrm{el}}\otimes\mathbb{H}_{\mathrm{f}}$. Decomposing $(\Pi_V\otimes\Pi_\Omega)^\perp = \Pi_V\otimes\Pi_\Omega^\perp+\Pi_V^\perp\otimes\mathbf{I}_{\mathrm{f}}$ and using (2.24), we obtain

$$\begin{aligned}\inf\sigma(\mathbb{H}) &= \mu_V - g^2\int_{\mathbb{R}^3}\big(\bar{\mathcal{F}}(\omega^{-1}v^2)*|u_V|^2\big)(x)\,|u_V(x)|^2\,\mathrm{d}x\\ &\quad - g^2\Big\langle u_V\otimes\Omega, a(h_x)(\Pi_V^\perp\otimes\mathbf{I}_{\mathrm{f}})\big(\mathbb{H}_{\mathrm{free}}-\mu_V\big)^{-1}(\Pi_V^\perp\otimes\mathbf{I}_{\mathrm{f}})a^*(h_x)u_V\otimes\Omega\Big\rangle + o(g^2)\,.\end{aligned}$$

A direct computation gives

$$\begin{aligned}&\Big\langle u_V\otimes\Omega, a(h_x)(\Pi_V^\perp\otimes\mathbf{I}_{\mathrm{f}})\big(\mathbb{H}_{\mathrm{free}}-\mu_V\big)^{-1}(\Pi_V^\perp\otimes\mathbf{I}_{\mathrm{f}})a^*(h_x)u_V\otimes\Omega\Big\rangle\\ &\qquad = \int_{\mathbb{R}^3} v(k)^2\big\langle u_V, e^{ikx}\Pi_V^\perp\big(H_V-\mu_V+\omega(k)\big)^{-1}\Pi_V^\perp e^{-ikx}u_V\big\rangle_{L^2_x}\mathrm{d}k,\end{aligned}$$

which, together with Proposition 2.1.6, proves Proposition 2.1.7. ☐

2.3.5 Ultraviolet limit

We suppose in this section that the coupling function is of the form $v_\Lambda = v\mathbb{1}_{|k|\le\Lambda}$ for some ultraviolet parameter $\Lambda>0$ and we write

$$W_\Lambda := g^2\omega^{-1}v_\Lambda = W\mathbb{1}_{|k|\le\Lambda},$$

where we recall that ω stands for the dispersion relation for the bosons and $W = g^2\omega^{-1}v^2$.

Our fist concern is to show that the ground state energies $E_{V,\Lambda}$ defined by

$$E_{V,\Lambda} := \inf_{u\in\mathcal{U}} J_\Lambda(u),\quad J_\Lambda(u) := \langle u, H_V\,u\rangle - \int_{\mathbb{R}^3}\big(\bar{\mathcal{F}}\left(W_\Lambda\right)*|u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x,$$

converge to E_V as $\Lambda\to\infty$. As mentioned in the introduction, the main difficulty comes from the fact that, in general, W_Λ does *not* converge to W in $L^1+L^{3,\infty}$. Nevertheless, we can rely on the following easy lemma.

Lemma 2.3.9. *Suppose that W satisfies Hypothesis 2.1.3. Let u in $\mathcal{Q}_V$. Then*

$$\int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}\,(W_\Lambda) * |u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x \underset{\Lambda\to\infty}{\longrightarrow} \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W) * |u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x, \tag{2.67}$$

and

$$\big\|(\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2)u\big\|_{L^2} \underset{\Lambda\to\infty}{\longrightarrow} 0. \tag{2.68}$$

Proof. To prove (2.67), we compute

$$\begin{aligned}&\int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}\,(W) * |u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x - \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W_\Lambda) * |u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x \\ &= \int_{\mathbb{R}^3} (W(k) - W_\Lambda(k))\big|\mathcal{F}(|u|^2)\big|^2(k)\,\mathrm{d}k = \int_{\mathbb{R}^3} W(k)\mathbb{1}_{|k|\geq\Lambda}\big|\mathcal{F}(|u|^2)\big|^2(k)\,\mathrm{d}k.\end{aligned}$$

Clearly, for all k in $\mathbb{R}^3$, $W(k)\mathbb{1}_{|k|\geq\Lambda}|\mathcal{F}(|u|^2)|^2(k) \to 0$ as $\Lambda \to \infty$. Moreover, since W is in $L^1 + L^{3,\infty}$ and u in $\mathcal{Q}_V$, the proof of Lemma 2.2.4 shows that $W\mathcal{F}(|u|^2)$ is in L^1 and hence $W|\mathcal{F}(|u|^2)|^2$ belongs to L^1. Lebesgue's dominated convergence Theorem then proves (2.67).

The proof of (2.68) is similar, using Lemma 2.2.4(iii) together with Lebesgue's dominated convergence in L^2. □

Now we can prove the convergence of the ground state energies in the ultraviolet limit. The next proposition implies Proposition 2.1.9 from the introduction.

Proposition 2.3.10 (Ultraviolet limit of the ground state energies)**.** *Suppose that V satisfies Hypothesis 2.1.1 and that W satisfies Hypothesis 2.1.3. Then*

$$E_{V,\Lambda} \underset{\Lambda\to\infty}{\longrightarrow} E_V.$$

Proof. First, we observe that for $0 < \Lambda \leq \Lambda'$,

$$\int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}\,(W_\Lambda) * |u|^2\big)(x)\,|u(x)|^2\,\mathrm{d}x = \int_{\mathbb{R}^3} W_\Lambda(k)\big|\mathcal{F}(|u|^2)\big|^2(k)\,\mathrm{d}k \leq \int_{\mathbb{R}^3} W_{\Lambda'}(k)\big|\mathcal{F}(|u|^2)\big|^2(k)\,\mathrm{d}k,$$

and therefore $J_\Lambda \geq J_{\Lambda'}$. Hence $\Lambda \mapsto E_{V,\Lambda}$ is non-increasing on $(0,\infty)$ and bounded below by E_V. We set

$$E_{V,\infty} := \lim_{\Lambda\to\infty} E_{V,\Lambda} \geq E_V.$$

Now we show that $E_{V,\infty} \leq E_V$. Let $\varepsilon > 0$ and let $u_\varepsilon \in \mathcal{U}$ be such that $J(u_\varepsilon) \leq E_V + \varepsilon$. We have

$$\begin{aligned}E_{V,\Lambda} \leq J_\Lambda(u_\varepsilon) &= J(u_\varepsilon) - \int_{\mathbb{R}^3} (W_\Lambda(k) - W(k))\big|\mathcal{F}(|u_\varepsilon|^2)\big|^2(k)\,\mathrm{d}k \\ &\leq E_V + \varepsilon - \int_{\mathbb{R}^3} (W_\Lambda(k) - W(k))\big|\mathcal{F}(|u_\varepsilon|^2)\big|^2(k)\,\mathrm{d}k.\end{aligned}$$

Applying Lemma 2.3.9, this yields

$$E_{V,\infty} = \lim_{\Lambda\to\infty} E_{V,\Lambda} \le E_V + \varepsilon.$$

Since $\varepsilon > 0$ is arbitrary, this concludes the proof of the proposition. □

Next, we establish the convergence of the ground states of J_Λ to the ground state of J, as $\Lambda \to \infty$. Combined with Proposition 2.3.1, the next result implies Proposition 2.1.10 from the introduction. Some arguments of the proof below are similar to those used in the proof of the uniqueness of the minimizer of J in Section 2.3.3. We do not give all the details.

Proposition 2.3.11 (Ultraviolet limit of the ground states)**.** *Suppose that V satisfies Hypotheses 2.1.1 and 2.1.2 and that W satisfies Hypothesis 2.1.3. There exists $\varepsilon_V > 0$ such that, if*

$$\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V,$$

then for all $\Lambda > 0$, J_Λ and J have unique minimizers $u_{\Lambda,\mathrm{gs}}$ and u_{gs} in $\mathcal{U}$, respectively, such that $\langle u_{\Lambda,\mathrm{gs}}, u_V\rangle_{L^2} > 0$ and $\langle u_{\mathrm{gs}}, u_V\rangle_{L^2} > 0$. They satisfy

$$\left\|u_{\Lambda,\mathrm{gs}} - u_{\mathrm{gs}}\right\|_{\mathcal{Q}_V} \underset{\Lambda\to\infty}{\longrightarrow} 0.$$

Proof. Existence of a unique minimizer for J follows from Proposition 2.3.5. The same holds for J_Λ since, for any $\Lambda > 0$,

$$\|W_\Lambda\|_{L^1+L^{3,\infty}} \le \|W\|_{L^1+L^{3,\infty}}. \tag{2.69}$$

We write $u = u_{\mathrm{gs}}$ and $u_\Lambda = u_{\Lambda,\mathrm{gs}}$ to simplify expressions below. We decompose $u = \alpha u_V + \varphi$, with a coefficient $\alpha = \langle u, u_V\rangle > 0$, φ in $\mathcal{Q}_V$ and $u_V \perp \varphi$ in L^2, and likewise $u_\Lambda = \alpha_\Lambda u_V + \varphi_\Lambda$, with a coefficient $\alpha_\Lambda = \langle u_\Lambda, u_V\rangle > 0$, φ_Λ in $\mathcal{Q}_V$ and $u_V \perp \varphi_\Lambda$ in L^2.

In the same way as in the proof of Proposition 2.3.5, using also (2.69) and the fact that $E_{V,\Lambda}$ is uniformly bounded in Λ (since $E_{V,\Lambda}$ converges as $\Lambda\to\infty$, by Proposition 2.3.10), we have

$$\|\varphi\|_{L^2} \le C_V\|W\|_{L^1+L^{3,\infty}}, \quad \|\varphi_\Lambda\|_{L^2} \le C_V\|W\|_{L^1+L^{3,\infty}}. \tag{2.70}$$

This yields

$$\|u - u_\Lambda\|_{\mathcal{Q}_V} \le C_V|\alpha - \alpha_\Lambda| + \|\varphi - \varphi_\Lambda\|_{\mathcal{Q}_V}. \tag{2.71}$$

The difference $|\alpha - \alpha_\Lambda|$ can be controlled by $\|\varphi - \varphi_\Lambda\|_{L^2}^2$. Indeed, we have the upper bound $\|\varphi_\sharp\|_{L^2} \le C_V\|W\|_{L^1+L^{3,\infty}} \le \frac{1}{2}$ for $\|W\|_{L^1+L^{3,\infty}} \le \varepsilon_V$ with ε_V small enough, where $\varphi_\sharp$ stands for φ or φ_Λ. We can thus estimate in the same way as in (2.64),

$$|\alpha - \alpha_\Lambda| = \left|\frac{\|\varphi_\Lambda\|_{L^2} + \|\varphi\|_{L^2}}{\left(1 - \|\varphi\|_{L^2}^2\right)^{1/2} + \left(1 - \|\varphi_\Lambda\|_{L^2}^2\right)^{1/2}}\right| \left|\|\varphi_\Lambda\|_{L^2} - \|\varphi\|_{L^2}\right| \le C\left\|\varphi - \varphi_\Lambda\right\|_{L^2}.$$

Since $\|\varphi - \varphi_\Lambda\|_{L^2} \leq \|\varphi - \varphi_\Lambda\|_{\mathcal{Q}_V}$, inserting the previous inequality into (2.71) gives

$$\|u - u_\Lambda\|_{\mathcal{Q}_V} \leq C_V \|\varphi - \varphi_\Lambda\|_{\mathcal{Q}_V}. \tag{2.72}$$

Now we estimate $\|\varphi - \varphi_\Lambda\|_{\mathcal{Q}_V}$. To this end, we use Lemma 2.3.6, which gives

$$\varphi = 2R_{\lambda_V}\Pi_V^\perp\, (\bar{\mathcal{F}}(W) * |u|^2)u, \quad \lambda_V := E_V - \big\langle u, (\bar{\mathcal{F}}(W) * |u|^2)u\big\rangle,$$
$$\varphi_\Lambda = 2R_{\lambda_{V,\Lambda}}\Pi_V^\perp\, (\bar{\mathcal{F}}(W_\Lambda) * |u_\Lambda|^2)u_\Lambda, \quad \lambda_{V,\Lambda} := E_{V,\Lambda} - \big\langle u_\Lambda, (\bar{\mathcal{F}}(W_\Lambda) * |u_\Lambda|^2)u_\Lambda\big\rangle.$$

By the triangle inequality,

$$\|\varphi - \varphi_\Lambda\|_{\mathcal{Q}_V} \leq T_1 + T_2 + T_3, \tag{2.73}$$

where

$$T_1 := 2\big\|\big(R_{\lambda_V}\Pi_V^\perp - R_{\lambda_{V,\Lambda}}\Pi_V^\perp\big)(\bar{\mathcal{F}}(W) * |u|^2)u\big\|_{\mathcal{Q}_V},$$
$$T_2 := 2\big\|R_{\lambda_{V,\Lambda}}\Pi_V^\perp(\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2)u\big\|_{\mathcal{Q}_V},$$
$$T_3 := 2\big\|R_{\lambda_{V,\Lambda}}\Pi_V^\perp\big((\bar{\mathcal{F}}(W_\Lambda) * |u|^2)u - (\bar{\mathcal{F}}(W_\Lambda) * |u_\Lambda|^2)u_\Lambda\big)\big\|_{\mathcal{Q}_V}.$$

We first estimate the term T_3. As in (2.55), we have that $\lambda_{V,\Lambda} \leq \mu_V + \frac{1}{2}\delta_V$, with the distance to the lower eigenvalue $\delta_V = \mathrm{dist}(\mu_V, \sigma(H_V) \setminus \{\mu_V\})$. Hence $R_{\lambda_{V,\Lambda}}\Pi_V^\perp$ is in $\mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$ and

$$\big\|R_{\lambda_{V,\Lambda}}\Pi_V^\perp\big\|_{\mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)} \leq 2\delta_V^{-1}. \tag{2.74}$$

This yields

$$\begin{aligned} T_3 &\leq 4\delta_V^{-1}\left\|(\bar{\mathcal{F}}(W) * |u|^2)u - (\bar{\mathcal{F}}(W) * |u_\Lambda|^2)u_\Lambda\right\|_{\mathcal{Q}_V^*} \\ &\leq 4\delta_V^{-1}\left\|(\bar{\mathcal{F}}(W) * |u|^2)u - (\bar{\mathcal{F}}(W) * |u_\Lambda|^2)u_\Lambda\right\|_{L^2}, \end{aligned}$$

since $L^2 \subset \mathcal{Q}_V^*$. We obtain from the triangle inequality that

$$\begin{aligned} T_3 \leq\ & 4\delta_V^{-1}\left\|\big(\bar{\mathcal{F}}(W) * [(\bar{u} - \bar{u}_\Lambda)u]\big)u\right\|_{L^2} \\ &+ 4\delta_V^{-1}\left\|\big(\bar{\mathcal{F}}(W) * [\bar{u}_\Lambda(u - u_\Lambda)]\big)u\right\|_{L^2} \\ &+ 4\delta_V^{-1}\left\|\big(\bar{\mathcal{F}}(W) * |u_\Lambda|^2\big)(u - u_\Lambda)\right\|_{L^2}, \end{aligned}$$

and hence Lemma 2.2.4 yields

$$T_3 \leq C_V \|W\|_{L^1 + L^{3,\infty}}\big(\|u\|_{H^1}^2 + \|u_\Lambda\|_{H^1}^2\big)\|u - u_\Lambda\|_{L^2}. \tag{2.75}$$

Since in addition we have $\|u_\Lambda\|_{\dot{H}^1}^2 \leq C_V$ (in the same way as in the proof of Proposition 2.3.5) uniformly in Λ, this gives

$$T_3 \leq C_V \|W\|_{L^1 + L^{3,\infty}}\|u - u_\Lambda\|_{\mathcal{Q}_V}. \tag{2.76}$$

Next we estimate T_1. It follows from the resolvent equation that

$$T_1 \leq 2|\lambda_V - \lambda_{V,\Lambda}| \big\| \big(R_{\lambda_V} \Pi_V^\perp R_{\lambda_{V,\Lambda}} \Pi_V^\perp \big) (\bar{\mathcal{F}}(W) * |u|^2) u \big\|_{\mathcal{Q}_V}.$$

Using (2.74), the fact that, likewise, $\big\| R_{\lambda_V} \Pi_V^\perp \big\|_{\mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V^*)} \leq 2\delta_V^{-1}$ and then Lemma 2.2.4, we obtain

$$T_1 \leq C_V \|W\|_{L^1+L^{3,\infty}} \|u\|_{H^1}^2 |\lambda_V - \lambda_{V,\Lambda}| \leq C_V \|W\|_{L^1+L^{3,\infty}} |\lambda_V - \lambda_{V,\Lambda}|. \tag{2.77}$$

The expressions of λ, λ_V imply

$$\begin{aligned} |\lambda_V - \lambda_{V,\Lambda}| &\leq |E_V - E_{V,\Lambda}| + \big| \big\langle u, (\bar{\mathcal{F}}(W) * |u|^2) u \big\rangle - \big\langle u_\Lambda, (\bar{\mathcal{F}}(W_\Lambda) * |u_\Lambda|^2) u_\Lambda \big\rangle \big| \\ &\leq |E_V - E_{V,\Lambda}| + \big| \big\langle u, (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\rangle \big| \\ &\quad + \big| \big\langle u, (\bar{\mathcal{F}}(W_\Lambda) * |u|^2) u \big\rangle - \big\langle u_\Lambda, (\bar{\mathcal{F}}(W_\Lambda) * |u_\Lambda|^2) u_\Lambda \big\rangle \big|. \end{aligned}$$

The last term can be estimated by the same argument we used to bound T_3. This gives

$$\begin{aligned} &|\lambda_V - \lambda_{V,\Lambda}| \\ &\quad \leq |E_V - E_{V,\Lambda}| + C_V \|W\|_{L^1+L^{3,\infty}} \|u - u_\Lambda\|_{\mathcal{Q}_V} + \big| \big\langle u, (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\rangle \big|. \end{aligned} \tag{2.78}$$

To estimate the term T_2, we write

$$\begin{aligned} T_2 &\leq C_V \big\| (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\|_{\mathcal{Q}_V^*}, \\ &\leq C_V \big\| (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\|_{L^2}, \end{aligned} \tag{2.79}$$

since $L^2 \subset \mathcal{Q}_V^*$.

Putting together (2.72), (2.73), (2.76), (2.77), (2.78) and (2.79), we deduce that

$$\begin{aligned} \big(1 - C_V \|W\|_{L^1+L^{3,\infty}}\big) \|u - u_\Lambda\|_{\mathcal{Q}_V} \leq C_V \Big(|E_V - E_{V,\Lambda}| + \big| \big\langle u, (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\rangle \big| \\ + \big\| (\bar{\mathcal{F}}(W - W_\Lambda) * |u|^2) u \big\|_{L^2} \Big). \end{aligned}$$

For $\|W\|_{L^1+L^{3,\infty}} \leq \varepsilon_V$ with ε_V small enough, Lemma 2.3.9 together with Proposition 2.3.10 then imply that $\|u - u_\Lambda\|_{\mathcal{Q}_V} \to 0$ as $\Lambda \to \infty$. □

2.4 Appendix : Operators in Fock space, self-adjointness

2.4.1 Operators in Fock space

We recall in this section a few well-known properties of basic operators in Fock space. We do not specify their domains. For more details the reader may consult e.g. [21, 25, 107]. Recall that the symmetric Fock space $\mathfrak{F}_s(\mathfrak{h})$ over the one-particle space $\mathfrak{h} = L^2(\mathbb{R}^3)$ has been defined in (2.10). For h in $\mathfrak{h}$, the creation and annihilation operators $a^*(h)$ and $a(h)$ are defined as follows :

$$a^*(h)_{|\bigvee^n \mathfrak{h}} = \sqrt{(n+1)}\, |h\rangle \bigvee \mathbf{I}_{\bigvee^n \mathfrak{h}}, \quad n \geq 0,$$
$$a(h)_{|\bigvee^n \mathfrak{h}} = \sqrt{n}\, \langle h| \otimes \mathbf{I}_{\bigvee^{n-1} \mathfrak{h}}, \quad n > 0, \qquad a(h)_{|\mathbb{C}} = 0.$$

Formally, we also have

$$a(h) = \int_{\mathbb{R}^3} \overline{h(k)} a(k)\, \mathrm{d}k, \quad a^*(h) = \int_{\mathbb{R}^3} h(k) a^*(k)\, \mathrm{d}k,$$

where $a(k)$ and $a^*(k)$ are operator-valued distributions which satisfy the well-known canonical commutations relations

$$[a(k), a(k')] = [a^*(k), a^*(k')] = 0, \quad [a(k), a^*(k')] = \delta(k - k').$$

The field operator $\Phi(h)$ is defined by

$$\Phi(h) = (a(h) + a^*(h))/\sqrt{2}.$$

Let ω be a self-adjoint operator on $\mathfrak{h}$. The second quantization of ω is defined by

$$\mathrm{d}\Gamma(\omega)_{|\bigvee^n \mathfrak{h}} = \sum_{k=1}^{n} \mathbf{I}_{\bigvee^{k-1} \mathfrak{h}} \otimes \omega \otimes \mathbf{I}_{\bigvee^{n-k} \mathfrak{h}}.$$

Note that this operator can be expressed in terms of creation and annihilation operators :

$$\mathrm{d}\Gamma(\omega) = \int_{\mathbb{R}^3} \omega(k) a^*(k) a(k)\, \mathrm{d}k.$$

The coherent state of parameter f in $\mathfrak{h}$ is the vector in Fock space defined as

$$\Psi_f := e^{i\Phi\left(\frac{\sqrt{2}}{i} f\right)} \Omega = e^{-\frac{\|f\|_{\mathfrak{h}}^2}{2}} \sum_{n=0}^{\infty} \frac{f^{\otimes n}}{\sqrt{n!}},$$

where Ω stands for the Fock vacuum. Coherent states are eigenvectors of the annihilation operator in the sense that, for all f, h in $\mathfrak{h}$, we have

$$a(h)\Psi_f = \langle h, f \rangle_{\mathfrak{h}} \Psi_f.$$

This identity implies the following relations :

$$\langle \Psi_f, \Phi(h)\Psi_f \rangle_{\mathfrak{F}_s(\mathfrak{h})} = 2\mathfrak{Re}\, \langle h, f \rangle_{\mathfrak{h}}, \qquad \langle \Psi_f, \mathrm{d}\Gamma(\omega)\Psi_f \rangle_{\mathfrak{F}_s(\mathfrak{h})} = \langle f, \omega f \rangle_{\mathfrak{h}}.$$

These equalities were used to compute the expressions (2.18)–(2.19) of the Pauli-Fierz energy of product stated of the form $u \otimes \Psi_f$.

2.4.2 Self-adjointness of the Pauli-Fierz Hamiltonian

In the next proposition, we recall the self-adjointness property of the Pauli-Fierz Hamiltonian $\mathbb{H}$ defined in (2.15). Recall also that the free Hamiltonian $\mathbb{H}_{\mathrm{free}}$ has been defined in (2.16).

Proposition 2.4.1. *Suppose V satisfies Hypothesis 2.1.1 and that $W = g^2\omega^{-1}v^2$ is in $L^1(\mathbb{R}^3)$. Then $\mathbb{H}$ is a self-adjoint, semi-bounded operator with form domain $\mathcal{Q}(\mathbb{H}) = \mathcal{Q}(\mathbb{H}_{\mathrm{free}})$ for all g in $\mathbb{R}$.*

Proof. Using the well-known N_τ-estimates for the creation and annihilation operators, we have

$$\|a(h_x)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq \left\|\omega^{-1/2}h_x\right\|_{\mathfrak{h}} \left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|_{\mathfrak{F}_s(\mathfrak{h})},$$
$$\|a^*(h_x)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq \left\|\omega^{-1/2}h_x\right\|_{\mathfrak{h}} \left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|_{\mathfrak{F}_s(\mathfrak{h})} + \|h_x\|_{\mathfrak{h}}\|\psi\|_{\mathfrak{F}_s(\mathfrak{h})}.$$

Note that the quantity $\left\|\omega^{-1/2}h_x\right\|_{\mathfrak{h}}$ is well-defined since W is in L^1. Now, by the Cauchy-Schwarz inequality, we have

$$\begin{aligned}\left\|\mathrm{d}\Gamma(\omega)^{1/2}\psi\right\|^2_{\mathfrak{F}_s(\mathfrak{h})} &= \langle\psi, \mathrm{d}\Gamma(\omega)\psi\rangle_{\mathfrak{F}_s(\mathfrak{h})} \\ &\leq \|\psi\|_{\mathfrak{F}_s(\mathfrak{h})}\|\mathrm{d}\Gamma(\omega)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq \frac{1}{2\varepsilon^2}\|\psi\|^2_{\mathfrak{F}_s(\mathfrak{h})} + \frac{\varepsilon^2}{2}\|\mathrm{d}\Gamma(\omega)\psi\|^2_{\mathfrak{F}_s(\mathfrak{h})}.\end{aligned}$$

Taking $\varepsilon > 0$ small enough allows us to conclude that there exists $a < 1$ and b in $\mathbb{R}$ such that, for all ψ in $\mathfrak{F}_s(\mathfrak{h})$, the following inequality holds

$$\|g\Phi(h_x)\psi\|_{\mathfrak{F}_s(\mathfrak{h})} \leq a\,\|\mathbb{H}_{\mathrm{free}}\psi\|_{\mathfrak{F}_s(\mathfrak{h})} + b\,\|\psi\|_{\mathfrak{F}_s(\mathfrak{h})}$$

Therefore $g\Phi(h_x)$ is relatively bounded (and hence also relatively form bounded) with respect to $\mathbb{H}_{\mathrm{free}}$ with relative bound less than 1. Applying the KLMN theorem (see e.g. [107, Theorem X.17]) then yields the result. ☐

As mentioned in the introduction, the condition $W \in L^1$ is not satisfied by the polaron model. It is nevertheless proven in [65], by other means, that the polaron Hamiltonian $\mathbb{H}$ also identifies with a semi-bounded self-adjoint operator with form domain $\mathcal{Q}(\mathbb{H}) = \mathcal{Q}(\mathbb{H}_{\mathrm{free}})$.

2.5 Appendix : Existence of a minimizer for the Hartree equation

In this section, we prove the existence of a minimizer for the Hartree energy functional as stated in Proposition 2.3.2. We write $w = \bar{\mathcal{F}}(W) = g^2\bar{\mathcal{F}}(\omega^{-1}v^2)$ (where, recall, ω is the field dispersion relation, v is the coupling function and g is the coupling parameter) and display the dependence of the Hartree energy functional (2.44) on the external potential V. In other words, we study in this section the energy functional

$$J_V(u) := \langle u, H_V u\rangle - \int_{\mathbb{R}^3} \big(w * |u|^2\big)(x)|u(x)|^2\,\mathrm{d}x, \quad u \in \mathcal{U},$$

where $V, w : \mathbb{R}^3 \to \mathbb{R}$ are real potentials, $H_V = -\Delta + V$, and

$$\mathcal{U} = \big\{u \in \mathcal{Q}_V \mid \|u\|_{L^2} = 1\big\},$$

with $\mathcal{Q}_V \subset L^2(\mathbb{R}^3)$ the form domain of H_V.

We begin with a lemma showing that J_V is well-defined and semi-bounded from below under our assumptions.

Lemma 2.5.1. *Assume that V satisfies Hypothesis 2.1.1 and that W satisfies Hypothesis 2.1.3. Then $J_V(u)$ is well-defined for all u in $\mathcal{U}$. Moreover, if the decomposition $W = W_1 + W_2$ in Hypothesis 2.1.3 can be chosen such that*

$$\|W_2\|_{L^{3,\infty}} < C(1-a)$$

for some universal constant C, where a is as in Hypothesis 2.1.1, then

$$E_V := \inf_{u\in\mathcal{U}} J_V(u) > -\infty. \tag{2.80}$$

Proof. Combining (2.40)–(2.41) from Lemma 2.2.4 and (2.26) from Lemma 2.2.1, we deduce that, for u in $\mathcal{U}$,

$$J_V(u) \le \Big(1 + \frac{C\|W_2\|_{L^{3,\infty}}}{1-a}\Big)\langle u, H_V u\rangle + \Big(\|W_1\|_{L^1} + \frac{bC\|W_2\|_{L^{3,\infty}}}{1-a}\Big), \tag{2.81}$$

for some universal constant C, and

$$J_V(u) \ge \Big(1 - \frac{C\|W_2\|_{L^{3,\infty}}}{1-a}\Big)\langle u, H_V u\rangle - \Big(\|W_1\|_{L^1} + \frac{bC\|W_2\|_{L^{3,\infty}}}{1-a}\Big). \tag{2.82}$$

Therefore, assuming $C\|W_2\|_{L^{3,\infty}} < 1-a$, we deduce that (2.80) holds. □

Next we prove Proposition 2.3.2. Recall that $\mu_V = \inf\sigma(H_V)$. Below, if $\tilde V$ is another potential, we denote by $J_{\tilde V}$, $E_{\tilde V}$, $\mu_{\tilde V}$ the quantities obtained from J_V, E_V, μ_V by replacing V by $\tilde V$.

Proof of Proposition 2.3.2. Let $(u_j)_{j\in\mathbb{N}} \subset \mathcal{U}$ be a minimizing sequence for J_V, i.e.

$$J_V(u_j) \underset{j\to+\infty}{\longrightarrow} E_V.$$

The strategy consists in showing that $(u_j)_{j\in\mathbb{N}}$ converges strongly in $L^2(\mathbb{R}^3)$, along some subsequence, to a state u_∞ in $\mathcal{Q}_V$ which is then a minimizer for H_V. We divide the proof into several steps.

Step 1 : We prove that
$$E_V < E_{V_1}. \tag{2.83}$$
Let $\varepsilon > 0$. Let u_ε in $\mathcal{U}$ be such that $\langle u_\varepsilon, H_V u_\varepsilon\rangle \leq \mu_V + \varepsilon$. Applying (2.81), we obtain that
$$E_V \leq J_V(u_\varepsilon) \leq \Big(1 + \frac{C\|W_2\|_{L^{3,\infty}}}{1-a}\Big)(\mu_V + \varepsilon) + \|W_1\|_{L^1} + \frac{bC\|W_2\|_{L^{3,\infty}}}{1-a}.$$
Letting $\varepsilon \to 0$, this yields
$$E_V \leq \Big(1 + \frac{C\|W_2\|_{L^{3,\infty}}}{1-a}\Big)\mu_V + \|W_1\|_{L^1} + \frac{bC\|W_2\|_{L^{3,\infty}}}{1-a}. \tag{2.84}$$
On the other hand, for all u in $\mathcal{U}$, we can write, using (2.40), (2.41) and the fact that $V_1 \geq 0$,
$$\begin{aligned} J_{V_1}(u) &\geq \langle u, H_{V_1} u\rangle - \|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}}\|u\|^2_{\dot{H}_1} \\ &\geq \big(1 - C\|W_2\|_{L^{3,\infty}}\big)\mu_{V_1} - \|W_1\|_{L^1}, \end{aligned}$$
and hence
$$E_{V_1} \geq \big(1 - C\|W_2\|_{L^{3,\infty}}\big)\mu_{V_1} - \|W_1\|_{L^1}. \tag{2.85}$$
Combining (2.84) and (2.85) gives
$$\begin{aligned} E_{V_1} - E_V &\geq \big(1 - C\|W_2\|_{L^{3,\infty}}\big)\mu_{V_1} - \Big(1 + \frac{C\|W_2\|_{L^{3,\infty}}}{1-a}\Big)\mu_V - 2\|W_1\|_{L^1} - \frac{bC\|W_2\|_{L^{3,\infty}}}{1-a} \\ &= \big(1 - C\|W_2\|_{L^{3,\infty}}\big)(\mu_{V_1} - \mu_V) - 2\|W_1\|_{L^1} - C_V\|W_2\|_{L^{3,\infty}}, \end{aligned} \tag{2.86}$$
where we have set
$$C_V := C\frac{(2-a)\mu_V + b}{1-a}.$$
The right-hand-side of (2.86) is strictly positive since we assumed $C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a) \leq \frac{1}{2}$ and provided that
$$2\|W_1\|_{L^1} + C_V\|W_2\|_{L^{3,\infty}} < \frac{1}{4}(\mu_{V_1} - \mu_V).$$

Step 2 : We prove that for all u in $\mathcal{U}$,
$$J_V(u) \geq E_V + \big(E_{V_1} - E_V - 4\|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}}\|u\|^2_{H^1}\big)\|\tilde{\eta}_R u\|^2_{L^2} + o(R^0), \tag{2.87}$$
as $R \to \infty$, for some universal constant $C > 0$.

Recall that the localizations functions η_R, $\tilde{\eta}_R$ have been defined in (2.6). Writing the decomposition $u = \eta_R^2 u + \tilde{\eta}_R^2 u$ and commuting η_R, $\tilde{\eta}_R$ through $-\Delta$, we have by the IMS localization formula (see e.g. [36])
$$\langle u, H_V u\rangle = \langle \eta_R u, H_V \eta_R u\rangle + \langle \tilde{\eta}_R u, H_V \tilde{\eta}_R u\rangle - \frac{1}{2}\langle u, \big(|\nabla\eta_R|^2 + |\nabla\tilde{\eta}_R|^2\big)u\rangle. \tag{2.88}$$

The definitions of η_R, $\tilde{\eta}_R$ yield $\||\nabla\eta_R|^2\|_{L^\infty} = \mathcal{O}(R^{-2})$, $\||\nabla\tilde{\eta}_R|^2\|_{L^\infty} = \mathcal{O}(R^{-2})$. Moreover, since $V_2(x) \to 0$ as $|x| \to \infty$,

$$\langle \tilde{\eta}_R u, H_V \tilde{\eta}_R u\rangle = \langle \tilde{\eta}_R u, H_{V_1} \tilde{\eta}_R u\rangle + o(R^0)\|\tilde{\eta}_R u\|^2.$$

Inserting this into (2.88), we get

$$\langle u, H_V u\rangle = \langle \eta_R u, H_V \eta_R u\rangle + \langle \tilde{\eta}_R u, H_{V_1} \tilde{\eta}_R u\rangle + o(R^0). \tag{2.89}$$

Next we consider the convolution term in $J_V(u)$. We can write

$$\begin{aligned}
&\int_{\mathbb{R}^3} \big(w * |u|^2\big)(x)|u(x)|^2\,\mathrm{d}x \\
&\quad= \int_{\mathbb{R}^3} \big(w * |\eta_R u|^2\big)(x)|(\eta_R u)(x)|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} \big(w * |\tilde{\eta}_R u|^2\big)(x)|(\tilde{\eta}_R u)(x)|^2\,\mathrm{d}x \\
&\quad+ \int_{\mathbb{R}^3} \big(w * |\eta_R u|^2\big)(x)|(\tilde{\eta}_R u)(x)|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} \big(w * |\tilde{\eta}_R u|^2\big)(x)|(\eta_R u)(x)|^2\,\mathrm{d}x. \qquad (2.90)
\end{aligned}$$

We estimate the last two terms in the right-hand-side of the previous equation. Since W_1 is in $L^1(\mathbb{R}^3)$, using (2.40) yields

$$\begin{aligned}
&\Big|\int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W_1) * |\eta_R u|^2\big)(x)|(\tilde{\eta}_R u)(x)|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W_1) * |\tilde{\eta}_R u|^2\big)(x)|(\eta_R u)(x)|^2\,\mathrm{d}x\Big| \\
&\qquad\le 2\|W_1\|_{L^1}\|\eta_R u\|_{L^2}^2\|\tilde{\eta}_R u\|_{L^2}^2 \le 2\|W_1\|_{L^1}\|\tilde{\eta}_R u\|_{L^2}^2. \qquad (2.91)
\end{aligned}$$

Note that in the last inequality we used that $\|\eta_R u\|_{L^2} \le \|u\|_{L^2} = 1$. Next, since W_2 is in $L^{3,\infty}(\mathbb{R}^3)$, using (2.41) yields

$$\begin{aligned}
&\Big|\int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W_2) * |\eta_R u|^2\big)(x)|(\tilde{\eta}_R u)(x)|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} \big(\bar{\mathcal{F}}(W_2) * |\tilde{\eta}_R u|^2\big)(x)|(\eta_R u)(x)|^2\,\mathrm{d}x\Big| \\
&\qquad\le C\|W_2\|_{L^{3,\infty}}\|\eta_R u\|_{H_1}^2\|\tilde{\eta}_R u\|_{L^2}^2 \le C\|W_2\|_{L^{3,\infty}}\|u\|_{H^1}^2\|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0), \qquad (2.92)
\end{aligned}$$

where in the last inequality we used in addition that $\|\eta_R u\|_{H_1} \le \|u\|_{H^1} + o(R^0)$. Putting together (2.89), (2.90), (2.91) and (2.92), we arrive at

$$J_V(u) \ge J_V(\eta_R u) + J_{V_1}(\tilde{\eta}_R u) - \big(2\|W_1\|_{L^1} + C\|W_2\|_{L^{3,\infty}}\|u\|_{H^1}^2\big)\|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0). \tag{2.93}$$

Now, suppose that $\|\eta_R u\|_{L^2} \neq 0$. Then we can write

$$\begin{aligned}
J_V(\eta_R u) &= \Big\langle \frac{\eta_R u}{\|\eta_R u\|_{L^2}}, H_V \frac{\eta_R u}{\|\eta_R u\|_{L^2}}\Big\rangle \|\eta_R u\|_{L^2}^2 \\
&\quad- \int_{\mathbb{R}^3} \Big(w * \Big|\frac{\eta_R u}{\|\eta_R u\|_{L^2}}\Big|^2\Big)(x)\,\Big|\frac{\eta_R u}{\|\eta_R u\|_{L^2}}(x)\Big|^2\,\mathrm{d}x\,\|\eta_R u\|_{L^2}^4 \\
&= J_V\Big(\frac{\eta_R u}{\|\eta_R u\|_{L^2}}\Big)\|\eta_R u\|_{L^2}^2 \\
&\quad+ \int_{\mathbb{R}^3} \Big(w * \Big|\frac{\eta_R u}{\|\eta_R u\|_{L^2}}\Big|^2\Big)(x)\,\Big|\frac{\eta_R u}{\|\eta_R u\|_{L^2}}(x)\Big|^2\,\mathrm{d}x\,\|\eta_R u\|_{L^2}^2\,\|\tilde{\eta}_R u\|_{L^2}^2.
\end{aligned}$$

By definition of E_V, we have that $J_V(\eta_R u/\|\eta_R u\|_{L^2}) \geq E_V$. Estimating the integrated term as above, using (2.40), (2.41) and $\|\eta_R u\|_{H_1} \leq \|u\|_{H^1} + o(R^0)$, we then deduce that

$$J_V(\eta_R u) \geq E_V \|\eta_R u\|_{L^2}^2 - \big(\|W_1\|_{L^1} + C\|W_2\|_{L^{3,\infty}} \|u\|_{H^1}^2\big) \|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0). \tag{2.94}$$

Similar arguments show that, if $\|\tilde{\eta}_R u\| \neq 0$, then

$$\begin{aligned} &J_{V_1}(\bar{\eta}_R u) \\ &\quad \geq E_{V_1} \|\bar{\eta}_R u\|_{L^2}^2 - \big(\|W_1\|_{L^1} + C\|W_2\|_{L^{3,\infty}} \|u\|_{H^1}^2\big) \|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0) \\ &\quad = \big(E_{V_1} - E_V - \|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}} \|u\|_{H^1}^2\big) \|\tilde{\eta}_R u\|_{L^2}^2 + E_V \|\tilde{\eta}_R u\|_{L^2}^2 + o(R^0). \end{aligned} \tag{2.95}$$

We claim that (2.93), (2.94) and (2.95) imply (2.87). Indeed, if $\|\tilde{\eta}_R u\|_{L^2} = 0$, then $\|\eta_R u\|_{L^2} = 1$ and (2.87) follows from (2.93) and (2.94). If $\|\eta_R u\|_{L^2} = 0$, then $\|\tilde{\eta}_R u\|_{L^2} = 1$ and (2.87) follows from (2.93) and (2.95). Finally if both $\|\eta_R u\|_{L^2} \neq 0$ and $\|\tilde{\eta}_R u\|_{L^2} \neq 0$, then combining (2.93), (2.94) and (2.95) gives (2.87), since $\|\eta_R u\|_{L^2}^2 + \|\tilde{\eta}_R u\|_{L^2}^2 = 1$.

Step 3 : We prove that $(u_j)_{j\in\mathbb{N}}$ is bounded in $\mathcal{Q}_V$ (equipped with the norm defined in (2.8)), uniformly in W_2 such that $C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a)$, for some universal constant C.

It suffices to show that $(\langle u_j, -\Delta u_j\rangle + \langle u_j, V_+ u_j\rangle)_{j\in\mathbb{N}} = (\langle u_j, H_{V_+} u_j\rangle)_{j\in\mathbb{N}}$ is bounded. We proceed as in the proof of Lemma 2.5.1. We write

$$\langle u_j, H_{V_+} u_j\rangle = J_V(u_j) + \langle u_j, V_- u_j\rangle + \int_{\mathbb{R}^3} \big(w * |u_j|^2\big)(x) |u_j(x)|^2 \,\mathrm{d}x. \tag{2.96}$$

For the second term in the right-hand-side of the previous equation, we use Hypothesis 2.1.1, which implies that

$$\langle u_j, V_- u_j\rangle \leq a\langle u_j, H_{V_+} u_j\rangle + b\|u_j\|_{L^2}^2. \tag{2.97}$$

The third term of the right-hand-side of (2.96) can be estimated using (2.40) and (2.41), namely

$$\begin{aligned} \Big| \int_{\mathbb{R}^3} \big(w * |u_j|^2\big)(x) |u_j(x)|^2 \,\mathrm{d}x \Big| &\leq \|W_1\|_{L^1} \|u_j\|_{L^2}^4 + C\|W_2\|_{L^{3,\infty}} \|u_j\|_{H^1}^2 \|u_j\|_{L^2}^2 \\ &\leq \|W_1\|_{L^1} + C\|W_2\|_{L^{3,\infty}} \langle u_j, H_{V_+} u_j\rangle, \end{aligned} \tag{2.98}$$

since $\|u_j\|_{L^2} = 1$. Inserting (2.97)–(2.98) into (2.96), assuming that $C\|W_2\|_{L^{3,\infty}} < 1 - a$, we obtain

$$\langle u_j, H_{V_+} u_j\rangle \leq \frac{1}{1 - a - C\|W_2\|_{L^{3,\infty}}} \Big(J_V(u_j) + b + \|W_1\|_{L^1} \Big). \tag{2.99}$$

Since $(J_V(u_j))_{j\in\mathbb{N}}$ converges, it is bounded. This proves that $(u_j)_{j\in\mathbb{N}}$ is bounded in $\mathcal{Q}_V$. In turn, since we can assume without loss of generality that $J_V(u_j) \leq E_V + 1$ for all j, one easily concludes form the previous equation together with (2.84) that $(u_j)_{j\in\mathbb{N}}$ is bounded in $\mathcal{Q}_V$ uniformly in W_2 such that $C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a)$.

Step 4 : By Step 3, we know that $(u_j)_{j\in\mathbb{N}}$ is bounded in $\mathcal{Q}_V$. Hence there exists a subsequence, still denoted $(u_j)_{j\in\mathbb{N}}$, which converges weakly in $\mathcal{Q}_V$. Let $u_\infty \in \mathcal{Q}_V$ be its limit. In particular $u_j \to u_\infty$ weakly in $H^1(\mathbb{R}^3)$. We prove that $(u_j)_{j\in\mathbb{N}}$ converges strongly (along some subsequence) to u_∞ in $L^2(\mathbb{R}^3)$.

As in Step 2, we write, for $R > 0$,

$$\|u_j - u_\infty\|_{L^2}^2 = \|\eta_R(u_j - u_\infty)\|_{L^2}^2 + \|\tilde{\eta}_R(u_j - u_\infty)\|_{L^2}^2. \tag{2.100}$$

Consider first the term $\|\tilde{\eta}_R(u_j - u_\infty)\|_{L^2}^2$. Let $\varepsilon > 0$. It follows from Step 2 that there exists $R_0 > 0$ such that, for $R \geq R_0$,

$$\|\tilde{\eta}_R u_j\|_{L^2}^2 \leq \frac{J_V(u_j) - E_V}{E_{V_1} - E_V - 4\|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}}\|u_j\|_{H^1}^2} + \varepsilon. \tag{2.101}$$

Here it should be noted that the term $E_{V_1} - E_V - 4\|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}}\|u_j\|_{H^1}^2$ is strictly positive. Indeed, we know from Step 3 that $(\|u_j\|_{H^1})_{j\in\mathbb{N}}$ is bounded uniformly in W_2 such that $C\|W_2\|_{L^{3,\infty}} \leq \frac{1}{2}(1-a)$. Together with (2.86), this shows that

$$E_{V_1} - E_V - 4\|W_1\|_{L^1} - C\|W_2\|_{L^{3,\infty}}\|u_j\|_{H^1}^2 \geq \frac{1}{2}(\mu_{V_1} - \mu_V) - 6\|W_1\|_{L^1} - (C + C_V)\|W_2\|_{L^{3,\infty}},$$

By the assumption (2.20), the right-hand-side of the previous equation is strictly positive. Returning now to (2.101), using in addition that $J_V(u_j) \to E_V$, we deduce that there exists j_0 in $\mathbb{N}$ such that, for all $j \geq j_0$ (and $R \geq R_0$),

$$\|\tilde{\eta}_R u_j\|_{L^2}^2 \leq 2\varepsilon. \tag{2.102}$$

Using the lower semi-continuity of $\|\cdot\|_{L^2}$, we also obtain that, for $R \geq R_0$,

$$\|\tilde{\eta}_R u_\infty\|_{L^2}^2 \leq \liminf_{j\to\infty} \|\tilde{\eta}_R u_j\|_{L^2}^2 \leq 2\varepsilon. \tag{2.103}$$

Now fix $R_0 > 0$ such that (2.102)–(2.103) hold and consider the term $\|\eta_{R_0}(u_j - u_\infty)\|_{L^2}^2$ from (2.100). Clearly, since $(u_j)_{j\in\mathbb{N}}$ converges weakly to u_∞ in $H^1(\mathbb{R}^3)$, it follows that $(\eta_{R_0}u_j)_{j\in\mathbb{N}}$ converges weakly to $\eta_{R_0}u_\infty$ in $H^1(B_{2R_0})$, where $B_{2R_0} = \{x \in \mathbb{R}^3 \,|\, |x| \leq 2R_0\}$. The Rellich-Kondrachov Theorem then gives the existence of a subsequence, still denoted by $(\eta_{R_0}u_j)_{j\in\mathbb{N}}$, which converges strongly to $\eta_{R_0}u_\infty$ in $L^2(B_{2R_0})$. We can then conclude that there exists an integer $j_1 \geq j_0$, such that, for all $j \geq j_1$,

$$\|u_j - u_\infty\|_{L^2}^2 = \|\eta_{R_0}(u_j - u_\infty)\|_{L^2}^2 + \|\tilde{\eta}_{R_0}(u_j - u_\infty)\|_{L^2}^2 \leq \varepsilon + 8\varepsilon. \tag{2.104}$$

Hence $(u_j)_{j\in\mathbb{N}}$ converges strongly to u_∞ in $L^2(\mathbb{R}^3)$.

Step 5 : We prove that u_∞ is a minimizer for J_V.

Obviously, since $u_j \to u_\infty$ strongly in $L^2(\mathbb{R}^3)$, we have that $\|u_\infty\|_{L^2} = 1$. Moreover, we clearly have

$$E_V \leq J_V(u_\infty).$$

Hence it remains to show that $J_V(u_\infty) \leq E_V$.

Recall that

$$J_V(u_\infty) = \langle u_\infty, (-\Delta + V)u_\infty\rangle - \int_{\mathbb{R}^3} \big(w * |u_\infty|^2\big)(x)|u_\infty(x)|^2 \, \mathrm{d}x. \tag{2.105}$$

By Step 3, (u_j) is bounded in $H^1(\mathbb{R}^3)$ and by Step 4, (u_j) converges strongly to u_∞ in $L^2(\mathbb{R}^3)$. Hence Lemma 2.2.3 yields

$$\langle u_\infty, (-\Delta + V)u_\infty\rangle \leq \liminf_{j\to\infty} \langle u_j, (-\Delta + V)u_j\rangle \,.$$

It remains to consider the quartic term in (2.105). As in (2.40)–(2.41), we have

$$\begin{aligned}
&\Big| \int_{\mathbb{R}^3} \big(w * |u_j|^2\big)(x)|u_j(x)|^2 \, \mathrm{d}x - \int_{\mathbb{R}^3} \big(w * |u_\infty|^2\big)(x)|u_\infty(x)|^2 \, \mathrm{d}x \Big| \\
&\quad = \Big| \int_{\mathbb{R}^3} \big(w * (|u_j|^2 - |u_\infty|^2)\big)(x)|u_j(x)|^2 \, \mathrm{d}x + \int_{\mathbb{R}^3} \big(w * |u_\infty|^2\big)(x)(|u_j(x)|^2 - |u_\infty(x)|^2 \, \mathrm{d}x \Big| \\
&\quad \lesssim \big(\|W_1\|_{L^1} + \|W_2\|_{L^{3,\infty}}\big)\big(\|u_j\|_{H^1}^2 + \|u_\infty\|_{H^1}^2\big) \big\| |u_j|^2 - |u_\infty|^2 \big\|_{L^1} \\
&\quad \lesssim \big(\|W_1\|_{L^1} + \|W_2\|_{L^{3,\infty}}\big)\big(\|u_j\|_{H^1}^2 + \|u_\infty\|_{H^1}^2\big) \|u_j + u_\infty\|_{L^2} \|u_j - u_\infty\|_{L^2} \\
&\quad \lesssim \big(\|W_1\|_{L^1} + \|W_2\|_{L^{3,\infty}}\big) \|u_j - u_\infty\|_{L^2},
\end{aligned}$$

where we used in the last inequality that $\|u_j\|_{L^2} = 1$ and that $(u_j)_{j\in\mathbb{N}}$ is bounded in $H^1(\mathbb{R}^3)$. Since $u_j \to u_\infty$ strongly in $L^2(\mathbb{R}^3)$, this yields

$$\int_{\mathbb{R}^3} \big(w * |u_\infty|^2\big)(x) \, |u_\infty(x)|^2 \, \mathrm{d}x = \lim_{j\to\infty} \int_{\mathbb{R}^3} \big(w * |u_j|^2\big)(x) \, |u_j(x)|^2 \, \mathrm{d}x. \tag{2.106}$$

Inserting (2.30), (2.31), (2.32) and (2.106) into (2.105), we finally obtain that

$$J_V(u_\infty) \leq \liminf_{j\to\infty} J_V(u_j) = E_V.$$

This concludes the proof of the proposition. □

Chapitre 3

Standard Model of Non-Relativistic Quantum Electrodynamics

Abstract. We consider a non-relativistic electron bound by an external potential and coupled to the quantized electromagnetic field in the standard model of non-relativistic QED. We compute the energy functional of product states of the form $u \otimes \Psi_f$, where u is a normalized state for the electron and Ψ_f is a coherent state in Fock space for the photon field. The minimization of this functional yields a Maxwell–Schrödinger system up to a trivial renormalization. We prove the existence of a ground state under general conditions on the external potential and the coupling. In particular, neither an ultraviolet cutoff nor an infrared cutoff needs to be imposed. Our results provide the convergence in the ultraviolet limit and the second-order asymptotic expansion in the coupling constant of the ground state energy of Maxwell–Schrödinger systems.

3.1 Introduction

We consider in this paper a non-relativistic spin-$\frac{1}{2}$ particle (an electron) minimally coupled to the quantized radiation field in the standard model of non-relativistic quantum electrodynamics, with an external potential V. This physical system is mathematically described by a Pauli-Fierz Hamiltonian $\mathbb{H}$, introduced in [104], whose spectral and scattering theories have been thoroughly studied since the end of the nineties (see, among others, [6, 11, 12, 40, 53, 62, 63, 71, 110, 111] and references therein). To be well-defined, the Pauli-Fierz Hamiltonian $\mathbb{H}$ requires an unphysical regularization : the interaction term comes with an ultraviolet cutoff. Finding a renormalization procedure leading to the definition of the model in the ultraviolet limit remains an important open problem.

Restricting the energy functional associated to $\mathbb{H}$ to well-chosen classes of states allows one to study the energy and its infimum more easily. In the translation invariant case ($V = 0$), considering the set of general product states $u \otimes \Psi$ where the state u of the electron is a unit vector in the Hilbert space $\mathcal{H}_{\text{el}} = L^2(\mathbb{R}^3; \mathbb{C}^2)$ and the state Ψ of the photon field is a unit vector in Fock space, the ultraviolet divergence of the infimum of the energy functional $\langle(u \otimes \Psi), \mathbb{H}(u \otimes \Psi)\rangle$ has been studied by Lieb and Loss in [87], and by Bach and Hach in [13]. Denoting by Λ the ultraviolet parameter associated to the ultraviolet cutoff introduced into the interaction Hamiltonian, it is shown in [13, 87] that the corresponding ground state energy diverges as $\Lambda^{12/7}$ in the ultraviolet limit. Also in the translation invariant case, at a fixed total momentum, the existence and uniqueness of a minimizer of the energy functional over coherent or quasifree states has been studied in [9].

Product states of the form $u \otimes \Psi_{\vec{f}}$, with $\Psi_{\vec{f}}$ a coherent state parametrized by vectors $\vec{f}$ in the one-particle Hilbert space $\mathfrak{h}$ for the field, have been considered in [31, 33–35]. The energy functional

$$(u, \vec{f}) \mapsto \langle(u \otimes \Psi_{\vec{f}}), \mathbb{H}(u \otimes \Psi_{\vec{f}})\rangle \tag{3.1}$$

is then called the *quasi-classical energy*. Indeed, assuming that the field degrees of freedom are 'almost classical', in the sense that the creation and annihilation operators a^*, a are rescaled as $a^*_\varepsilon = \sqrt{\varepsilon} a^*$, $a_\varepsilon = \sqrt{\varepsilon} a$ (see also [5]), it is shown in [31, 33–35], under suitable assumptions, that the ground state energy of the rescaled Pauli-Fierz Hamiltonian $\mathbb{H}_\varepsilon$ converges to the infimum of the quasi-classical energy functional as $\varepsilon \to 0$.

In this paper, we also consider the quasi-classical energy functional (3.1). Up to a trivial renormalization, we will see that minimizing (3.1) boils down to minimizing $\mathcal{E}_V(u, \vec{A}_{\vec{f}})$, for some $\vec{f}$-dependent magnetic potential $\vec{A}_{\vec{f}}$, where $\mathcal{E}_V(u, \vec{A})$ is the Maxwell-Schrödinger energy in the Coulomb gauge, given by

$$\mathcal{E}_V(u, \vec{A}) = \|\vec{\sigma} \cdot (-i\vec{\nabla} - g\hat{\chi} * \vec{A})\, u\|^2_{L^2} + \langle u, Vu\rangle_{L^2} + \frac{1}{32\pi^3}\|\vec{A}\|^2_{\dot{H}^1}\,. \tag{3.2}$$

Here $\vec{\sigma}$ is the vector of Pauli matrices, g is a coupling constant and χ a coupling function. The coefficient $(32\pi^3)^{-1}$ comes from our choice of normalization of the Fourier transform, see below. We use a similar notation when V is replaced by other potentials.

For a general class of external potentials V (including both binding and confining potentials) and coupling functions χ, we prove the existence of a ground state for $\mathcal{E}_V$. In particular, neither an infrared nor an ultraviolet cutoff is needed in the interaction term of the energy. Furthermore, if an ultraviolet cutoff of parameter Λ is imposed, our results show that the ground state energy converges in $\mathbb{R}$, as $\Lambda \to \infty$.

To prove the existence of a quasi-classical ground state, we follow the usual strategy of the calculus of variations. The main difficulty comes from the possible absence of an ultraviolet cutoff. This induces singular terms with a critical behavior in the energy functional that we handle using suitable estimates in Lorentz spaces. Note that Kramers' symmetry of the Maxwell-Schrödinger energy functional implies that the minimizer is not unique (even up to a phase in u).

In [50], Fröhlich, Lieb and Loss studied the minimization problem of similar energy functionals. Compared to [50], our results provide the existence of a ground state for large classes of external potentials and coupling terms, and allow us to pass to the ultraviolet limit. Moreover, we compute the second order asymptotic expansion at small coupling of the ground state energy.

In the companion paper [26], we study the same problem in the case of a spinless, non-relativistic particle linearly coupled to a scalar, quantized radiation field. Although the overall strategies in [26] and the present paper are similar, the arguments used in the proofs are significantly different. In particular, in the case of linear coupling, an easy argument shows that the minimization of the quasi-classical ground state energy reduces to the minimization of the Hartree energy (over the state u of the non-relativistic particle). In the present context such a simplification does not occur : We have to minimize (3.2) over $(u, \vec{A})$ in suitable spaces, with the constraint $\|u\|_{L^2} = 1$ for the electron state and no constraint on the divergence-free vector potential $\vec{A}$ in $\dot{H}^1$. Note however that some technical results concerning the electronic Hamiltonian are used both in [26] and in this paper. They are stated here without proof.

We have focused in this work on the static problem, but the dynamical version, the Maxwell–Schrödinger equations, has of course been also largely studied in the literature. In particular, the Maxwell–Schrödinger equations have been derived in [100], where results on the existence of solutions have been proven. The dynamics of the Maxwell–Schrödinger equations has been further studied in [18, 19, 30, 57, 66, 79, 94, 97, 101, 109, 112, 113]. In relation with many-body systems, the Maxwell–Schrödinger equations have been obtained from many-body dynamics in [84], see also [35].

Notations. We recall that for $1 \leq p < \infty$, the Lorentz spaces (or weak L^p spaces) $L^{p,\infty}(\mathbb{R}^3)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^3 \to \mathbb{C}$ such that

$$\|f\|_{L^{p,\infty}} := \sup_{t>0} \lambda\big(\{|f| > t\}\big)^{\frac{1}{p}} t, \tag{3.3}$$

is finite, where λ denotes Lebesgue's measure.

The Fourier transform acting on tempered distribution is denoted by $\mathcal{F}$, its inverse being given by $(2\pi)^{-3}\bar{\mathcal{F}}$. (We use the normalization $\mathcal{F}(f)(x) = \int_{\mathbb{R}^3} e^{-ix\cdot\xi} f(\xi)\,\mathrm{d}\xi$ for f in $L^1(\mathbb{R}^3)$, and hence $\bar{\mathcal{F}}(f)(x) = \int_{\mathbb{R}^3} e^{ix\cdot\xi} f(\xi)\,\mathrm{d}\xi$. This normalization is not the standard one but it will be convenient in our context.) Throughout the paper, we use the following convention about the convolution product. Let f and g be functions associated to tempered distributions. Assume that $\mathcal{F}(g)$ identifies with a function such that $f\mathcal{F}(g)$ can be associated to a tempered distribution. We write

$$\mathcal{F}(f) * g := (2\pi)^{-3}\mathcal{F}(f\bar{\mathcal{F}}(g)). \tag{3.4}$$

This convention is convenient in our context. It extends the well-known equality which holds e.g. if f and g are in L^1 or f is in L^2 and g in L^1.

In several places, we use localization functions η and $\tilde{\eta}$ in $\mathrm{C}^\infty(\mathbb{R}^3)$ such that $\eta(x) = 1$ if $|x| \leq 1$, $\eta(x) = 0$ if $|x| \geq 2$ and

$$\eta^2 + \tilde{\eta}^2 = 1\,.$$

For all $R > 0$, we set

$$\eta_R(x) := \eta(x/R) \quad \text{and} \quad \tilde{\eta}_R(x) := \tilde{\eta}(x/R)\,. \tag{3.5}$$

If $\mathcal{H}_1$, $\mathcal{H}_2$ are two Hilbert spaces, $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ stands for the set of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. Given a linear operator A on a Hilbert space $\mathcal{H}$, we denote by $\mathcal{D}(A)$ its domain and $\mathcal{Q}(A)$ its form domain. The topological dual of a Banach space $\mathcal{B}$ is denoted by $\mathcal{B}^*$.

3.1.1 The electronic Hamiltonian

If the coupling between the electron and the photon field is turned out, the free Hamiltonian for the electron is of the form

$$\begin{pmatrix} H_V & 0 \\ 0 & H_V \end{pmatrix} \quad \text{on} \quad \mathcal{H}_{\text{el}} := L^2(\mathbb{R}^3;\mathbb{C}^2) = L^2(\mathbb{R}^3;\mathbb{C}) \oplus L^2(\mathbb{R}^3;\mathbb{C}),$$

where

$$H_V := -\Delta + V(x) \tag{3.6}$$

is defined on a domain contained in $L^2(\mathbb{R}^3;\mathbb{C})$. Here $V : \mathbb{R}^3 \to \mathbb{R}$ is the external potential. We display the dependence on V since one of our main hypotheses (see Hypothesis 3.1.1) assumes the existence of a decomposition $V = V_1 + V_2$ such that $V_1 \geq 0$, V_2 vanishes at ∞ and there is a gap between the ground state energies of H_V and H_{V_1}.

The main examples we have in mind are confining potentials, $V(x) \to \infty$ as $|x| \to \infty$, and Coulomb-type potentials, $V(x) = -c|x|^{-1}$ with $c > 0$. We introduce general hypotheses on V that are fulfilled by a large class of potentials, including the two preceding examples. As we will see below, some of our main results have interesting consequences in special cases, especially when V is confining.

We set

$$\mu_V := \inf \sigma(H_V),$$

and likewise if V is replaced by another potential. The positive and negative parts of V are denoted, respectively, by

$$V_+ := \max(V, 0) \quad \text{and} \quad V_- := \max(-V, 0),$$

so that $V = V_+ - V_-$.

We make the following hypothesis.

Hypothesis 3.1.1 (Conditions on V)**.** *The potential V satisfies $V(x) = V(-x)$ for all x in $\mathbb{R}^3$ and there exist $a \geq 0$ and b in $\mathbb{R}$ such that*

$$V_- \leq a\sqrt{-\Delta} + b$$

in the sense of quadratic forms on $H^{1/2}(\mathbb{R}^3)$. Moreover, V decomposes as $V = V_1 + V_2$ with

(i) $V_1 \in L^1_{\text{loc}}(\mathbb{R}^3;\mathbb{R}^+)$,

(ii) $V_2 \in L^{3/2}_{\text{loc}}(\mathbb{R}^3;\mathbb{R})$ *and* $\lim_{|x|\to\infty} V_2(x) = 0$.

Since $V_+ \geq 0$, $H_{V_+} = -\Delta + V_+$ identifies with a non-negative self-adjoint operator on $L^2(\mathbb{R}^3)$ with form domain

$$\mathcal{Q}(H_{V_+}) = \mathcal{Q}(-\Delta) \cap \mathcal{Q}(V_+) = \Big\{ u \in H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} V_+(x)|u(x)|^2 \,\mathrm{d}x < +\infty \Big\}.$$

Moreover, it follows from Hypothesis 3.1.1 that H_V identifies with a semi-bounded self-adjoint operator with form domain $\mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1})$. In particular, μ_V and μ_{V_1} are well-defined. See Section 3.2.1 for justifications.

The state of the electron is represented by a unit vector in the space $L^2(\mathbb{R}^3; \mathbb{C}^2)$. We set

$$\mathcal{Q}_V := \mathcal{Q}(H_V) \otimes \mathbb{C}^2\,, \tag{3.7}$$

and note that $\mathcal{Q}_V$ is a Hilbert space for the norm

$$\|u\|^2_{\mathcal{Q}_V} := \|u\|^2_{H^1} + \big\|(V_+)^{\frac{1}{2}} \otimes \mathbf{I}_{\mathbb{C}^2}\, u\big\|^2_{L^2}\,.$$

We will most of the time consider an electron state u in

$$\mathcal{U} := \{ u \in \mathcal{Q}_V \mid \|u\|_{L^2} = 1 \}\,. \tag{3.8}$$

Finally, in order to obtain the asymptotic expansion of the infimum of the Maxwell-Schrödinger energy functional with respect to the coupling constant, we will require that H_V has a unique ground state. By Perron-Frobenius arguments, it is well-known that, under suitable conditions on V, if μ_V is an eigenvalue of H_V then it is simple and there exists a corresponding strictly positive eigenstate (see e.g. [107, Theorems XIII.46 and XIII.48]). We will make the following related hypothesis.

Hypothesis 3.1.2 (Ground state of H_V)**.** *The ground state energy μ_V of $H_V = -\Delta + V$ is a simple isolated eigenvalue associated to a unique positive ground state u_V belonging to $L^2(\mathbb{R}^3; \mathbb{R}_+)$ and such that $\|u_V\|_{L^2} = 1$.*

The orthogonal projection onto the vector space spanned by $\binom{u_V}{0}$ and $\binom{0}{u_V}$ in $L^2(\mathbb{R}^3; \mathbb{C}^2)$ is denoted by Π_V. We also set $\Pi_V^\perp := \mathbf{I}_{L^2(\mathbb{R}^3;\mathbb{C}^2)} - \Pi_V$.

3.1.2 Standard model of non-relativistic QED

In the standard model of non-relativistic QED, the quantized electromagnetic field is represented by a vector-valued bosonic field whose Hilbert space is given by the symmetric Fock space

$$\mathcal{H}_{\mathrm{f}} := \mathfrak{F}_s(L^2_\perp(\mathbb{R}^3; \mathbb{C}^3)) = \bigoplus_{n=0}^{+\infty} \bigvee^n L^2_\perp(\mathbb{R}^3; \mathbb{C}^3)\,,$$

where $L^2_\perp(\mathbb{R}^3; \mathbb{C}^3) = \{ \vec{f} \in L^2(\mathbb{R}^3; \mathbb{C}^3) \mid \forall k \in \mathbb{R}^3, k \cdot \vec{f}(k) = 0 \}$. The free field Hamiltonian in momentum representation is the second quantization of the multiplication operator by the euclidean norm of k,

$$\mathbb{H}_{\mathrm{f}} := \mathrm{d}\Gamma(|k|)\,.$$

The kinetic energy of the electron minimally coupled to the field is given by the following expression, which is quadratic in the creation and annihilation operators,

$$\Big(\vec{\sigma} \cdot \big(- i\vec{\nabla}_x \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} - \vec{\mathbb{A}}(\vec{m}_x)\big)\Big)^2 ,$$

where

$$\vec{\mathbb{A}}(\vec{m}_x) := (a(\vec{m}_{x,j}) + a^*(\vec{m}_{x,j}))_{1\le j\le 3}$$

has three components, corresponding to the three components for $1 \le j \le 3$ of the coupling functions

$$\vec{m}_{x,j}(k,\tau) := g\frac{\chi(k)}{|k|^{1/2}} e^{-ik\cdot x}\vec{\varepsilon}_{\tau,j}(k) ,$$

and the Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The coupling functions are defined using a family $(\vec{\varepsilon}_\tau(k))_{\tau\in\{1,2,3\}}$ of polarization vectors, i.e. orthonormal bases of $\mathbb{R}^3$ depending on k in $\mathbb{R}^3 \setminus \{\vec{0}\}$ and such that $\vec{\varepsilon}_3(k) = k/|k|$, a coupling constant g in $\mathbb{R}$ and an ultraviolet cutoff function χ such that $\chi/|k|^{1/2}$ and $\chi/|k|$ are both in $L^2(\mathbb{R}^3)$. Note, though, that these conditions on χ will be relaxed to some extent in our study of the Maxwell–Schrödinger functional.

The Pauli-Fierz Hamiltonian of the standard model of non-relativistic QED is given by

$$\begin{aligned}\mathbb{H} :=& \Big(\vec{\sigma} \cdot \big(- i\vec{\nabla}_x \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} - \vec{\mathbb{A}}(\vec{m}_x)\big)\Big)^2 + V \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} \\ =& \big(- i\vec{\nabla}_x \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} - \vec{\mathbb{A}}(\vec{m}_x)\big)^2 - \vec{\sigma}\cdot \sqrt{2}\Phi(\vec{\nabla}_x \wedge \vec{m}_x) + V \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} ,\end{aligned} \tag{3.9}$$

where the normalization of the field operator is given in the Appendix, see (3.71). The operator $\mathbb{H}$ on $\mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}^3;\mathbb{C}) \otimes \mathbb{C}^2 \otimes \mathcal{H}_{\mathrm{f}}$ identifies with a self-adjoint operator with form domain

$$\mathcal{Q}(\mathbb{H}) := \mathcal{Q}(\mathbb{H}_{\mathrm{free}}), \quad \mathbb{H}_{\mathrm{free}} := H_V \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}} , \tag{3.10}$$

see Appendix 3.4, where H_V is defined in (3.6). Under suitable assumptions on V and χ, one can actually check that $\mathcal{D}(\mathbb{H}) := \mathcal{D}(\mathbb{H}_{\mathrm{free}})$, see [70, 75].

3.1.3 The Maxwell–Schrödinger energy functional

We take u in $\mathcal{U}$ and consider a coherent state

$$\Psi_{\vec{f}} = e^{i\Phi(\frac{\sqrt{2}}{i}\vec{f})}\Omega \in \mathcal{H}_{\mathrm{f}}$$

with parameter $\vec{f}$ in $L^2_\perp(\mathbb{R}^3;\mathbb{C}^3) \cap \mathcal{Z}$. Here

$$\mathcal{Z} := \left\{ \vec{f}(k) = \sum_{1\le\tau\le 2} f_\tau(k)\vec{\varepsilon}_\tau(k) \;\middle|\; k \mapsto |k|^{1/2}\,\vec{f}(k) \in L^2(\mathbb{R}^3, \mathrm{d}k) \right\} . \tag{3.11}$$

A direct computation (see Section 3.3.1) yields the following formula for the energy of the product state $u \otimes \Psi_{\vec{f}}$ assuming that $\chi(-k) = \overline{\chi(k)}$:

$$\big\langle (u \otimes \Psi_{\vec{f}}), \mathbb{H}(u \otimes \Psi_{\vec{f}}) \big\rangle_{\mathcal{H}} = 2g^2 \| |k|^{-1/2} \chi(k) \|_{L^2}^2 + \big\langle \vec{f}_-, |k| \vec{f}_- \big\rangle_{L^2} + \mathcal{E}_V(u, \vec{A}_{\vec{f}}), \tag{3.12}$$

where $\mathcal{E}_V$ is defined by (3.2),

$$\vec{A}_{\vec{f}} := 2\mathcal{F}(\overline{\vec{f}_+(k)}|k|^{-1/2}) , \tag{3.13}$$

and we have set $\vec{f}_+(k) := \frac{1}{2}(\vec{f}(k) + \overline{\vec{f}(-k)})$, $\vec{f}_-(k) := \frac{1}{2}(\vec{f}(k) - \overline{\vec{f}(-k)})$. Note that

$$\mathcal{E}_V(u, \vec{A}) = \| (-i\vec{\nabla} - g\hat{\chi} * \vec{A})\, u \|_{L^2}^2 + \langle u, (V - g\hat{\chi} * \vec{\sigma} \cdot \vec{B}) u \rangle_{L^2} + \frac{1}{32\pi^3} \| \vec{A} \|_{\dot{H}^1}^2, \tag{3.14}$$

with $\vec{B} = \vec{\nabla} \wedge \vec{A}$. We thus obtain the stationary Maxwell–Schrödinger energy functional in the Coulomb gauge introduced in [100], which we refer to as the Maxwell–Schrödinger energy functional.

If $V(x) = V(-x)$, this energy functional is invariant under Kramers' symmetry,

$$\mathcal{E}_V(\nu u, \vec{A}(-\cdot)) = \mathcal{E}_V(u, \vec{A}), \tag{3.15}$$

where $\nu u\,(x) = \sigma_2 \overline{u(-x)}$, see [96]. Hence, in general, we can only hope for uniqueness of the minimizer modulo this symmetry.

As we will see in Section 3.3, the Maxwell–Schrödinger energy functional is well-defined when $(u, \vec{A})$ belongs to $\mathcal{U} \times \mathcal{A}$, where

$$\mathcal{A} := \{ \vec{A} \in \dot{H}^1(\mathbb{R}^3; \mathbb{R}^3) \mid \vec{\nabla} \cdot \vec{A} = 0 \} \tag{3.16}$$

and χ satisfies the following assumption :

Hypothesis 3.1.3 (Conditions on χ)**.** *The cutoff function $\chi : \mathbb{R}^3 \to \mathbb{R}$ satisfies $\chi(-k) = \chi(k)$ for all k in $\mathbb{R}^3$ and*

$$\frac{\chi}{|k|} \in L^2(\mathbb{R}^3) + L^{3,\infty}(\mathbb{R}^3) .$$

Remark 3.1.1. *At the expense of slightly more involved expressions in some places, our main results below hold under the more general assumption that χ is complex-valued and satisfies $\chi(-k) = \overline{\chi(k)}$ for all k in $\mathbb{R}^3$.*

The main quantity studied in this paper is

$$E_V := \inf_{\mathcal{V} \times \mathcal{A}} \mathcal{E}_V ,$$

with V a potential satisfying Hypothesis 3.1.1. We use a similar notation when V is replaced by another potential.

3.1.4 Main results

We begin with the following proposition which relates minimizers of the Maxwell–Schrödinger energy functional to minimizers of the energy of product states $u \otimes \Psi_{\vec{f}}$ in the standard model of non-relativistic QED.

Proposition 3.1.2. *Suppose that V satisfies Hypothesis 3.1.1 and that χ satisfies Hypothesis 3.1.3. If $(u_{\rm gs}, \vec{A}_{\rm gs})$ is a global minimizer of $\mathcal{E}_V$ over $\mathcal{U} \times \mathcal{A}$, then there exists $\vec{f}_{\rm gs}$ in $L^2_\perp(\mathbb{R}^3; \mathbb{C}^3) \cap \mathcal{Z}$ such that $\vec{A}_{\rm gs} = \vec{A}_{\vec{f}_{\rm gs}}$ in the sense of (3.13).*

This result shows that, up to the trivial renormalization consisting in removing the χ-dependent constant obtained from normal-ordering the Hamiltonian $\mathbb{H}$, the minimizers of the energy of product states $u \otimes \Psi_{\vec{f}}$ in the standard model of non-relativistic QED can be computed *via* the Maxwell–Schrödinger energy functional. More precisely,

$$\min_{(u,\vec{f}) \in \mathcal{U} \times (L^2_\perp \cap \mathcal{Z})} \big\langle (u \otimes \Psi_{\vec{f}}), \mathbb{H}(u \otimes \Psi_{\vec{f}}) \big\rangle - 2g^2 \Big\| \frac{\chi(k)}{\sqrt{|k|}} \Big\|^2_{L^2} = \min_{(u,\vec{A}) \in \mathcal{U} \times \mathcal{A}} \mathcal{E}_V(u, \vec{A}), \tag{3.17}$$

the minimizers in both sides of the equality (if they exist) being related as in (3.13). Note that for any minimizer of the functional on the left hand side, $\vec{f}_-$ vanishes by (3.12), and the map $\vec{f} \mapsto \vec{A}_{\vec{f}}$ is one to one from the set of vectors $\vec{f}$ in $\mathcal{Z}$ such that $\vec{f} = \vec{f}_+$ to the set of vectors $\vec{A}$ in $\mathcal{A}$.

Our main result concerning the existence of a minimizer for $\mathcal{E}_V$ is the following.

Theorem 3.1.3 (Existence of a ground state for Maxwell–Schrödinger)**.** *Suppose that V satisfies Hypothesis 3.1.1 and that $\chi = \chi_1 + \chi_2$ satisfies Hypothesis 3.1.3 with $\chi_1/|k|$ in L^2 and $\chi_2/|k|$ in $L^{3,\infty}$. Suppose that the decomposition $V = V_1 + V_2$ of Hypothesis 3.1.1 can be chosen such that $E_{V_1} > E_V$. With the constant $a \geq 0$ from Hypothesis 3.1.1 and some universal constant $C > 0$ (see Lemma 3.2.4), if*

$$32\pi^3 a C^2 g^2 \Big\| \frac{\chi_2}{|k|} \Big\|^2_{L^{3,\infty}} < 1\,, \tag{3.18}$$

then the Maxwell–Schrödinger energy functional $\mathcal{E}_V$ admits a minimizer $(u_{\rm gs}, \vec{A}_{\rm gs})$ in $\mathcal{U} \times \mathcal{A}$.

Remark 3.1.4. *For $|g|\, \|\chi_2/|k|\|_{L^{3,\infty}}$ sufficiently small, the existence of a ground state holds without assuming the presence of an ultraviolet cutoff. The case $\chi = 1$ is indeed covered by the previous theorem, since $1/|k|$ belongs to $L^{3,\infty}$.*

Remark 3.1.5. *The smallness condition (3.18) only concerns the critical part χ_2 such that $\chi_2/|k|$ belongs to $L^{3,\infty}$. We do not require any restriction on $\|\chi_1/|k|\|_{L^2}$.*

Remark 3.1.6. *The condition $E_{V_1} > E_V$ is verified in many cases of interest :*

- *For potentials V such that $\mu_V < 0$ (e.g. if V is a negative Coulomb potential), one has $E_V \leq \mu_V < 0 \leq E_{V_1}$.*

— *For confining potentials (i.e. such that $V(x) \to \infty$ as $|x| \to \infty$), Lemma 3.2.2 and Proposition 3.3.6 imply that there always exists a decomposition $V = V_1 + V_2$ such that $E_V < E_{V_1}$.*

— *Assuming the 'binding' condition $\mu_{V_1} > \mu_V$ and that $|g| \| \frac{\chi}{|k|} \|_{L^2+L^{\infty,3}} \le C_V$ with C_V small enough, Proposition 3.3.6 implies that $E_{V_1} > E_V$.*

Remark 3.1.7. *If one considers a spinless particle instead of an electron, then the previous theorem becomes trivial. Indeed, using the diamagnetic inequality, it is not difficult to verify that the Maxwell–Schrödinger energy of a spinless particle reaches its minimum when $\vec{A} = 0$. On the contrary, Proposition 3.1.9 below shows that the minimizer of the Maxwell–Schrödinger energy for a spin-$\frac{1}{2}$ electron is not trivial in general.*

Remark 3.1.8. *If $(u, \vec{A})$ is a minimizer of the Maxwell-Schrödinger energy functional $\mathcal{E}_V$, then, by Kramers' symmetry (3.15), $(\nu u, \vec{A}(-\cdot))$ is another minimizer of $\mathcal{E}_V$, different from the first one since $\nu u \perp u$. We conjecture that, generically, for $g > 0$ sufficiently small, there are exactly two minimizers for $\mathcal{E}_V$, up to the phase symmetry with respect to u. Note that if V is radially symmetric, then $\mathcal{E}_V$ is also rotation invariant and the system has a* $\mathrm{U}(1) \times \mathrm{SU}(2)$ *local gauge symmetry, see, e.g., [51] and there will be more minimizers.*

To prove Theorem 3.1.3 we apply the usual strategy from the calculus of variations [92, 93], considering a minimizing sequence $(u_j, \vec{A}_j)$ in $\mathcal{U} \times \mathcal{A}$ and proving that it converges, along some subsequence, to a minimizer of $\mathcal{E}_V$. A difficulty here comes from the fact that the minimization problem is subject to a constraint on the parameter u, but not on $\vec{A}$. We first establish a suitable coercivity property that allows us to localize possible minimizers to a ball in $\mathcal{U} \times \mathcal{A}$. This implies that $(u_j, \vec{A}_j)$ converges weakly to some $(u_\infty, \vec{A}_\infty)$ in $\mathcal{U} \times \mathcal{A}$. Then we can the relative compactness in L^2 of a ball in H^1 to deduce that (u_j) converges strongly in L^2 to u_∞. This in turn suffices to prove the existence of a minimizer.

The main difficulty to implement this approach comes from the presence of singular terms in the interaction (i.e. terms involving χ_2 with $\chi_2/|k|$ in $L^{3,\infty}$). In order to handle them, we use suitable estimates in Lorentz spaces that we detail in the next section. This is one of the main novelties of this paper, which allows us to remove the ultraviolet cutoff, and which we believe is naturally suited to study the minimization problem in the present context.

Our next proposition establishes the asymptotic expansion of the ground state energy E_V up to third order in the coupling constant, assuming that V and χ are radial.

Proposition 3.1.9 (Asymptotic expansion of the ground state energy at small coupling)**.** *Suppose that V satisfies Hypothesis 3.1.1 and 3.1.2, and χ satisfies Hypothesis 3.1.3. Suppose also that V and χ are radial, and that the decomposition $V = V_1 + V_2$ of Hypothesis 3.1.1 can be chosen such that $E_{V_1} > E_V$. There exist $\varepsilon_V > 0$ and $C_V > 0$ such that, if*

$$\mathbf{g}_\chi := |g| \Big\| \frac{\chi}{|k|} \Big\|_{L^2+L^{3,\infty}} \le \varepsilon_V \,,$$

then the minimum of the energy satisfies

$$\left| E_V - \mu_V - \frac{32}{3}\pi^3 \int (g\hat{\chi} * u_V^2)^2 \right| \leq C_V\, \mathbf{g}_\chi^4 \,. \tag{3.19}$$

In particular, if $\chi = 1$*, then*

$$\left| E_V - \mu_V - g^2 \frac{4}{3}(8\pi^3)^3 \int u_V^4 \right| \leq C_V\, \mathbf{g}_\chi^4 \,.$$

Remark 3.1.10. *The asymptotic expansion at small coupling of the ground state energy of the Hamiltonian* $\mathbb{H}$ *in the standard model of non-relativistic QED has been computed in [10].*

To prove Proposition 3.1.9, we derive Euler-Lagrange type equations for minimizers $(u_{\rm gs}, \vec{A}_{\rm gs})$, which we subsequently project to the vector space spanned by the electronic ground states and its orthogonal complement. The asymptotic expansion in Proposition 3.1.9 then follows from estimating these equations.

Our last concern is to prove the convergence of the ground state energies in the ultraviolet limit. More precisely, suppose that the interaction between the electron and the field is cut-off in the ultraviolet, i.e. that the Maxwell–Schrödinger energy functional is given by

$$\mathcal{E}_{V,\Lambda}(u, \vec{A}) := \left\| \vec{\sigma} \cdot (-i\vec{\nabla} - g\hat{\chi}_\Lambda * \vec{A})\, u \right\|_{L^2}^2 + \langle u, Vu \rangle_{L^2} + \frac{1}{32\pi^3} \|\vec{A}\|_{\dot{H}^1}^2, \tag{3.20}$$

with $\chi_\Lambda = \chi \mathbb{1}_{|k| \leq \Lambda}$, for some ultraviolet parameter $\Lambda > 0$. Define the ground state energies $E_{V,\Lambda}$ by

$$E_{V,\Lambda} := \inf_{(u,\vec{A}) \in \mathcal{U} \times \mathcal{A}} \mathcal{E}_{V,\Lambda}(u, \vec{A}). \tag{3.21}$$

The next proposition then shows that $E_{V,\Lambda}$ converges to E_V as $\Lambda \to \infty$.

Proposition 3.1.11 (Ultraviolet limit of the ground state energies)**.** *Suppose that* V *satisfies Hypothesis 3.1.1 and that* χ *satisfies Hypothesis 3.1.3 and* $32\pi^3 a C^2 g^2 \|\chi_2/|k|\|_{L^{3,\infty}}^2 < 1$. *Then*

$$E_{V,\Lambda} \underset{\Lambda \to \infty}{\longrightarrow} E_V.$$

Note that the conditions imposed in Proposition 3.1.11 are weaker than those ensuring the existence of a ground state in Theorem 3.1.3.

3.1.5 Organisation of the paper

In the preliminary Section 3.2, we state estimates on the electronic Hamiltonian. Most of the proofs can be found in the companion paper [26]. We also establish functional inequalities in Lorentz spaces used to handle the ultraviolet limit in the Maxwell-Schrödinger energy functional. Our main results are proved in Section 3.3 : We first reduce the variational problem for (3.1) to the minimization of the Maxwell–Schrödinger energy functional

(3.2) in Section 3.3.1. Existence of a minimizer for the Maxwell–Schrödinger energy as stated in Theorem 3.1.3 is proved in Section 3.3.2. In Section 3.3.3, we establish useful properties of the set of minimizers. We compute the expansion of the ground state energy for small coupling constants and prove Proposition 3.1.9 in Section 3.3.4. Finally, the convergence of the ground state energies in the ultraviolet limit (Proposition 3.1.11) is proved in Section 3.3.5. For the sake of completeness, the self-adjointness of the Pauli-Fierz Hamiltonian and its quadratic form domain are recalled in Appendix 3.4.

3.2 Preliminaries

In this preliminary section, we gather several technical estimates that will be used in the next section to prove our main results. The first subsection mainly concerns the electronic Hamiltonian H_V. We refer to the article [26] for a proof of some of the stated results. In a second subsection, we give some functional estimates in Lorentz spaces that will be used in a crucial way to control the interactions terms in the Maxwell–Schrödinger energy functional.

3.2.1 Estimates on the electronic part

Recall that our assumptions on the external potential V of the electronic Hamiltonian $H_V = -\Delta + V$ have been introduced in Section 3.1.1. We begin with a few remarks showing that H_V is well-defined and that $\mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1})$ with V_1 as in Hypothesis 3.1.1.

First, V_- is form bounded with respect to $\sqrt{-\Delta}$, by Hypothesis 3.1.1. This implies by a well-known argument that V_- is also form bounded with respect to H_{V_+} with a relative bound less than 1, and hence the KLMN Theorem (see [107, Theorem X.17]) yields that H_V identifies with a semi-bounded self-adjoint operator with form domain $\mathcal{Q}(H_V) = \mathcal{Q}(H_{V_+})$.

Next, Hypothesis 3.1.1(ii) implies that V_2 is relatively form bounded with respect to $\sqrt{-\Delta}$ with relative bound 0. Indeed, for R sufficiently large, $V_2 \mathbb{1}_{|x|\geq R}$ belongs to $L^\infty(\mathbb{R}^3)$ since $V_2(x) \to 0$ as $|x| \to \infty$, while $V_2 \mathbb{1}_{|x|\leq R}$ belongs to $L^{3/2}(B_R)$ with $B_R := \{x \in \mathbb{R}^3 \,|\, |x| \leq R\}$, since V_2 is in $L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$. Therefore V_2 belongs to $L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and hence we can apply [107, Theorem X.19] to deduce that V_2 is infinitesimally form-bounded with respect to $\sqrt{-\Delta}$. In turn, since $V_+ - V_1 = V_2 + V_-$ is form bounded with respect to $\sqrt{-\Delta}$, it is not difficult to verify that $\mathcal{Q}(H_{V_+}) = \mathcal{Q}(H_{V_1})$.

We recall a version of the IMS localization formula (see e.g. [36]), used to split the contributions to the energy for large x and for small x. We state it for a magnetic kinetic energy since this context is relevant in Section 3.3 to study the Maxwell–Schrödinger energy functional.

Lemma 3.2.1 (Magnetic IMS localization formula)**.** *Let $\vec{A} \in L^2_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R}^3)$ and η, $\tilde{\eta} : \mathbb{R}^3 \to \mathbb{R}$ be differentiable with bounded first derivatives and such that $\eta^2 + \tilde{\eta}^2 = 1$. Let $u \in H^1_{\vec{A}} =$*

$\{\tilde{u} \in L^2 \mid (-i\vec{\nabla} - \vec{A})\tilde{u} \in L^2\}$. *Then*

$$\|(-i\vec{\nabla} - \vec{A})u\|^2 = \|(-i\vec{\nabla} - \vec{A})\,\eta\,u\|^2 + \|(-i\vec{\nabla} - \vec{A})\,\tilde{\eta}\,u\|^2 - \langle u, (|\vec{\nabla}\eta|^2 + |\vec{\nabla}\tilde{\eta}|^2)u\rangle\,. \quad (3.22)$$

Proof. Using the commutator $[-i\vec{\nabla} - \vec{A}, \eta] = (-i\vec{\nabla}\eta)$ three times yields

$$\begin{aligned}\langle(-i\vec{\nabla} - \vec{A})\,u, (-i\vec{\nabla} - \vec{A})\,\eta^2 u\rangle &= \langle(-i\vec{\nabla} - \vec{A})\,\eta u, (-i\vec{\nabla} - \vec{A})\,\eta u\rangle - \langle u, (-i\vec{\nabla}\eta)^2 u\rangle \\ &+ \frac{1}{2}\langle u, (-(-i\vec{\nabla}\eta^2)(-i\vec{\nabla} - \vec{A}) + (-i\vec{\nabla} - \vec{A})\,(-i\vec{\nabla}\eta^2))u\rangle\,. \quad (3.23)\end{aligned}$$

Summing (3.23) and the same equation with η replaced by $\tilde{\eta}$ leads to

$$\begin{aligned}\|(-i\vec{\nabla} - \vec{A})u\|^2 &= \|(-i\vec{\nabla} - \vec{A})\,\eta\,u\|^2 + \|(-i\vec{\nabla} - \vec{A})\,\tilde{\eta}\,u\|^2 - \langle u, (|\vec{\nabla}\eta|^2 + |\vec{\nabla}\tilde{\eta}|^2)u\rangle \\ &+ \big\langle u, \big(- (-i\vec{\nabla}\frac{\eta^2 + \tilde{\eta}^2}{2})(-i\vec{\nabla} - \vec{A}) + (-i\vec{\nabla} - \vec{A})(-i\vec{\nabla}\frac{\eta^2 + \tilde{\eta}^2}{2})\big)u\big\rangle\end{aligned}$$

which implies the result since $\eta^2 + \tilde{\eta}^2$ is constant. □

The following lemma shows that, for confining potentials V, the gap $\mu_{V_1} - \mu_V$ can be made as large as we want, provided that the potential V_1 is suitably chosen. The proof can be found in the companion paper [26].

Lemma 3.2.2. *Suppose that $V = V_+ - V_-$ is such that*

(i) $V_+ \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$,

(ii) $V_- \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$,

(iii) $V(x) \to \infty$ *as* $|x| \to \infty$.

Then, for all $C > 0$, there exist a decomposition $V = V_{1,C} + V_{2,C}$ as in Hypothesis 3.1.1 such that, moreover,

$$\mu_{V_{1,C}} - \mu_V \geq C.$$

To conclude this section, we give a lemma, proved again in the companion paper [26], which is useful to prove the existence of minimizers for the energy functional studied in Section 3.3.

Lemma 3.2.3. *Suppose that V satisfies Hypothesis 3.1.1. Let $(u_j)_{j\in\mathbb{N}}$ be a bounded sequence in $H^1(\mathbb{R}^3)$ which converges weakly to u_∞ in $H^1(\mathbb{R}^3)$, and strongly in $L^2(\mathbb{R}^3)$. Then*

$$\langle u_\infty, (-\Delta + V)u_\infty\rangle \leq \liminf_{j\to\infty}\langle u_j, (-\Delta + V)u_j\rangle\,.$$

3.2.2 Functional inequalities in Lorentz spaces

In the proof of our main results, we use in a crucial way some functional inequalities in Lorentz spaces that we present in this section. For $1 \le p < \infty$, the Lorentz spaces $L^{p,\infty} = L^{p,\infty}(\mathbb{R}^d)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that (3.3) holds.

More generally, for $1 \le p < \infty$ and $1 \le q \le \infty$, the Lorentz spaces $L^{p,q} = L^{p,q}(\mathbb{R}^d)$ are defined as the set of (equivalence classes of) measurable functions $f : \mathbb{R}^d \to \mathbb{C}$ such that the quasi-norm

$$\|f\|_{L^{p,q}} := p^{1/q} \|\lambda(\{|f| > t\})^{1/p} \, t\|_{L^q((0,\infty),\mathrm{d}t/t)}$$

is finite.

For $1 \le p < \infty$ and $1 \le q_1 \le q_2 \le \infty$, the continuous embedding $L^{p,q_1} \subseteq L^{p,q_2}$ holds. Moreover $L^{p,p}$ identifies with the Lebesgue space L^p. We use the following generalizations of Hölder and Young's inequality in Lorentz spaces, see [23, 82, 103, 114] or [58, Exercise 1.4.19].

For $1 \le p_1, p_2 < \infty$, $1 \le q_1, q_2 \le \infty$, Hölder's inequality states that

$$\|f_1 f_2\|_{L^{p,q}} \lesssim \|f_1\|_{L^{p_1,q_1}} \|f_2\|_{L^{p_2,q_2}}, \qquad \frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}, \quad \frac{1}{q} = \frac{1}{q_1} + \frac{1}{q_2}, \tag{3.24}$$

whenever the right hand side is finite.

Young's inequality states that, for $1 < p, p_1, p_2 < \infty$, $1 \le q_1, q_2 \le \infty$,

$$\|f_1 * f_2\|_{L^{p,q}} \lesssim \|f_1\|_{L^{p_1,q_1}} \|f_2\|_{L^{p_2,q_2}}, \qquad 1 + \frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}, \quad \frac{1}{q} = \frac{1}{q_1} + \frac{1}{q_2}. \tag{3.25}$$

Functional inequalities in the Maxwell–Schrödinger setting

We present estimates which will play an important role in the next section. We work in the setting of the Maxwell–Schrödinger energy functional introduced in (3.1.3), with u in $\mathcal{Q}_V \subset L^2(\mathbb{R}^3;\mathbb{C}^2)$ (see (3.7)) and A in $\dot{H}^1(\mathbb{R}^3;\mathbb{R}^3)$.

Lemma 3.2.4. *Under Hypothesis 3.1.3 on $\chi = \chi_1 + \chi_2$ with $\chi_1/|k|$ in L^2 and $\chi_2/|k|$ in $L^{3,\infty}$, there exists a universal constant $C > 0$ such that,*

$$\forall (u, \vec{A}) \in H^1 \times \dot{H}^1, \ \|(\hat{\chi} * \vec{A})u\|_{L^2} \le C \|\vec{A}\|_{\dot{H}^1} \left(\left\| \frac{\chi_1}{|k|} \right\|_{L^2} \|u\|_{L^2} + \left\| \frac{\chi_2}{|k|} \right\|_{L^{3,\infty}} \|u\|_{\dot{H}^{1/2}} \right), \tag{3.26}$$

and

$$\forall (u, \vec{A}) \in \mathcal{Q}_V \times \dot{H}^1, \quad \|(\hat{\chi} * \vec{A})u\|_{L^2} \le C \left\| \frac{\chi}{|k|} \right\|_{L^2 + L^{3,\infty}} \|\vec{A}\|_{\dot{H}^1} \|u\|_{L^2}^{1/2} \|u\|_{\mathcal{Q}_V}^{1/2}. \tag{3.27}$$

Proof. In this proof $X \lesssim Y$ means that there is a universal constant c such that $X \leq cY$. Hölder and Young's inequalities are sufficient to estimate

$$\|(\hat{\chi}_1 * \vec{A})u\|_{L^2} \lesssim \|(\chi_1\,\overline{\mathcal{F}}\vec{A}) * \overline{\mathcal{F}}u\|_{L^2} \leq \|\chi_1\,\overline{\mathcal{F}}\vec{A}\|_{L^1}\,\|u\|_{L^2}$$
$$\leq \|\chi_1/|k|\|_{L^2}\,\||k|\,\overline{\mathcal{F}}\vec{A}\|_{L^2}\,\|u\|_{L^2} \leq \|\chi_1/|k|\|_{L^2}\,\|\vec{A}\|_{\dot{H}^1}\,\|u\|_{L^2}.$$

Similarly, using the Hölder and Young inequalities in Lorentz spaces, see (3.24)–(3.25),

$$\|(\hat{\chi}_2 * \vec{A})u\|_{L^2} \lesssim \left\|(\chi_2\overline{\mathcal{F}}\vec{A}) * (\overline{\mathcal{F}}u)\right\|_{L^2} \lesssim \left\|\chi_2\overline{\mathcal{F}}\vec{A}\right\|_{L^{6/5,2}}\left\|\overline{\mathcal{F}}u\right\|_{L^{3/2,2}}$$
$$\lesssim \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\||k|\overline{\mathcal{F}}\vec{A}\|_{L^2}\left\|\frac{1}{|k|^{1/2}}\right\|_{L^{6,\infty}}\||k|^{1/2}\overline{\mathcal{F}}u\|_{L^2} \lesssim \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\|\vec{A}\|_{\dot{H}^1}\|u\|_{\dot{H}^{1/2}}\,.$$

One could also use the Brascamp-Lieb inequality in Lorentz spaces, see [20, 23]. This proves (3.26). Hölder's inequality then yields (3.27), since

$$\|u\|_{\dot{H}^{1/2}} \lesssim \left\||\overline{\mathcal{F}}u|^{1/2}|k|^{1/2}|\overline{\mathcal{F}}u|^{1/2}\right\|_{L^2} \lesssim \left\||\overline{\mathcal{F}}u|^{1/2}\right\|_{L^4}\left\||k|^{1/2}|\overline{\mathcal{F}}u|^{1/2}\right\|_{L^4} \lesssim \|u\|_{H^1}^{1/2}\,\|u\|_{L^2}^{1/2}.$$

This ends the proof. □

Lemma 3.2.5. *Under Hypothesis 3.1.3 on χ, there exists a universal constant $C > 0$ such that, for all tempered distribution w such that $\mathcal{F}w$ is in $L^\infty \cap L^{6,2}$,*

$$\|\hat{\chi} * w\|_{\dot{H}^{-1}} \leq C\left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}}\|\mathcal{F}w\|_{L^\infty\cap L^{6,2}}\,, \tag{3.28}$$

and for all u_1 in L^2, u_2 in H^1, and $0 < \Lambda \leq \infty$,

$$\|\mathbb{1}_{|k|\leq\Lambda}\mathcal{F}(u_1u_2)\|_{L^\infty\cap L^{6,2}} \leq C\|u_1\|_{L^2}\|u_2\|_{H^1}\,. \tag{3.29}$$

Proof. With a decomposition $\chi = \chi_1 + \chi_2$ where $\chi_1/|k|$ in L^2 and $\chi_2/|k|$ in $L^{3,\infty}$, Hölder's inequality gives

$$\|\hat{\chi}_1 * w\|_{\dot{H}^{-1}} \lesssim \left\|\frac{\chi_1}{|k|}\right\|_{L^2}\|\mathcal{F}w\|_{L^\infty}\,.$$

Likewise, Hölder's inequality in Lorentz spaces, see (3.24), yields

$$\|\hat{\chi}_2 * w\|_{\dot{H}^{-1}} \lesssim \left\|\frac{\chi_2}{|k|}\,\mathcal{F}w\right\|_{L^2} \leq \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\|\mathcal{F}w\|_{L^{6,2}}\,.$$

This proves (3.28).

Now, by the continuity of the Fourier transform from L^1 to L^∞ and Hölder's inequality,

$$\|\mathbb{1}_{|k|\leq\Lambda}\mathcal{F}(u_1u_2)\|_{L^\infty} \leq \|u_1u_2\|_{L^1} \lesssim \|u_1\|_{L^2}\|u_2\|_{L^2}\,.$$

Then Young's inequality in Lorentz spaces (3.25) yields

$$\left\|\mathbb{1}_{|k|\leq\Lambda}\mathcal{F}(u_1u_2)\right\|_{L^{6,2}} \lesssim \|\mathcal{F}(u_1)*\mathcal{F}(u_2)\|_{L^{6,2}} \lesssim \|\mathcal{F}(u_1)\|_{L^{2,2}}\,\|\mathcal{F}(u_2)\|_{L^{3/2,\infty}}\ .$$

Using the fact that $L^{2,2}=L^2$ and Hölder's inequality in Lorentz spaces (3.24) yields

$$\|\mathcal{F}(u_1)\|_{L^{2,2}}\,\|\mathcal{F}(u_2)\|_{L^{3/2,\infty}} \lesssim \|u_1\|_{L^2}\,\left\|\,|k|^{-1/2}\,\right\|_{L^{6,\infty}}\left\|\,|k|^{1/2}\,\mathcal{F}(u_2)\right\|_{L^{2,\infty}}.$$

Since $L^{2,2}=L^2$ is continuously embedded in $L^{2,\infty}$, and since $\|u_2\|_{\dot{H}^{1/2}}\leq\|u_2\|_{H^1}$ this yields (3.29). □

Recall that $\mathcal{Q}_V^*$ stands for the topological dual of $\mathcal{Q}_V$ (see (3.7)) and that the space $\mathcal{A}$ has been defined in (3.16).

Lemma 3.2.6. *Suppose that V satisfies Hypothesis 3.1.1 and that χ satisfies Hypothesis 3.1.3. There exists a universal constant $C>0$ such that, for all $\vec{A}$ in $\mathcal{A}$ and u in H^1,*

$$\|(-i\vec{\nabla}u)\cdot(\hat{\chi}*\vec{A})\|_{\mathcal{Q}_V^*} \leq C\left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}}\|\vec{A}\|_{\dot{H}^1}\|u\|_{H^1}^{1/2}\|u\|_{L^2}^{1/2},$$

$$\|\hat{\chi}*\vec{\sigma}\cdot(\vec{\nabla}\wedge\vec{A})u\|_{\mathcal{Q}_V^*} \leq C\left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}}\|\vec{A}\|_{\dot{H}^1}\|u\|_{H^1}^{1/2}\|u\|_{L^2}^{1/2},$$

$$\|(\hat{\chi}*\vec{A})^2u\|_{\mathcal{Q}_V^*} \leq C\left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}}^2\|\vec{A}\|_{\dot{H}^1}^2\|u\|_{H^1}^{1/2}\|u\|_{L^2}^{1/2}.$$

Proof. By duality, using that $\vec{\nabla}\cdot\vec{A}=0$, we have

$$\begin{aligned}
\|(-i\vec{\nabla}u)\cdot(\hat{\chi}*\vec{A})\|_{\mathcal{Q}_V^*} &= \sup_{\|v\|_{\mathcal{Q}_V}=1}\left|\int\overline{v(x)}[(-i\vec{\nabla}u(x))\cdot(\hat{\chi}*\vec{A})(x)]\,\mathrm{d}x\right|\\
&= \sup_{\|v\|_{\mathcal{Q}_V}=1}\left|\int\overline{-i\vec{\nabla}v(x)}[u(x)\cdot(\hat{\chi}*\vec{A})(x)]\,\mathrm{d}x\right|\\
&\leq \sup_{\|v\|_{\mathcal{Q}_V}=1}\|\vec{\nabla}v\|_{L^2}\|(\hat{\chi}*\vec{A})u\|_{L^2}\\
&\leq \sup_{\|v\|_{\mathcal{Q}_V}=1}\|v\|_{\mathcal{Q}_V}\|(\hat{\chi}*\vec{A})u\|_{L^2} \leq \|(\hat{\chi}*\vec{A})u\|_{L^2}\,.
\end{aligned}$$

This last quantity is estimated thanks to Lemma 3.2.4 :

$$\|(\hat{\chi}*\vec{A})u\|_{L^2} \lesssim \left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}}\|\vec{A}\|_{\dot{H}^1}\|u\|_{H^1}^{1/2}\|u\|_{L^2}^{1/2}.$$

The estimate of $\|\hat{\chi}*\vec{\sigma}\cdot(\vec{\nabla}\wedge\vec{A})u\|_{\mathcal{Q}_V^*}$ is analogous, using that

$$\int\overline{v(x)}\big(\hat{\chi}*\vec{\sigma}\cdot(\vec{\nabla}\wedge\vec{A})u\big)(x)\mathrm{d}x = -\big\langle(\vec{\nabla}\wedge\vec{\sigma})v\,,(\hat{\chi}*\vec{A})u\big\rangle_{L^2}.$$

Similarly, by duality, Hölder's inequality and Lemma 3.2.4,

$$\|(\hat{\chi}*\vec{A})^2u\|_{\mathcal{Q}_V^*} = \sup_{\|v\|_{\mathcal{Q}_V}=1}\left|\int \overline{v}(\hat{\chi}*\vec{A})^2u\right|$$
$$\leq \|(\hat{\chi}*\vec{A})v\|_{L^2}\|(\hat{\chi}*\vec{A})u\|_{L^2} \lesssim \left\|\frac{\chi}{|k|}\right\|^2_{L^2+L^{3,\infty}}\|\vec{A}\|^2_{\dot{H}^1}\|u\|^{1/2}_{H^1}\|u\|^{1/2}_{L^2}.$$

This concludes the proof of the lemma. □

3.3 Proofs of the main results

In this section we prove our main results stated in Section 3.1.4. In Section 3.3.1, we show that minimizing the Pauli-Fierz energy over coherent states is equivalent to minimizing the Maxwell–Schrödinger energy functional over its natural definition domain. The existence of a minimizer stated in Theorem 3.1.3 is proved in Section 3.3.2, using coercivity and lower semicontinuity arguments. In Section 3.3.3 we study the set of minimizers of the Maxwell–Schrödinger energy functional for small coupling constants. In particular, the Euler-Lagrange equations leads to useful estimates for the minimizers, which in turn allows us to obtain in Section 3.3.4 the second-order asymptotic expansions of the ground state energy at small coupling stated in Proposition 3.1.9. Finally, we prove the convergence of the quasi-classical ground state energy in the ultraviolet limit (Proposition 3.1.11) in Section 3.3.5.

3.3.1 Reduction to the Maxwell–Schrödinger energy functional

We first justify the derivation of the Maxwell–Schrödinger energy functional appearing in (3.12). To this end we compute the energy of product state $u\otimes\Psi_{\vec{f}}$ in the standard model of non-relativistic QED. Recall that u is in $\mathcal{U}$ (see (3.8)) and $\vec{f}$ is in $L^2_\perp(\mathbb{R}^3;\mathbb{C}^3)\cap\mathcal{Z}$ (see (3.11)).

We introduce a direct sum decomposition $\mathcal{Z}=\mathcal{Z}^+\oplus\mathcal{Z}^-$ where

$$\mathcal{Z}^+ := \left\{\vec{f}\in\mathcal{Z},\ \vec{f}(-k)=\overline{\vec{f}(k)}\quad\forall k\in\mathbb{R}^3\right\},\quad \mathcal{Z}^- := \left\{\vec{f}\in\mathcal{Z},\ \vec{f}(-k)=-\overline{\vec{f}(k)}\quad\forall k\in\mathbb{R}^3\right\}.$$

Note that any $\vec{f}$ in $\mathcal{Z}$ decomposes as $\vec{f}=\vec{f}_++\vec{f}_-$ with

$$\vec{f}_+(k) := \frac{\vec{f}(k)+\overline{\vec{f}(-k)}}{2}\in\mathcal{Z}^+,\quad \vec{f}_-(k) := \frac{\vec{f}(k)-\overline{\vec{f}(-k)}}{2}\in\mathcal{Z}^-.$$

We suppose here that $\chi/\sqrt{|k|}$ and $\chi/|k|$ belong to $L^2(\mathbb{R}^3)$ in order for the Hamiltonian $\mathbb{H}$ to be well-defined (see Proposition 3.4.1). These assumptions will however subsequently be relaxed in our study of the Maxwell–Schrödinger energy functional. In this section we drop the index V for $\mathcal{E}_V$ as the potential remains fixed throughout this section.

Proposition 3.3.1. *Let $\chi : \mathbb{R}^3 \to \mathbb{R}$ be such that $\chi(-k) = \chi(k)$ for all k in $\mathbb{R}^3$ and both $\chi/\sqrt{|k|}$ and $\chi/|k|$ belong to $L^2(\mathbb{R}^3)$. Let u in $\mathcal{U}$ and $\Psi_{\vec{f}}$ in $\mathcal{H}_{\mathrm{f}}$ be a coherent state of parameter $\vec{f}$ in $L^2_\perp(\mathbb{R}^3;\mathbb{C}^3) \cap \mathcal{Z}$. The energy of the state $u \otimes \Psi_{\vec{f}}$ satisfies*

$$\Big\langle (u \otimes \Psi_{\vec{f}})\,,\, \mathbb{H}(u \otimes \Psi_{\vec{f}}) \Big\rangle_{\mathcal{H}} = 2g^2 \Big\| \frac{\chi(k)}{\sqrt{|k|}} \Big\|^2_{L^2} + \Big\langle \vec{f}_-, |k| \vec{f}_- \Big\rangle_{L^2} + \mathcal{E}(u, \vec{A}_{\vec{f}}), \tag{3.30}$$

where $\vec{A}_{\vec{f}}$ is given by (3.13) and $\mathcal{E}(u, \vec{A}_{\vec{f}})$ is given by (3.14). Moreover,

$$\inf_{u\in\mathcal{U}, \vec{f} \in L^2_\perp \cap \mathcal{Z}} \Big\langle (u \otimes \Psi_{\vec{f}})\,,\, \mathbb{H}(u \otimes \Psi_{\vec{f}}) \Big\rangle = 2g^2 \Big\| \frac{\chi(k)}{\sqrt{|k|}} \Big\|^2_{L^2} + \inf_{u\in\mathcal{U}, \vec{f} \in L^2_\perp \cap \mathcal{Z}^+} \mathcal{E}(u, \vec{A}_{\vec{f}}). \tag{3.31}$$

Proof. Using the identities (3.72) recalled in Appendix 3.4, we can compute the Pauli-Fierz energy of the state $u \otimes \Psi_{\vec{f}}$, which gives

$$\begin{aligned}\big\langle u \otimes \Psi_{\vec{f}}, \mathbb{H}\,(u \otimes \Psi_{\vec{f}})\big\rangle &= \langle u, H_V u\rangle_{L^2} + 2g^2 \,\|\vec{m}\|^2_{L^2_k} - 4g\mathfrak{Re}\Big\langle u, -i\vec{\nabla} u \langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k} \Big\rangle_{L^2_x} \\ &+ 4g^2 \Big\langle u, \Big(\mathfrak{Re}\langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}\Big)^2 u \Big\rangle_{L^2_x} - g\langle u, \vec{\sigma}\cdot\vec{\nabla}_x \wedge 2\mathfrak{Re}\langle \vec{f}, \vec{m}(x,\cdot)\rangle_{L^2_k} u\rangle + \big\langle \vec{f}, |k|\, \vec{f}\big\rangle_{L^2_k},\end{aligned}$$

where $\vec{m} = \sum_\tau \vec{m}_\tau$ and

$$\vec{m}_\tau(x,k) := \chi(k)\, |k|^{-1/2}\, e^{-ik\cdot x} \vec{\varepsilon}_\tau(k)\,.$$

First, we can use the properties of the Fourier transform to obtain

$$\begin{aligned}\langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k} &= \sum_\tau \int \overline{\vec{f}_\tau(k)} \chi(k)\, |k|^{-1/2}\, e^{-ikx} \vec{\varepsilon}_\tau(k)\, \mathrm{d}k \\ &= \mathcal{F}\Big(\overline{\vec{f}(k)}\, |k|^{-1/2}\, \chi(k)\Big)(x) \\ &= \hat{\chi} * \mathcal{F}(\overline{\vec{f}(k)}\, |k|^{-1/2})\,(x),\end{aligned}$$

which means that, with the notation $\vec{A}_{\vec{f}}$ introduced in (3.13), and using that $\hat{\chi}$ is real valued :

$$2\mathfrak{Re}\langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k} = \hat{\chi} * \vec{A}_{\vec{f}}(x)\,.$$

Integrating by parts then gives

$$\begin{aligned}&2\mathfrak{Re}\Big\langle u, -i\vec{\nabla} u \langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}\Big\rangle_{L^2_x} \\ &= \Big\langle u, -i\vec{\nabla} u \langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}\Big\rangle_{L^2_x} + \Big\langle -i\vec{\nabla} u\langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}, u\Big\rangle_{L^2_x} \\ &= \int \overline{-i\vec{\nabla} u(x)} u(x) \langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}\, \mathrm{d}x + \int \overline{-i\vec{\nabla} u(x)} u(x) \overline{\langle \vec{f}, \vec{m}(x,.)\rangle}_{L^2_k}\, \mathrm{d}x \\ &= \int \overline{-i\vec{\nabla} u(x)} u(x) 2\mathfrak{Re}\langle \vec{f}, \vec{m}(x,.)\rangle_{L^2_k}\, \mathrm{d}x \\ &= \Big\langle -i\vec{\nabla} u, (\hat{\chi} * \vec{A}_{\vec{f}}) u\Big\rangle_{L^2}.\end{aligned}$$

Now, we compute the scalar product

$$\big\langle \vec{f}, |k|\, \vec{f} \big\rangle_{L^2} = \big\langle \vec{f}_+, |k|\, \vec{f}_+ \big\rangle_{L^2} + \big\langle \vec{f}_-, |k|\, \vec{f}_- \big\rangle_{L^2} + 2\mathfrak{Re}\big\langle \vec{f}_+, |k|\, \vec{f}_- \big\rangle_{L^2}.$$

Using a change of variables and the definitions of f_+ and f_- yields

$$\big\langle \vec{f}_+, |k|\, \vec{f}_- \big\rangle = \int \overline{\vec{f}_+(k)}\, |k|\, \vec{f}_-(k)\, \mathrm{d}k = \int \overline{\vec{f}_+(-k)}\, |-k|\, \vec{f}_-(-k)\, \mathrm{d}k = -\int \vec{f}_+(k)\, |k|\, \overline{\vec{f}_-(k)}\, \mathrm{d}k.$$

This shows that $2\mathfrak{Re}\big\langle \vec{f}_+, |k|\, \vec{f}_- \big\rangle = 0$. Then, applying the inverse Fourier transform to (3.13) yields

$$\overline{\vec{f}_+(k)} = \frac{1}{2}\, |k|^{1/2}\, \mathcal{F}^{-1}(\vec{A}_{\vec{f}})\,.$$

Finally, using Parseval's equality yields

$$\big\langle \vec{f}_+, |k|\, \vec{f}_+ \big\rangle_{L^2} = \frac{1}{32\pi^3} \big\langle \mathcal{F}^{-1}(\vec{A}_{\vec{f}}), |k|^2\, \mathcal{F}^{-1}(\vec{A}_{\vec{f}}) \big\rangle_{L^2} = \frac{1}{32\pi^3} \big\langle \vec{A}_{\vec{f}}, -\Delta \vec{A}_{\vec{f}} \big\rangle_{L^2} = \frac{1}{32\pi^3} \big\| \vec{A}_{\vec{f}} \big\|^2_{\dot{H}^1}.$$

This allows us to obtain (3.30).

Now, since the term $\langle \vec{f}_-, |k|\, \vec{f}_- \rangle$ is non-negative, we can write

$$\begin{aligned}
&\inf_{u \in \mathcal{U}, \vec{f} \in L^2_\perp \cap \mathcal{Z}} \Big\langle (u \otimes \Psi_{\vec{f}}), \mathbb{H}(u \otimes \Psi_{\vec{f}}) \Big\rangle - 2g^2 \big\| |k|^{-1/2} \chi(k) \big\|^2_{L^2} \\
&\qquad = \inf_{u \in \mathcal{U}, \vec{f}_+ \in L^2_\perp \cap \mathcal{Z}^+} \ \inf_{\vec{f}_- \in L^2_\perp \cap \mathcal{Z}^-} \Big(\mathcal{E}(u, \vec{A}_{\vec{f}_+ + \vec{f}_-}) + \Big\langle \vec{f}_-, |k|\, \vec{f}_- \Big\rangle_{L^2} \Big) \\
&\qquad = \inf_{u \in \mathcal{U}, \vec{f}_+ \in L^2_\perp \cap \mathcal{Z}^+} \mathcal{E}(u, \vec{A}_{\vec{f}_+}),
\end{aligned}$$

which establishes (3.31). □

In the sequel we focus on the minimization of the energy functional $\mathcal{E}$. By (3.31), we can restrict the minimization to $\vec{f} \in \mathcal{Z}^+$.

In order for the coherent state $\Psi_{\vec{f}}$ to be well-defined, we assumed in the previous proof that $\vec{f} \in L^2_\perp(\mathbb{R}^3; \mathbb{C}^3)$. The further condition $\vec{f} \in \mathcal{Z}^+$ ensures that the term $\langle \vec{f}, |k|\, \vec{f} \rangle$ is finite. We will see below (see Lemma 3.3.5) that, in order for $\mathcal{E}(u, \vec{A}_{\vec{f}})$ to be well-defined, it suffices in fact to assume that $u \in \mathcal{U}$ and $\vec{f} \in \mathcal{Z}^+$. (By (3.13), the latter condition is equivalent to $\vec{A}_{\vec{f}} \in \dot{H}^1$, while $\vec{f}_+ \in L^2$ is equivalent to $\vec{A}_{\vec{f}} \in \dot{H}^{1/2}$). We therefore study $\mathcal{E}$ on the energy space $\mathcal{U} \times \mathcal{A}$ (where $\mathcal{A}$ is defined in (3.16)), the norm on $\mathcal{U} \times \mathcal{A}$ being defined by

$$\|(u, \vec{A})\|^2_{\mathcal{U} \times \mathcal{A}} = \|u\|^2_{H^1} + \langle u, V_+ u \rangle_{L^2} + \|\vec{A}\|^2_{\dot{H}^1}.$$

In the remainder of this section, we establish Proposition 3.1.2, namely, that for any minimizer $(u_{\mathrm{gs}}, \vec{A}_{\mathrm{gs}})$ in $\mathcal{U} \times \mathcal{A}$ of the Maxwell–Schrödinger energy functional (3.14), there exists $\vec{f}_{\mathrm{gs}}$ in $L^2_\perp(\mathbb{R}^3; \mathbb{C}^3) \cap \mathcal{Z}$ such that $\vec{A}_{\mathrm{gs}} = \vec{A}_{\vec{f}_{\mathrm{gs}}}$ as in (3.13).

We begin with a lemma introducing the Euler-Lagrange equation satisfied by $\vec{A}_{\mathrm{gs}}$ and the Pauli operator at a minimizer $(u_{\mathrm{gs}}, \vec{A}_{\mathrm{gs}})$, which will often be useful in the sequel.

Lemma 3.3.2 (Euler-Lagrange equation and Pauli operator associated to a minimizer)**.** *Suppose that the potential V satisfies Hypothesis 3.1.1 and that χ satisfies Hypothesis 3.1.3. If $(u_{\rm gs}, \vec{A}_{\rm gs})$ is a minimizer of $\mathcal{E}$ over $\mathcal{U} \times \mathcal{A}$, then*

$$\vec{A}_{\rm gs} = 32\pi^3(-\Delta)^{-1} g\hat{\chi} * \mathfrak{Re}\big\langle(-i\vec{\nabla} + \vec{\nabla} \wedge \vec{\sigma} - g\hat{\chi} * \vec{A}_{\rm gs})u_{\rm gs}, u_{\rm gs}\big\rangle_{\mathbb{C}^2}, \tag{3.32}$$

the operator

$$H_{V,\vec{A}_{\rm gs}} := (-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\rm gs})^2 - g\hat{\chi} * \vec{\sigma} \cdot (\vec{\nabla} \wedge \vec{A}_{\rm gs}) + V + \frac{1}{32\pi^3}\|\vec{A}_{\rm gs}\|^2_{\dot{H}^1} \tag{3.33}$$

defines a self-adjoint operator, and $u_{\rm gs}$ is an eigenvector of $H_{V,\vec{A}_{\rm gs}}$ associated to the eigenvalue E_V.

Proof. At a minimizer, the Frechet derivative of $\mathcal{E}(u, \vec{A})$ with respect to $\vec{A}$,

$$\begin{aligned} \partial_{\vec{A}}\mathcal{E}(u_{\rm gs}, \vec{A}_{\rm gs}) = & -\frac{\Delta}{16\pi^3}\vec{A}_{\rm gs} - g\hat{\chi} * 2\mathfrak{Re}\langle -i\vec{\nabla}u_{\rm gs}, u_{\rm gs}\rangle_{\mathbb{C}^2} \\ & + 2g\hat{\chi} * [(g\hat{\chi} * \vec{A}_{\rm gs})\,|u_{\rm gs}|^2_{\mathbb{C}^2}] - 2g\hat{\chi} * \mathfrak{Re}\langle\vec{\nabla} \wedge \vec{\sigma}u, u\rangle_{\mathbb{C}^2}\,, \end{aligned}$$

vanishes, which yields (3.32).

Note that under our assumptions, V_- is infinitesimally form bounded with respect to the operator $(\vec{\sigma} \cdot (-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\rm gs}))^2$ (see (3.37) below) from which, using the KLMN Theorem, it is not difficult to deduce that $H_{V,\vec{A}_{\rm gs}}$ identifies with a self-adjoint operator. The minimizing property of $(u_{\rm gs}, \vec{A}_{\rm gs})$ means that

$$\langle u_{\rm gs}, (H_{V,\vec{A}_{\rm gs}} - E_V)u_{\rm gs}\rangle = 0\,. \tag{3.34}$$

As $H_{V,\vec{A}_{\rm gs}} \geq E_V$, (3.34) implies that $(H_{V,\vec{A}_{\rm gs}} - E_V)^{1/2}\, u_{\rm gs} = 0$ and thus

$$(H_{V,\vec{A}_{\rm gs}} - E_V)u_{\rm gs} = 0\,, \tag{3.35}$$

which ends the proof of the lemma. □

Two important ingredients in the proof of Proposition 3.1.2 are the exponential decay of the electronic part $u_{\rm gs}$ and a virial argument. We begin with proving these two properties in Lemmata 3.3.3 and 3.3.4, respectively.

Lemma 3.3.3 (Exponential decay of the ground state)**.** *Under the assumptions of Proposition 3.1.2, there exists $\gamma > 0$ such that*

$$\left\|e^{\gamma|x|}u_{\rm gs}\right\|_{L^2} < \infty. \tag{3.36}$$

Proof. Recall from Lemma 3.3.2 that $u_{\rm gs}$ is a ground state of the Pauli operator (3.33). In particular, it is then known that $u_{\rm gs}$ decays exponentially in the sense that (3.36) holds for some $\gamma > 0$ (see e.g. [59, Theorem 1]). □

Lemma 3.3.4 (Virial argument)**.** *Under the assumptions of Proposition 3.1.2,*

$$\big\langle u_{\rm gs}, \big(-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\rm gs} \big) u_{\rm gs} \big\rangle = 0.$$

Proof. We use the Pauli operator defined in (3.33). A direct computation shows that, in the sense of quadratic forms on $\mathcal{D}(H_{V,\vec{A}_{\rm gs}}) \cap \mathcal{D}(x)$, we have

$$\big[H_{V,\vec{A}_{\rm gs}}, x \big] = -2i \big(-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\rm gs} \big).$$

Since $H_{V,\vec{A}_{\rm gs}} u_{\rm gs} = E_V u_{\rm gs}$ and $u_{\rm gs}$ belongs to $\mathcal{D}(x)$ by Lemma 3.3.3, we deduce that

$$\begin{aligned}\big\langle u_{\rm gs}, \big(-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\rm gs} \big) u_{\rm gs} \big\rangle \\ = \frac{i}{2} \big\langle \big(H_{V,\vec{A}_{\rm gs}} - E_V \big) u_{\rm gs}, x u_{\rm gs} \big\rangle - \frac{i}{2} \big\langle x u_{\rm gs}, \big(H_{V,\vec{A}_{\rm gs}} - E_V \big) u_{\rm gs} \big\rangle = 0.\end{aligned}$$

This proves the lemma. □

Now we are ready to prove Proposition 3.1.2.

Proof of Proposition 3.1.2. Recall that $\vec{f}_{\rm gs}$ and $\vec{A}_{\vec{f}_{\rm gs}}$ are related as in (3.13). Moreover, $\vec{A}_{\rm gs}$ satisfies the relation (3.32), which implies that

$$\|\vec{f}_{\rm gs}\|_{L^2} \lesssim \big\| \vec{A}_{\vec{f}_{\rm gs}} \big\|_{\dot{H}^{1/2}} \lesssim |g| \Big\| \frac{\chi}{|k|^{\frac{3}{2}}} \vec{F}_{\rm gs} \Big\|_{L^2},$$

where, to shorten notations, we have set $\vec{F}_{\rm gs} := \vec{F}_{{\rm gs},1} + \vec{F}_{{\rm gs},2}$, with

$$\vec{F}_{{\rm gs},1} := \bar{\mathcal{F}} \big(\langle -i\vec{\nabla} u_{\rm gs} - g(\hat{\chi} * \vec{A}_{\vec{f}_{\rm gs}}) u_{\rm gs}, u_{\rm gs} \rangle_{\mathbb{C}^2} \big), \quad \vec{F}_{{\rm gs},2} := \bar{\mathcal{F}} \big(\langle \vec{\nabla} \wedge \vec{\sigma} u_{\rm gs}, u_{\rm gs} \rangle_{\mathbb{C}^2} \big).$$

We can estimate

$$\|\vec{f}_{\rm gs}\|_{L^2} \lesssim \Big\| \frac{\chi}{|k|} \Big\|_{L^2 + L^{3,\infty}} \Big\| \frac{1}{|k|^{\frac{1}{2}}} \vec{F}_{\rm gs} \Big\|_{L^\infty \cap L^{6,2}}.$$

Using the cutoff functions η, $\tilde{\eta}$, we separate the contributions from k in a neighborhood of the origin and k in a neighborhood of ∞, obtaining, since $\tilde{\eta}^2 |k|^{-1/2} \le 1$,

$$\|\vec{f}_{\rm gs}\|_{L^2} \lesssim \Big\| \frac{\chi}{|k|} \Big\|_{L^2 + L^{3,\infty}} \Big(\Big\| \frac{1}{|k|^{\frac{1}{2}}} \eta^2 \vec{F}_{\rm gs} \Big\|_{L^\infty \cap L^{6,2}} + \big\| \vec{F}_{\rm gs} \big\|_{L^\infty \cap L^{6,2}} \Big).$$

Clearly, $\|\vec{F}_{\rm gs}\|_{L^\infty} < \infty$ since $F_{{\rm gs},1}$, $F_{{\rm gs},2}$ are the Fourier transforms of products of L^2-functions. Moreover, $\|\vec{F}_{\rm gs}\|_{L^{6,2}} < \infty$ by Lemma 3.2.5. Thanks to the cutoff function η, we also have

$$\Big\| \frac{1}{|k|^{\frac{1}{2}}} \eta^2 \vec{F}_{\rm gs} \Big\|_{L^{6,2}} \lesssim \Big\| \frac{1}{|k|^{\frac{1}{2}}} \eta^2 \vec{F}_{\rm gs} \Big\|_{L^\infty}.$$

Hence it remains to show that the right-hand-side of the previous equation is finite.

To this end, we estimate the contributions from $F_{\text{gs},1}$ and $F_{\text{gs},2}$ separately. We begin with $F_{\text{gs},1}$. We observe that, by Lemma 3.3.4,

$$\vec{F}_{\text{gs},1}(0) = \big\langle u_{\text{gs}}, \big(-i\vec{\nabla} - g\hat{\chi} * \vec{A}_{\text{gs}}\big) u_{\text{gs}} \big\rangle_{L^2} = 0.$$

Moreover, using Lemma 3.3.3, Lemma 3.2.4 and the fact that u_{gs} belongs to $\dot{H}^1$, we have, for all multi-index $\alpha \in \mathbb{N}^3$,

$$\begin{aligned}\big\|\partial_k^\alpha \vec{F}_{\text{gs},1}\big\|_{L^\infty} &\lesssim \big\|\langle -i\vec{\nabla} u_{\text{gs}} - (g\hat{\chi} * \vec{A}_{\vec{f}_{\text{gs}}}) u_{\text{gs}}, x^\alpha u_{\text{gs}}\rangle_{\mathbb{C}^2}\big\|_{L^1} \\ &\lesssim \big\| -i\vec{\nabla} u_{\text{gs}} - (g\hat{\chi} * \vec{A}_{\vec{f}_{\text{gs}}}) u_{\text{gs}}\big\|_{L^2} \big\|x^\alpha u_{\text{gs}}\big\|_{L^2} < \infty.\end{aligned}$$

Hence $\vec{F}_{\text{gs},1}$ belongs to the Sobolev space $W^{\infty,\infty}(\mathbb{R}^3;\mathbb{R}^3)$. Applying the mean-value theorem then yields

$$\Big\|\frac{1}{|k|^{\frac{1}{2}}}\eta^2 \vec{F}_{\text{gs},1}\Big\|_{L^\infty} \le \sup_{|\alpha|=1} \big\||k|^{\frac{1}{2}}\eta^2 \partial_x^\alpha \vec{F}_{\text{gs},1}\big\|_{L^\infty} \lesssim \sup_{|\alpha|=1} \big\|\partial_x^\alpha \vec{F}_{\text{gs},1}\big\|_{L^\infty} < \infty.$$

Now we consider $F_{\text{gs},2}$. Since

$$\vec{F}_{\text{gs},2}(k) = k \wedge \bar{\mathcal{F}}\big(\langle \vec{\sigma} u_{\text{gs}}, u_{\text{gs}}\rangle_{\mathbb{C}^2}\big)(k),$$

we can estimate

$$\Big\|\frac{1}{|k|^{\frac{1}{2}}}\eta^2 \vec{F}_{\text{gs},2}\Big\|_{L^\infty} \le \Big\||k|^{\frac{1}{2}}\eta^2 \bar{\mathcal{F}}\big(\langle \vec{\sigma} u_{\text{gs}}, u_{\text{gs}}\rangle_{\mathbb{C}^2}\big)\Big\|_{L^\infty} \lesssim \Big\|\bar{\mathcal{F}}\big(\langle \vec{\sigma} u_{\text{gs}}, u_{\text{gs}}\rangle_{\mathbb{C}^2}\big)\Big\|_{L^\infty} < \infty.$$

This concludes the proof of the proposition. □

3.3.2 Coercivity, energy gap and existence of a minimizer

In this section we prove Theorem 3.1.3, namely the existence of a global minimizer for the Maxwell–Schrödinger energy functional. We use coercivity and lower semicontinuity arguments.

Before we prove Theorem 3.1.3, we establish a coercivity result which will allow us to show that any minimizing sequence is bounded in $\mathcal{U} \times \mathcal{A}$ (recall that $\mathcal{U}$ has been defined in (3.8) and $\mathcal{A}$ in (3.16)).

Lemma 3.3.5 (Coercivity)**.** *Suppose that V satisfies Hypothesis 3.1.1 and $\chi = \chi_1 + \chi_2$ satisfies Hypothesis 3.1.3, with $\chi_1/|k|$ in L^2 and $\chi_2/|k|$ in $L^{3,\infty}$. If*

$$32\pi^3 a C^2 g^2 \Big\|\frac{\chi_2}{|k|}\Big\|^2_{L^{3,\infty}} < 1\,,$$

with the constant $a \ge 0$ from Hypothesis 3.1.1 and the universal constant $C > 0$ from Lemma 3.2.4, then for all $(u, \vec{A})$ in $\mathcal{U} \times \mathcal{A}$ such that $\|(u, \vec{A})\|_{\mathcal{U}\times\mathcal{A}} \ge 16(2+a)^2$ we have

$$\mathcal{E}_V(u, \vec{A}) \ge C_1 \|(u, \vec{A})\|_{\mathcal{U}\times\mathcal{A}} - C_2\,,$$

with

- $C_1 =: \varepsilon / \max\{4, 32 g^2 C^2 \big\|\chi/|k|\big\|^2_{L^2+L^{3,\infty}}\}$,
- $C_2 =: b + a^2\big(1 + \frac{C^2 g^2}{\varepsilon}\big\|\chi_1/|k|\big\|^2_{L^2}\big)$,
- $2\varepsilon := (32\pi^3)^{-1} - C^2 a g^2 \big\|\chi_2/|k|\big\|^2_{L^{3,\infty}}$.

Proof. Thanks to Lemma 3.2.4, with the constant a from Hypothesis 3.1.1, we can write

$$\|u\|^2_{\dot{H}^{1/2}} \leq \|\vec{\nabla} u\|_{L^2} = \|\vec{\sigma}\cdot\vec{\nabla} u\|_{L^2} \leq \|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} + g\|\vec{\sigma}\cdot(\hat{\chi} * \vec{A})\,u\|_{L^2}$$
$$\leq \|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} + Cg\|\vec{A}\|_{\dot{H}^1}\left(\left\|\frac{\chi_1}{|k|}\right\|_{L^2} + \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\|u\|_{\dot{H}^{1/2}}\right)$$
$$\leq \|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} + \frac{aC^2g^2}{2\varepsilon}\left\|\frac{\chi_1}{|k|}\right\|^2_{L^2} + \left(\frac{\varepsilon}{2a} + \frac{C^2g^2}{2}\left\|\frac{\chi_2}{|k|}\right\|^2_{L^{3,\infty}}\right)\|\vec{A}\|^2_{\dot{H}^1} + \frac{1}{2}\|u\|^2_{\dot{H}^{1/2}}.$$

Hence,

$$\|u\|^2_{\dot{H}^{1/2}} \leq 2\|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} + \frac{aC^2g^2}{\varepsilon}\left\|\frac{\chi_1}{|k|}\right\|^2_{L^2} + \left(\frac{\varepsilon}{a} + C^2g^2\left\|\frac{\chi_2}{|k|}\right\|^2_{L^{3,\infty}}\right)\|\vec{A}\|^2_{\dot{H}^1}.$$

It follows from Hypothesis 3.1.1 that

$$\langle u, V_- u\rangle \leq 2a\|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} + \Big(\frac{1}{32\pi^3} - \varepsilon\Big)\|\vec{A}\|^2_{\dot{H}^1} + \frac{C^2a^2g^2}{\varepsilon}\left\|\frac{\chi_1}{|k|}\right\|^2_{L^2} + b \tag{3.37}$$

and hence,

$$\mathcal{E}_V(u,\vec{A}) \geq \langle u, V_+ u\rangle + \big(\|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} - a\big)^2 + \varepsilon\|\vec{A}\|^2_{\dot{H}^1}$$
$$- a^2\Big(1 + \frac{C^2g^2}{\varepsilon}\left\|\frac{\chi_1}{|k|}\right\|^2_{L^2}\Big) - b$$
$$\geq \varepsilon\Big(\langle u, V_+ u\rangle + \big(\|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} - a\big)^2 + \|\vec{A}\|^2_{\dot{H}^1}\Big) - C_2.$$

Let us suppose that $R = \|(u,\vec{A})\|_{\mathcal{U}\times\mathcal{A}} \geq 4$. We consider three cases :

1. If $\|\vec{A}\|_{\dot{H}^1} \geq R/4$, then $\mathcal{E}(u,\vec{A}) \geq \varepsilon R^2/16 - C_2 \geq \varepsilon R/4 - C_2$.
2. If $\langle u, V_+ u\rangle \geq R^2/16$, then $\mathcal{E}(u,\vec{A}) \geq \varepsilon R^2/16 - C_2 \geq \varepsilon R/4 - C_2$.
3. Otherwise $\|u\|_{H^1} \geq R/2$ and

$$\|\vec{\nabla} u\|^2_{L^2} = \|u\|^2_{H^1} - 1 \geq R^2/4 - 1 \geq (R/2 - 1)^2.$$

   We distinguish two subcases :

   (a) If $\big(\|\vec{\sigma}\cdot(-i\vec{\nabla} - g\,\hat{\chi} * \vec{A})u\|_{L^2} - a\big)^2 \geq R/4$, then $\mathcal{E}(u,\vec{A}) \geq \varepsilon R/4 - C_2$,

(b) If $\big(\|\vec\sigma\cdot(-i\vec\nabla - g\,\hat\chi * \vec A)u\|_{L^2} - a\big)^2 < R/4$, then

$$\begin{aligned}\frac{R}{2} - 1 - a - \frac{R^{1/2}}{2} &\le \|\vec\nabla u\|_{L^2} - \|\vec\sigma\cdot(-i\vec\nabla - g\,\hat\chi * \vec A)u\| \\ &\le g\|(\hat\chi * \vec A)u\|_{L^2} \\ &\le 4gC\Big\|\frac{\chi}{|k|}\Big\|_{L^2+L^{3,\infty}}\|\vec A\|_{\dot H^1}\frac{R^{1/2}}{2}.\end{aligned}$$

Therefore, for $R \ge 16(2+a)^2$,

$$\frac{R^{1/2}}{4\sqrt2 gC\|\frac{\chi}{|k|}\|_{L^2+L^{3,\infty}}} \le \frac{R^{1/2}-(2+a)}{4gC\|\frac{\chi}{|k|}\|_{L^2+L^{3,\infty}}} \le \|\vec A\|_{\dot H^1}$$

and hence

$$\mathcal{E}_V(u,\vec A) \ge \varepsilon\|\vec A\|^2_{\dot H^1} - C_2 \ge \frac{\varepsilon}{32g^2C^2\|\frac{\chi}{|k|}\|^2_{L^2+L^{3,\infty}}}R - C_2\,.$$

This yields the result. □

We are now ready to prove Theorem 3.1.3.

Proof of Theorem 3.1.3. Let $(u_j,\vec A_j)_{j\in\mathbb N}$ be a minimizing sequence for $\mathcal E$ in $\mathcal U\times\mathcal A$. In particular, $(\mathcal E(u_j,\vec A_j))_j$ is bounded and hence, by Lemma 3.3.5, $(u_j,\vec A_j)_j$ is bounded in $\mathcal U\times\mathcal A$. Hence the sequence $(u_j,\vec A_j)_j$ converges weakly to some limit $(u_\infty,\vec A_\infty)$ in $\mathcal U\times\mathcal A$ w.r.t. the topology of $\mathcal Q_V\times\dot H^1$.

We first show that

$$\|u_j - u_\infty\|_{L^2} \xrightarrow[j\to\infty]{} 0\,. \tag{3.38}$$

Let $\varepsilon>0$. By Hypothesis 3.1.1 there exists $R>0$ such that $|V_2(x)| \le \varepsilon(E_{V_1}-E_V)/2$ for $|x|\ge R$ and $|\vec\nabla\eta_R(x)|^2 + |\vec\nabla\tilde\eta_R(x)|^2 \le \varepsilon(E_{V_1}-E_V)/2$ for all x. Recall that the cutoff functions η_R, $\tilde\eta_R$ have been defined in (3.5). We have

$$\begin{aligned}\|u_j-u_\infty\|^2_{L^2} &= \|\eta_R(u_j-u_\infty)\|^2_{L^2} + \|\tilde\eta_R(u_j-u_\infty)\|^2_{L^2} \\ &\le \|\eta_R(u_j-u_\infty)\|^2_{L^2} + 2\|\tilde\eta_R u_j\|^2_{L^2} + 2\|\tilde\eta_R u_\infty\|^2_{L^2}\,.\end{aligned} \tag{3.39}$$

For u in $\mathcal U$, the magnetic IMS localization formula (3.22) yields

$$\begin{aligned}\mathcal E_V(u,\vec A) &= \langle\eta_R\,u, ((-i\vec\nabla - \hat\chi*\vec A)^2 + V - \vec\sigma\cdot(\vec\nabla\wedge\vec A))\,\eta_R\,u\rangle \\ &\quad + \langle\tilde\eta_R\,u, ((-i\vec\nabla - \hat\chi*\vec A)^2 + V_1 - \vec\sigma\cdot(\vec\nabla\wedge\vec A))\,\tilde\eta_R\,u\rangle \\ &\quad + \langle u, (\tilde\eta_R^2\,V_2 - |\vec\nabla\eta_R|^2 - |\vec\nabla\tilde\eta_R|^2)u\rangle + \frac{1}{32\pi^3}\|\vec A\|^2_{\dot H^1} \\ &= \mathcal E_V(\frac{\eta_R\,u}{\|\eta_R\,u\|_{L^2}},\vec A)\,\|\eta_R\,u\|^2_{L^2} + \mathcal E_{V_1}(\frac{\tilde\eta_R\,u}{\|\tilde\eta_R\,u\|_{L^2}},\vec A)\,\|\tilde\eta_R\,u\|^2_{L^2} \\ &\quad + \langle u, (\tilde\eta_R^2\,V_2 - |\vec\nabla\eta_R|^2 - |\vec\nabla\tilde\eta_R|^2)u\rangle \\ &\ge E_V\,\|\eta_R\,u\|^2_{L^2} + E_{V_1}\,\|\tilde\eta_R\,u\|^2_{L^2} - \varepsilon(E_{V_1}-E_V).\end{aligned} \tag{3.40}$$

As $(u_j, \vec{A}_j)$ is a minimizing sequence, (3.40) yields, for j large enough,

$$\|\tilde{\eta}_R\, u_j\|_{L^2}^2 \leq \frac{\mathcal{E}_V(u_j, \vec{A}_j) - E_V}{E_{V_1} - E_V} + \varepsilon \leq 2\varepsilon\,. \tag{3.41}$$

By the lower semi-continuity of the L^2 norm,

$$\|\tilde{\eta}_R\, u_\infty\|_{L^2}^2 \leq \liminf_{j\to\infty} \|\tilde{\eta}_R\, u_j\|_{L^2}^2 \leq 2\varepsilon\,. \tag{3.42}$$

The sequence $(u_j)_j$ converges towards u_∞ weakly in $\mathcal{Q}_V$ and thus the sequence $(\eta_R\, u_j)$ converges weakly in H^1 towards $\eta_R\, u_\infty$. Using the compactness of the set $\overline{B(0,2R)}$ and the Rellich-Kondrachov Theorem, we deduce that $(\eta_R\, u_j)$ converges strongly in L^2 to $\eta_R\, u_\infty$. This together with (3.39), (3.41) and (3.42) prove (3.38).

To show that $\liminf_{j\to\infty} \mathcal{E}(u_j, \vec{A}_j) \geq \mathcal{E}(u_\infty, \vec{A}_\infty)$, we split $\mathcal{E}(u, \vec{A})$ into five parts :

$$\mathcal{E}_V(u,\vec{A}) = \overbrace{\langle u, H_V u\rangle}^{\mathcal{E}_1(u)} + \frac{1}{32\pi^3}\overbrace{\|\vec{A}\|_{\dot{H}^1}^2}^{\mathcal{E}_2(\vec{A})} - 2g\mathfrak{Re}\overbrace{\big\langle -i\vec{\nabla}u, (\hat{\chi}*\vec{A})u\big\rangle}^{\mathcal{E}_3(u,\vec{A})} + \underbrace{\big\langle u, (\hat{\chi}*\vec{A})^2 u\big\rangle}_{\mathcal{E}_4(u,\vec{A})} - g\underbrace{\big\langle u, \vec{\sigma}\cdot(\hat{\chi}*\vec{\nabla}\wedge\vec{A})u\big\rangle}_{\mathcal{E}_5(u,\vec{A})}.$$

By Lemma 3.2.3, we have

$$\liminf_{j\to\infty} \mathcal{E}_1(u_j) \geq \mathcal{E}_1(u_\infty)\,. \tag{3.43}$$

By the lower semi-continuity of $\|\cdot\|_{\dot{H}^1}$,

$$\liminf_{j\to\infty} \mathcal{E}_2(\vec{A}_j) \geq \mathcal{E}_2(\vec{A}_\infty)\,. \tag{3.44}$$

Now using $\vec{\nabla}\cdot\vec{A}_j = 0$, the Cauchy-Schwarz inequality, the boundedness of $(\|(u_j,\vec{A}_j)\|_{\mathcal{U}\times\mathcal{A}})_j$ and Lemma 3.2.4, we obtain

$$|\mathcal{E}_3(u_j,\vec{A}_j) - \big\langle -i\vec{\nabla}u_j, (\hat{\chi}*\vec{A}_j)\,u_\infty\big\rangle + \big\langle(\hat{\chi}*\vec{A}_j)\,u_j,\ -i\vec{\nabla}u_\infty\big\rangle - \mathcal{E}_3(u_\infty,\vec{A}_j)| \lesssim \|u_j - u_\infty\|_{L^2}^{\frac{1}{2}}. \tag{3.45}$$

We claim that the weak convergence of $\vec{A}_j$ towards $\vec{A}_\infty$ then yields

$$\mathcal{E}_3(u_\infty,\vec{A}_j) \xrightarrow[j\to\infty]{} \mathcal{E}_3(u_\infty,\vec{A}_\infty)\,. \tag{3.46}$$

The limit (3.46) can be proven as follows. Let $\varphi = \overline{-i\vec{\nabla}u_\infty}$. Then

$$\mathcal{E}_3(u_\infty,\vec{A}_j) = \int (\hat{\chi}*(u_\infty\varphi))\ \vec{A}_j \tag{3.47}$$

and it thus suffices to verify that $\hat{\chi} * (u_\infty \varphi)$ belongs to $\dot{H}^{-1}$. This is a consequence of Lemma 3.2.5 :

$$\left\|\hat{\chi} * (u_\infty \varphi)\right\|_{\dot{H}^{-1}} \lesssim \left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}} \|u_\infty\|_{H^1} \|\varphi\|_{L^2} \lesssim \left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}} \|u_\infty\|_{H^1}^2 < \infty \,. \tag{3.48}$$

The bound (3.45), and the limit (3.46) yield

$$\mathcal{E}_3(u_j, \vec{A}_j) \xrightarrow[j\to\infty]{} \mathcal{E}_3(u_\infty, \vec{A}_\infty) \,. \tag{3.49}$$

Similarly as in (3.45), we have

$$|\mathcal{E}_4(u_j, \vec{A}_j) - \langle u_\infty, \vec{A}_j^2 u_j \rangle_{L^2} + \langle u_\infty, \vec{A}_j^2 u_j \rangle_{L^2} - \mathcal{E}_4(u_\infty, \vec{A}_j)| \lesssim \|u_j - u_\infty\|_{L^2}^{\frac{1}{2}} \,. \tag{3.50}$$

Let us now prove that

$$\liminf_{j\to\infty} \mathcal{E}_4(u_\infty, \vec{A}_j) \geq \mathcal{E}_4(u_\infty, \vec{A}_\infty) \,. \tag{3.51}$$

Using the same arguments as those used to prove the lower semicontinuity of norms, we can write

$$\mathcal{E}_4(u_\infty, \vec{A}_j - \vec{A}_\infty) = \mathcal{E}_4(u_\infty, \vec{A}_j) + \mathcal{E}_4(u_\infty, \vec{A}_\infty) - 2\mathfrak{Re}\left\langle (\hat{\chi} * \vec{A}_\infty) u_\infty, (\hat{\chi} * \vec{A}_j) u_\infty \right\rangle \geq 0 \tag{3.52}$$

and arguing as in (3.47), with $\varphi = \overline{(\hat{\chi} * \vec{A}_\infty) u_\infty}$ (which belongs to L^2 by Lemma 3.2.4), we deduce that

$$\left\langle (\hat{\chi} * \vec{A}_\infty) u_\infty, (\hat{\chi} * \vec{A}_j) u_\infty \right\rangle = \int (\hat{\chi} * (u_\infty \varphi))\, \vec{A}_j \xrightarrow[j\to\infty]{} \mathcal{E}_4(u_\infty, \vec{A}_\infty) \,. \tag{3.53}$$

Now (3.52)-(3.53) imply (3.51). A convenient expression of the last term,

$$\mathcal{E}_5(u, \vec{A}) = \langle u, \vec{\sigma} \cdot (\hat{\chi} * \vec{\nabla} \wedge \vec{A}) u \rangle = -2\mathfrak{Re}\langle \vec{\nabla} \wedge \vec{\sigma} u \,, (\hat{\chi} * \vec{A}) u \rangle,$$

shows that it can be handled as $\mathcal{E}_3$ and

$$\mathcal{E}_5(u_j, \vec{A}_j) \xrightarrow[j\to\infty]{} \mathcal{E}_5(u_\infty, \vec{A}_\infty) \,.$$

Finally, (3.43), (3.44), (3.49), (3.50), (3.51) and (3.49) imply that

$$\liminf_{j\to\infty} \mathcal{E}(u_j, \vec{A}_j) \geq \mathcal{E}(u_\infty, \vec{A}_\infty)$$

and hence the infimum is indeed a minimum, since $(u_\infty, \vec{A}_\infty)$ is a minimizer. □

To conclude this subsection, we focus on the condition $E_{V_1} > E_V$ which was a crucial assumption in our proof of the existence of a minimizer in Theorem 3.1.3. As mentioned in Remark 3.1.6, the next proposition shows that this condition is satisfied provided that $|g|\, \|\chi_2/|k|\|_{L^{3,\infty}}$ is not too large and that either V is confining (recall from Lemma 3.2.2 that in this case μ_{V_1} can be chosen arbitrarily large) or $\mu_{V_1} > \mu_V$ and $|g|\, \|\chi/|k|\|_{L^2+L^{3,\infty}}$ is small enough.

Proposition 3.3.6 (Existence of a gap)**.** *Suppose that V satisfies Hypothesis 3.1.1 and that the cut-off function $\chi = \chi_1 + \chi_2$ satisfies Hypothesis 3.1.3 with $\chi_1/|k|$ in L^2 and $\chi_2/|k|$ in $L^{3,\infty}$. If $\mu_V \geq 0$, then there exists a positive constant C_V such that, for all $0 < \beta < 1 - C_V g \, \|\chi_2/|k|\|_{L^{3,\infty}}$,*

$$E_{V_1} - E_V \geq \min\Big(1, \Big(1 - \beta - C_V g \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big)\mu_{V_1} - \mu_V - \frac{C_V^2 g^2}{4\beta}\left\|\frac{\chi_1}{|k|}\right\|_{L^2}^2 - C_V g \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big).$$

Proof. Restricting the infimum of $\mathcal{E}_V$ to $\mathcal{U} \times \{\vec{0}\}$ yields an upper bound for E_V :

$$E_V = \inf_{(u,\vec{A}) \in \mathcal{U} \times \mathcal{A}} \mathcal{E}_V(u, \vec{A}) \leq \inf_{u \in \mathcal{U}} \mathcal{E}_V(u, \vec{0}) = \mu_V \, . \tag{3.54}$$

To control E_{V_1} from below, recall that

$$\mathcal{E}_{V_1}(u, \vec{A}) = \|\vec{\sigma} \cdot (-i\vec{\nabla} - g\hat{\chi} * \vec{A})\, u\|_{L^2}^2 + \langle u, V_1 u\rangle + \frac{1}{32\pi^3}\|\vec{A}\|_{\dot{H}^1}^2.$$

If $\|\vec{A}\|_{\dot{H}^1}^2/(32\pi^3) \geq \mu_V + 1$, then

$$\mathcal{E}_{V_1}(u, \vec{A}) \geq \mu_V + 1.$$

Suppose now that $\|\vec{A}\|_{\dot{H}^1}^2/(32\pi^3) \leq \mu_V + 1$. Then, with $C > 0$ the universal constant from Lemma 3.2.4, and $C_V = 2C\sqrt{\mu_V + 1}$,

$$\begin{aligned}
\mathcal{E}_{V_1}(u, \vec{A}) &\geq \langle u, (-\Delta_x + V_1)u\rangle - 2g\big|\langle \vec{\sigma} \cdot \vec{\nabla} u \,, \vec{\sigma} \cdot (\hat{\chi} * \vec{A})u\rangle\big| \\
&\geq \langle u, (-\Delta_x + V_1)u\rangle - 2gC\|u\|_{\dot{H}^1}\|\vec{A}\|_{\dot{H}^1}\left(\left\|\frac{\chi_1}{|k|}\right\|_{L^2} + \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\|u\|_{\dot{H}^{1/2}}\right) \\
&\geq \langle u, (-\Delta_x + V_1)u\rangle - gC_V\left(\left\|\frac{\chi_1}{|k|}\right\|_{L^2}\|u\|_{\dot{H}^1} + \left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\|u\|_{\dot{H}^1}^2\right) .
\end{aligned}$$

Now, thanks to the conditions on β,

$$\begin{aligned}
\mathcal{E}_{V_1}(u, \vec{A}) &\geq \Big(1 - \beta - gC_V\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big)\langle u, (-\Delta_x + V_1)u\rangle - \frac{C_V^2 g^2}{4\beta}\left\|\frac{\chi_1}{|k|}\right\|_{L^2}^2 - gC_V\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}} \\
&\geq \Big(1 - \beta - gC_V\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big)\mu_{V_1} - \frac{C_V^2 g^2}{4\beta}\left\|\frac{\chi_1}{|k|}\right\|_{L^2}^2 - gC_V\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}} .
\end{aligned}$$

Therefore

$$E_{V_1} \geq \min\Big(\mu_V + 1, \Big(1 - \beta - C_V g\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big)\mu_{V_1} - \frac{C_V^2 g^2}{4\beta}\left\|\frac{\chi_1}{|k|}\right\|_{L^2}^2 - C_V g\left\|\frac{\chi_2}{|k|}\right\|_{L^{3,\infty}}\Big),$$

which together with (3.54) yields the result. □

3.3.3 Properties of the set of minimizers

In this section we prove some estimates on minimizers $(u_{\mathrm{gs}}, \vec{A}_{\mathrm{gs}})$ of the Maxwell–Schrödinger energy functional, which in turn implies that $\vec{A}_{\mathrm{gs}}$ is fully determined by u_{gs} for small g.

We use the following notations. The resolvent of the operator $H_V \otimes \mathbf{I}_{\mathbb{C}^2}$ is denoted by $R_\lambda := (H_V - \lambda)^{-1} \otimes \mathbf{I}_{\mathbb{C}^2}$ (a priori defined as an unbounded operator on the set $\mathrm{Ran}(\mathbb{1}_{\{\lambda\}}(H_V \otimes \mathbf{I}_{\mathbb{C}^2}))^\perp)$. Recall that Π_V, $\Pi_V^\perp$ are the projections in $L^2(\mathbb{R}^3;\mathbb{C}^2)$ defined by $\Pi_V := |u_V\rangle\langle u_V| \otimes \mathbf{I}_{\mathbb{C}^2}$, $\Pi_V^\perp = \mathbf{I}_{L^2} - \Pi_V$. Moreover, for all u in $\mathcal{Q}_V$, we set $\varphi = \Pi_V^\perp u$.

In the next lemma, under hypotheses which implies the existence of a ground state u_V for H_V, we obtain an equation satisfied by φ at a minimizer. Moreover, using the Euler-Lagrange equation for $\vec{A}_{\mathrm{gs}}$, we obtain a control over u_{gs} and $\vec{A}_{\mathrm{gs}}$.

Lemma 3.3.7. *Suppose that V satisfies Hypotheses 3.1.1 and 3.1.2 and that χ satisfies Hypothesis 3.1.3. Let $(u_{\mathrm{gs}}, \vec{A}_{\mathrm{gs}})$ in $\mathcal{U} \times \mathcal{A}$ be a global minimizer of $\mathcal{E}$. Then*

$$\varphi_{\mathrm{gs}} = R_{E_V}\Pi_V^\perp\Big[2(-i\vec{\nabla}u_{\mathrm{gs}})\cdot(g\hat{\chi} * \vec{A}_{\mathrm{gs}}) - g\hat{\chi} * \vec{\sigma}\cdot(\vec{\nabla}\wedge\vec{A}_{\mathrm{gs}})u_{\mathrm{gs}} - (g\hat{\chi} * \vec{A}_{\mathrm{gs}})^2 u_{\mathrm{gs}} - \frac{1}{32\pi^3}\|\vec{A}_{\mathrm{gs}}\|_{\dot{H}^1}^2 u_{\mathrm{gs}}\Big]. \quad (3.55)$$

Moreover, there exist $\varepsilon_V > 0$ and $C_V > 0$ such that, if

$$\mathbf{g}_\chi := |g|\Big\|\frac{\chi}{|k|}\Big\|_{L^2+L^{3,\infty}} \le \varepsilon_V, \quad (3.56)$$

then the following estimates hold

$$\|\varphi_{\mathrm{gs}}\|_{\mathcal{Q}_V} \le C_V \mathbf{g}_\chi^2, \quad (3.57)$$

$$\|\vec{A}_{\mathrm{gs}}\|_{\dot{H}^1} \le C_V \mathbf{g}_\chi, \quad (3.58)$$

$$\|\vec{A}_{\mathrm{gs}} - \vec{A}_{\mathrm{gs}}^{[1]}\|_{\dot{H}^1} = \|\vec{\nabla}\wedge\vec{A}_{\mathrm{gs}} - \vec{\nabla}\wedge\vec{A}_{\mathrm{gs}}^{[1]}\|_{L^2} \le C_V \mathbf{g}_\chi^3, \quad (3.59)$$

with

$$\vec{A}_{\mathrm{gs}}^{[1]} := 16\pi^3(-\Delta)^{-1} g\hat{\chi} * \vec{\nabla}\wedge u_V^2\vec{\omega}_{\mathrm{gs}}, \quad (3.60)$$

and where the vector $\vec{\omega}_{\mathrm{gs}}$ in $\mathbb{C}^3$ is defined by the relation

$$u_V^2\vec{\omega}_{\mathrm{gs}} = \langle \Pi_V u_{\mathrm{gs}}, \vec{\sigma}\,\Pi_V u_{\mathrm{gs}}\rangle_{\mathbb{C}^2}. \quad (3.61)$$

By (3.57), $\big||\vec{\omega}_{\mathrm{gs}}|^2 - 1\big| \le C_V \mathbf{g}_\chi^4$.

Remark 3.3.8. *Note that in (3.61) both sides are functions of x as the scalar product on the right hand side is only on the $\mathbb{C}^2$ space.*

Proof of Lemma 3.3.7. To prove (3.55), it suffices to observe that $E_V \le \mu_V = \inf\sigma(H_V)$ (see (3.54)), and hence that $R_{E_V}\Pi_V^\perp$ is well-defined and identifies with an element of $\mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$. Applying $R_{E_V}\Pi_V^\perp$ to (3.35) then yields (3.55).

Now we prove (3.58). First observe that, by Lemma 3.3.5, the assumption (3.56) and the fact that $E_V \le \mu_V$, we have, for ε_V sufficiently small,

$$\big\|(u_{\rm gs}, \vec{A}_{\rm gs})\big\|_{\mathcal{U}\times\mathcal{A}} \le C_V ,$$

for some constant $C_V > 0$, uniformly in g and χ such that $\mathbf{g}_\chi \le \varepsilon_V$. Using (3.32) and Lemmata 3.2.4–3.2.5, we then estimate

$$\begin{aligned}\big\|\vec{A}_{\rm gs}\big\|_{\dot{H}^1} &\le C\big\|\, g\hat{\chi} * \mathfrak{Re}\langle -i\vec{\nabla} u_{\rm gs} + \vec{\nabla}\wedge\vec{\sigma} u_{\rm gs}, u_{\rm gs}\rangle_{\mathbb{C}^2}\big\|_{\dot{H}^{-1}} + C\big\|\, g\hat{\chi} * [(g\hat{\chi} * \vec{A}_{\rm gs})\, |u_{\rm gs}|^2_{\mathbb{C}^2}]\big\|_{\dot{H}^{-1}} \\ &\le C|g| \left\|\frac{\chi}{|k|}\right\|_{L^2+L^{3,\infty}} \|u_{\rm gs}\|_{H^1} + Cg^2 \left\|\frac{\chi}{|k|}\right\|^2_{L^2+L^{3,\infty}} \big\|\vec{A}_{\rm gs}\big\|_{\dot{H}^1} \|u_{\rm gs}\|_{H^1} \\ &\le 2CR_V \mathbf{g}_\chi \,. \end{aligned} \tag{3.62}$$

Next using (3.55), the fact that $R_{E_V}\Pi_V^\perp \in \mathcal{L}(\mathcal{Q}_V^*, \mathcal{Q}_V)$, the continuous embedding $L^2 \subset \mathcal{Q}_V^*$, (3.62) and Lemma 3.2.4, we obtain

$$\|\varphi_{\rm gs}\|_{\mathcal{Q}_V} \le C_V \mathbf{g}_\chi^2 ,$$

for some constant $C_V > 0$.

Let us now prove (3.59) starting from the formula given in (3.32) for $\vec{A}_{\rm gs}$. Note that the constant C_V might change from one line to the other. Applying Lemma 3.2.5 first and then Lemma 3.2.4, the boundedness of $u_{\rm gs}$ in $\mathcal{Q}_V$ and (3.58),

$$\begin{aligned}\|(-\Delta)^{-1} g\hat{\chi} * \mathfrak{Re}\big\langle (g\hat{\chi} * \vec{A}_{\rm gs})u_{\rm gs}, u_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^1} &\le C_V \mathbf{g}_\chi \|(g\hat{\chi} * \vec{A}_{\rm gs})u_{\rm gs}\|_{L^2}\|u_{\rm gs}\|_{H^1} \\ &\le C_V \mathbf{g}_\chi^2 \|\vec{A}_{\rm gs}\|_{\dot{H}^1}\|u_{\rm gs}\|^2_{H^1} \le C_V \mathbf{g}_\chi^3 \,. \end{aligned} \tag{3.63}$$

By Lemma 3.2.4, the boundedness of $u_{\rm gs}$ in $\mathcal{Q}_V$ and (3.57),

$$\begin{aligned} &\|(-\Delta)^{-1} g\hat{\chi} * \mathfrak{Re}\big\langle -i\vec{\nabla} u_{\rm gs}, u_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^1} \\ &\le \|g\hat{\chi} * \mathfrak{Re}\big\langle i\vec{\nabla}\Pi_V u_{\rm gs}, \Pi_V u_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^{-1}} + 2\|g\hat{\chi} * \big\langle \vec{\nabla}\Pi_V u_{\rm gs}, \varphi_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^{-1}} + \|g\hat{\chi} * \big\langle \vec{\nabla}\varphi_{\rm gs}, \varphi_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^{-1}} \\ &\le 0 + C_V \mathbf{g}_\chi \|\vec{\nabla}\Pi_V u_{\rm gs}\|_{L^2}\|\varphi_{\rm gs}\|_{\dot{H}^1} + C_V \mathbf{g}_\chi \|\vec{\nabla}\varphi_{\rm gs}\|_{L^2}\|\varphi_{\rm gs}\|_{\dot{H}^1} \le C_V \mathbf{g}_\chi^3 \,. \end{aligned} \tag{3.64}$$

Applying Lemma 3.2.5 first, then the boundedness of $u_{\rm gs}$ in $\mathcal{Q}_V$ and (3.57), we obtain

$$\begin{aligned} &\|(-\Delta)^{-1} g\hat{\chi} * \mathfrak{Re}\big\langle \vec{\nabla}\wedge\vec{\sigma}\, u_{\rm gs}, u_{\rm gs}\big\rangle_{\mathbb{C}^2} - (-\Delta)^{-1} g\hat{\chi} * \mathfrak{Re}\big\langle \vec{\nabla}\wedge\vec{\sigma}\,\Pi_V u_{\rm gs}, \Pi_V u_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^1} \\ &\le 2\|g\hat{\chi} * \big\langle \vec{\nabla}\wedge\vec{\sigma}\,\varphi_{\rm gs}, \Pi_V u_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^{-1}} + \|g\hat{\chi} * \big\langle \vec{\nabla}\wedge\vec{\sigma}\,\varphi_{\rm gs}, \varphi_{\rm gs}\big\rangle_{\mathbb{C}^2}\|_{\dot{H}^{-1}} \\ &\le C_V \mathbf{g}_\chi \|\vec{\nabla}\wedge\vec{\sigma}\,\varphi_{\rm gs}\|_{L^2}(\|\Pi_V u_{\rm gs}\|_{H^1} + \|\varphi_{\rm gs}\|_{H^1}) \le C_V \mathbf{g}_\chi^3 \,. \end{aligned} \tag{3.65}$$

Then, from $\vec{\nabla}\wedge\langle u, \vec{\sigma} u\rangle = 2\mathfrak{Re}\langle u, \vec{\nabla}\wedge\vec{\sigma} u\rangle$ the equality

$$(-\Delta)^{-1} g\hat{\chi} * 2\mathfrak{Re}\big\langle \vec{\nabla}\wedge\vec{\sigma}\,\Pi_V u_{\rm gs}, \Pi_V u_{\rm gs}\big\rangle_{\mathbb{C}^2} = (-\Delta)^{-1} g\hat{\chi} * \vec{\nabla} u_V^2 \wedge \vec{\omega}_{\rm gs}$$

follows, which, along with (3.63), (3.64) and (3.65), yields (3.59).

Finally, since $\vec{\nabla}\cdot\vec{A}_{\rm gs}=\vec{\nabla}\cdot\vec{A}_{\rm gs}^{[1]}=0$, using the formula $\vec{\nabla}\wedge\vec{\nabla}\wedge\vec{A}=-\Delta\vec{A}-\vec{\nabla}(\vec{\nabla}\cdot\vec{A})$,

$$\big\|\vec{\nabla}\wedge(\vec{A}_{\rm gs}-\vec{A}_{\rm gs}^{[1]})\big\|_{L^2}=\big\|\vec{A}_{\rm gs}-\vec{A}_{\rm gs}^{[1]}\big\|_{\dot{H}^1}\,.$$

This concludes the proof of Lemma 3.3.7. □

Now we can prove that $\vec{A}_{\rm gs}$ is fully determined by $u_{\rm gs}$ for small g.

Proposition 3.3.9. *Suppose that V satisfies Hypotheses 3.1.1 and 3.1.2 and that χ satisfies Hypothesis 3.1.3. Suppose that the decomposition $V=V_1+V_2$ of Hypothesis 3.1.1 can be chosen such that $E_{V_1}>E_V$. There exists $\varepsilon_V>0$ such that, if*

$$\mathbf{g}_\chi:=|g|\Big\|\frac{\chi}{|k|}\Big\|_{L^2+L^{3,\infty}}\le\varepsilon_V,$$

then if $(u_{\rm gs},\vec{A}_{\rm gs})$ and $(u_{\rm gs},\vec{A}'_{\rm gs})$ are minimizers of $\mathcal{E}$, necessarily $\vec{A}_{\rm gs}=\vec{A}'_{\rm gs}$.

Proof. In this proof we drop the indices gs to simplify the notations. For sufficiently small $\mathbf{g}_\chi$, if $(u,\vec{A})$ and $(u,\vec{A}')$ are minimizers, (3.32) yields

$$\vec{A}-\vec{A}'=-32\pi^3(-\Delta)^{-1}g\hat{\chi}*\big[(g\hat{\chi}*(\vec{A}-\vec{A}'))\,|u|^2_{\mathbb{C}^2}\big]\,.$$

It follows from Lemmata 3.2.5 and 3.2.4 that

$$\begin{aligned}\big\|\vec{A}-\vec{A}'\big\|_{\dot{H}^1}&=32\pi^3\big\|g\hat{\chi}*[(g\hat{\chi}*(\vec{A}-\vec{A}'))|u|^2_{\mathbb{C}^2}]\big\|_{\dot{H}^{-1}}\\&\le C\mathbf{g}_\chi\big\|(g\hat{\chi}*(\vec{A}-\vec{A}'))u\|_{L^2}\|u\|_{H^1}\\&\le C^2\mathbf{g}_\chi^2\big\|\vec{A}-\vec{A}'\big\|_{\dot{H}^1}\|u\|^2_{H^1}\\&\le C_V^2\mathbf{g}_\chi^2\big\|\vec{A}-\vec{A}'\big\|_{\dot{H}^1}\,,\end{aligned}$$

which implies that, for sufficiently small $\mathbf{g}_\chi$, $\vec{A}=\vec{A}'$. □

3.3.4 Expansion of the minimum at small coupling

In this section, we prove Proposition 3.1.9, by establishing the asymptotic expansion (3.19).

Proof of Proposition 3.1.9. Recall that

$$\begin{aligned}E_V=\mathcal{E}_V(u_{\rm gs},\vec{A}_{\rm gs})=&\overbrace{\langle u_{\rm gs},H_Vu_{\rm gs}\rangle}^{(i)}-\overbrace{2\mathfrak{Re}\big\langle-i\vec{\nabla}u_{\rm gs},(g\hat{\chi}*\vec{A}_{\rm gs})u_{\rm gs}\big\rangle}^{(ii)}\\&-\underbrace{\big\langle u_{\rm gs},\vec{\sigma}\cdot(g\hat{\chi}*\vec{\nabla}\wedge\vec{A}_{\rm gs})u_{\rm gs}\big\rangle}_{(iii)}+\underbrace{\big\langle u_{\rm gs},(g\hat{\chi}*\vec{A}_{\rm gs})^2u_{\rm gs}\big\rangle}_{(iv)}+\frac{1}{32\pi^3}\underbrace{\big\|\vec{A}_{\rm gs}\big\|^2_{\dot{H}^1}}_{(v)}\,.\end{aligned}$$

For (i), using that $H_V \Pi_V u_{\rm gs} = \mu_V \Pi_V u_{\rm gs}$, $\Pi_V u_{\rm gs} \perp \varphi_{\rm gs}$ and (3.57), we obtain

$$|(i) - \mu_V| \le |\langle \varphi_{\rm gs}, H_V \varphi_{\rm gs}\rangle| \le C_V \mathbf{g}_\chi^4.$$

Next we decompose (ii) into three terms :

$$(ii) = g\mathfrak{Re}\big\langle -i\vec{\nabla}\Pi_V u_{\rm gs}, (\hat{\chi} * \vec{A}_{\rm gs})\Pi_V u_{\rm gs}\big\rangle \\ + 2g\mathfrak{Re}\big\langle -i\vec{\nabla}\Pi_V u_{\rm gs}, (\hat{\chi} * \vec{A}_{\rm gs})\varphi_{\rm gs}\big\rangle + g\mathfrak{Re}\big\langle -i\vec{\nabla}\varphi_{\rm gs}, (\hat{\chi} * \vec{A}_{\rm gs})\varphi_{\rm gs}\big\rangle.$$

The first term vanishes because, with $\Pi_V u_{\rm gs} = \binom{a}{b} u_V$ for some coefficients a and b in $\mathbb{C}$,

$$g\mathfrak{Re}\big\langle -i\vec{\nabla}\Pi_V u_{\rm gs}, (\hat{\chi} * \vec{A}_{\rm gs})\Pi_V u_{\rm gs}\big\rangle = g(|a|^2 + |b|^2)\mathfrak{Re}\big\langle -i\vec{\nabla} u_V, (\hat{\chi} * \vec{A}_{\rm gs}) u_V\big\rangle = 0\,,$$

since u_V, $\hat{\chi}$ and $\vec{A}_{\rm gs}$ are real-valued. The next term in (ii) is controlled using Cauchy-Schwarz's inequality followed by Lemmata 3.2.4 and 3.3.7,

$$|\big\langle -i\vec{\nabla}\Pi_V u_{\rm gs}, (g\hat{\chi} * \vec{A}_{\rm gs})\varphi_{\rm gs}\big\rangle| \le C_V \mathbf{g}_\chi \|\vec{\nabla}\Pi_V u_{\rm gs}\|_{L^2} \|\vec{A}_{\rm gs}\|_{\dot{H}^1} \|\varphi_{\rm gs}\|_{H^1} \le C_V \mathbf{g}_\chi^4\,.$$

The last term in (ii) is bounded by $C_V \mathbf{g}_\chi^6$ using similar arguments.

Similarly, (iv) is bounded by $C_V \mathbf{g}_\chi^4$.

As for (iii), using the formula $\int \vec{w}_1 \cdot \vec{\nabla} \wedge \vec{w}_2 = \int \vec{w}_2 \cdot \vec{\nabla} \wedge \vec{w}_1$, we can rewrite

$$(iii) = \int (g\hat{\chi} * \vec{A}_{\rm gs}) \cdot \vec{\nabla} \wedge \big\langle u_{\rm gs}, \vec{\sigma} u_{\rm gs}\big\rangle_{\mathbb{C}^2}\,.$$

In this form, it can be shown using the same arguments as before that

$$\Big|(iii) - \int (g\hat{\chi} * \vec{A}^{[1]}_{\rm gs}) \cdot \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs}\Big| \le C_V \mathbf{g}_\chi^4,$$

where we recall that $\omega_{\rm gs}$ has been defined in (3.61). Now, thanks to (3.60) and the formula $\vec{\nabla} \wedge \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs} = -\Delta u_V^2 \vec{\omega}_{\rm gs} - \vec{\nabla}(\vec{\nabla} \cdot u_V^2 \vec{\omega}_{\rm gs})$, we have

$$\int (g\hat{\chi} * \vec{A}^{[1]}_{\rm gs}) \cdot \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs} = 16\pi^3 \int (g\hat{\chi} * \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs}) \cdot ((-\Delta)^{-1} g\hat{\chi} * \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs}) \\ = 16\pi^3 \int (g\hat{\chi} * u_V^2)^2 |\vec{\omega}_{\rm gs}|^2 + 16\pi^3 \int ((-\Delta)^{-1} g\hat{\chi} * \vec{\omega}_{\rm gs} \cdot \vec{\nabla} u_V^2)(g\hat{\chi} * \vec{\omega}_{\rm gs} \cdot \vec{\nabla} u_V^2). \quad (3.66)$$

To estimate (v), we use Lemma 3.3.7, which shows that

$$\Big|(v) - \|\vec{A}^{[1]}_{\rm gs}\|^2_{\dot{H}^1}\Big| \le C_V \mathbf{g}_\chi^4\,.$$

A direct computation then gives

$$\|\vec{A}^{[1]}_{\rm gs}\|^2_{\dot{H}^1} = (16\pi^3)^2 \int (g\hat{\chi} * \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs}) \cdot ((-\Delta)^{-1} g\hat{\chi} * \vec{\nabla} \wedge u_V^2 \vec{\omega}_{\rm gs}),$$

namely we obtain the same term as in (3.66), with a different pre-factor.

Putting all together, we have shown that

$$\Big|E_V - \mu_V + 8\pi^3 g^2\Big(\int (\hat{\chi} * u_V^2)^2 |\vec{\omega}_{\mathrm{gs}}|^2 + \int ((-\Delta)^{-1}\hat{\chi} * \vec{\omega}_{\mathrm{gs}} \cdot \vec{\nabla} u_V^2)(\hat{\chi} * \vec{\omega}_{\mathrm{gs}} \cdot \vec{\nabla} u_V^2)\Big)\Big| \leq C_V \mathbf{g}_\chi^4.$$

We have $|1-|\vec{\omega}_{\mathrm{gs}}|^2| \leq C_V \mathbf{g}_\chi^4$ (see Lemma 3.3.7). Moreover, in the case of a radial potential V, the ground state u_V of H_V is radial. If in addition χ is radial, then the second term in the right-hand side of the previous equation can be expressed independently of $\vec{\omega}_{\mathrm{gs}}$. This directly leads to (3.19). □

3.3.5 Ultraviolet limit of the ground state energies

We suppose in this section that the interaction between the non-relativistic particle and the field is cut-off in the ultraviolet, i.e. that the Maxwell–Schrödinger energy functional is given by (3.20) with $\chi_\Lambda = \chi \mathbb{1}_{|k|\leq\Lambda}$, for some ultraviolet parameter $\Lambda > 0$. We then study the limit $\Lambda \to \infty$. In this section we drop the index V for $\mathcal{E}_V$ as the potential remains fixed throughout the section.

As in the previous sections, χ will be fixed such that $\chi/|k|$ lies in $L^2+L^{3,\infty}$. In particular, we have $\chi_\Lambda/|k|$ in L^2 and $\chi_\Lambda/\sqrt{|k|}$ in L^2, which in turn implies that the ultraviolet cut-off Pauli-Fierz Hamiltonian

$$\mathbb{H}_\Lambda := \big(\vec{\sigma} \cdot \big(-i\vec{\nabla}_x \otimes \mathbf{I}_{\mathrm{f}} - \vec{\mathbb{A}}(\vec{m}_{\chi_\Lambda,x})\big)\big)^2 + V \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbb{H}_{\mathrm{f}},$$

identifies to a self-adjoint operator (see Appendix 3.4).

We show that the ground state energies $E_{V,\Lambda}$ defined in (3.21) converge to E_V in the ultraviolet limit $\Lambda \to \infty$. It should be noted that, in general, $|k|^{-1}\chi_\Lambda$ does *not* converge to $|k|^{-1}\chi$ in $L^2 + L^{3,\infty}$. To circumvent this difficulty, we will use the following relation

$$\hat{\chi}_\Lambda * \vec{A} = (2\pi)^{-3}\mathcal{F}(\chi_\Lambda \bar{\mathcal{F}}(\vec{A})) = (2\pi)^{-3}\mathcal{F}(\chi \bar{\mathcal{F}}(\mathbb{1}_{|-i\vec{\nabla}|\leq\Lambda}\vec{A})) = \hat{\chi} * \vec{A}_{\leq\Lambda}, \tag{3.67}$$

where we have set

$$\vec{A}_{\leq\Lambda} := \mathbb{1}_{|-i\vec{\nabla}|\leq\Lambda}(\vec{A}).$$

Recalling from (3.16) that $\mathcal{A} = \{\vec{A} \in \dot{H}^1(\mathbb{R}^3;\mathbb{R}^3) \mid \vec{\nabla}\cdot\vec{A} = 0\}$, we introduce the subspace

$$\mathcal{A}_{\leq\Lambda} := \{\vec{A} \in \mathcal{A} \mid \vec{A} = \mathbb{1}_{|-i\vec{\nabla}|\leq\Lambda}(\vec{A})\}\,. \tag{3.68}$$

We then have the following identity.

Lemma 3.3.10. *Suppose that V satisfies Hypothesis 3.1.1 and that χ satisfies Hypothesis 3.1.3. Then, for all $\Lambda > 0$,*

$$E_{V,\Lambda} = \inf_{(u,\vec{A})\in\mathcal{U}\times\mathcal{A}_{\leq\Lambda}} \mathcal{E}(u,\vec{A}).$$

Proof. It suffices to observe that, by (3.67), the following equality holds for all $(u, \vec{A})$ in $\mathcal{U} \times \mathcal{A}$:

$$\mathcal{E}_\Lambda(u, \vec{A}) = \mathcal{E}(u, \vec{A}_{\leq \Lambda}) + \frac{1}{32\pi^3} \big\| \mathbb{1}_{|-i\vec{\nabla}| \geq \Lambda}(\vec{A}) \big\|^2_{\dot{H}^1}. \tag{3.69}$$

The statement of the lemma directly follows. □

If $\vec{A}$ belongs to $\dot{H}^1$, we have that $\|\vec{A}_{\leq\Lambda} - \vec{A}\|_{\dot{H}^1} \to 0$ as $\Lambda \to \infty$. Now we can prove the convergence of the ground state energies in the ultraviolet limit.

Proof of Proposition 3.1.11. For $0 < \Lambda \leq \Lambda'$, we have $\mathcal{A}_{\leq\Lambda} \subseteq \mathcal{A}_{\leq\Lambda'} \subset \mathcal{A}$ and hence, by Lemma 3.3.10,

$$E_V \leq E_{V,\Lambda'} \leq E_{V,\Lambda}.$$

Therefore $\Lambda \mapsto E_{V,\Lambda}$ is non-increasing on $(0, \infty)$, bounded below by E_V, so that we can define

$$E_{V,\infty} := \lim_{\Lambda\to\infty} E_{V,\Lambda} \geq E_V.$$

To show that $E_{V,\infty} \leq E_V$, let $\varepsilon > 0$ and let $(u_\varepsilon, \vec{A}_\varepsilon)$ in $\mathcal{U} \times \mathcal{A}$ be such that $\mathcal{E}(u_\varepsilon, \vec{A}_\varepsilon) \leq E_V + \varepsilon$. Using (3.69), we have

$$\begin{aligned} E_{V,\Lambda} \leq \mathcal{E}_\Lambda(u_\varepsilon, \vec{A}_\varepsilon) &= \mathcal{E}(u_\varepsilon, \vec{A}_{\varepsilon,\leq\Lambda}) + \frac{1}{32\pi^3} \big\| \mathbb{1}_{|-i\vec{\nabla}|\geq\Lambda} \vec{A}_\varepsilon \big\|^2_{\dot{H}^1} \\ &\leq E_V + \varepsilon + \mathcal{E}(u_\varepsilon, \vec{A}_{\varepsilon,\leq\Lambda}) - \mathcal{E}(u_\varepsilon, \vec{A}_\varepsilon) + \frac{1}{32\pi^3} \big\| \mathbb{1}_{|-i\vec{\nabla}|\geq\Lambda} \vec{A}_\varepsilon \big\|^2_{\dot{H}^1}. \end{aligned}$$

A direct computation shows that

$$\begin{aligned} \Big| \mathcal{E}(u_\varepsilon, \vec{A}_{\varepsilon,\leq\Lambda}) - \mathcal{E}(u_\varepsilon, \vec{A}_\varepsilon) + \frac{1}{32\pi^3} \big\| \mathbb{1}_{|-i\vec{\nabla}|\geq\Lambda} \vec{A}_\varepsilon \big\|^2_{\dot{H}^1} \Big| \\ \leq 2|g| \, \big| \big\langle \vec{\sigma} \cdot (-i\vec{\nabla} u_\varepsilon), \vec{\sigma} \cdot \hat{\chi} * (\vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon) u_\varepsilon \big\rangle_{L^2} \big| \\ + g^2 \Big| \big\| (\hat{\chi} * \vec{A}_{\varepsilon,\leq\Lambda}) u_\varepsilon \big\|^2_{L^2} - \big\| (\hat{\chi} * \vec{A}_\varepsilon) u_\varepsilon \big\|^2_{L^2} \Big|. \end{aligned} \tag{3.70}$$

Applying Lemma 3.2.4 gives

$$\big| \big\langle \vec{\sigma} \cdot (-i\vec{\nabla} u_\varepsilon), \vec{\sigma} \cdot \hat{\chi} * (\vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon) u_\varepsilon \big\rangle_{L^2} \big| \leq C_{\chi,u_\varepsilon} \big\| \vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon \big\|_{\dot{H}^1},$$

for some constant C_{χ,u_ε} depending on χ and u_ε. Likewise,

$$\begin{aligned} \Big| \big\| (\hat{\chi} * \vec{A}_{\varepsilon,\leq\Lambda}) u_\varepsilon \big\|^2 - \big\| (\hat{\chi} * \vec{A}_\varepsilon) u_\varepsilon \big\|^2_{L^2} \Big| \\ \leq \big\| \big(\hat{\chi} * (\vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon)\big) u_\varepsilon \big\|_{L^2} \big(\big\| (\hat{\chi} * \vec{A}_{\varepsilon,\leq\Lambda}) u_\varepsilon \big\|_{L^2} + \big\| (\hat{\chi} * \vec{A}_\varepsilon) u_\varepsilon \big\|_{L^2} \big) \\ \leq C_{\chi,u_\varepsilon,\vec{A}_\varepsilon} \big\| \vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon \big\|_{\dot{H}^1}. \end{aligned}$$

Since $\|\vec{A}_{\varepsilon,\leq\Lambda} - \vec{A}_\varepsilon\|_{\dot{H}^1} \to 0$ as $\Lambda \to \infty$, inserting the previous estimates into (3.70) and letting $\Lambda \to \infty$, we obtain

$$E_{V,\infty} \leq E_V + \varepsilon.$$

Since $\varepsilon > 0$ is arbitrary, this concludes the proof of the proposition. □

3.4 Appendix : Operators in Fock space, self-adjointness

In this appendix we set up some notations and give the proof of the self-adjointness of the Pauli-Fierz operator $\mathbb{H}$. We recall the definitions of standard operators in Fock space. We only give here formal definitions, referring the reader to e.g. [40, 107] for more details.

Let us consider a Hilbert space $\mathfrak{h}$ and its associated symmetric Fock space $\mathfrak{F}_s(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \bigvee^n \mathfrak{h}$, with $\bigvee^0 \mathfrak{h} := \mathbb{C}$. Let $h \in \mathfrak{h}$. For $n \in \mathbb{N}$, the creation and annihilation operators are respectively defined as

$$a^*(h)_{|\bigvee^n \mathfrak{h}} = \sqrt{(n+1)}\, |h\rangle \bigvee \mathbf{I}_{\bigvee^n \mathfrak{h}}, \quad a(h)_{|\bigvee^n \mathfrak{h}} = \sqrt{n}\, \langle h| \otimes \mathbf{I}_{\bigvee^{n-1} \mathfrak{h}}, \quad a(h)_{|\mathbb{C}} = 0\,.$$

The field operator $\Phi(h)$ is then defined as

$$\Phi(h) = (a(h) + a^*(h))/\sqrt{2}. \tag{3.71}$$

Let ω be a self-adjoint operator on $\mathfrak{h}$. The second quantization of ω is the operator on Fock space defined by

$$\mathrm{d}\Gamma(\omega)_{|\bigvee^n \mathfrak{h}} = \sum_{k=1}^{n} \mathbf{I}_{\bigvee^{k-1} \mathfrak{h}} \otimes \omega \otimes \mathbf{I}_{\bigvee^{n-k} \mathfrak{h}}, \quad \mathrm{d}\Gamma(\omega)_{|\mathbb{C}} = 0.$$

The coherent state of parameter $f \in \mathfrak{h}$ is defined as

$$\Psi_f := e^{i\Phi\left(\frac{\sqrt{2}}{i} f\right)}\Omega = e^{-\frac{\|f\|_{\mathfrak{h}}^2}{2}} \sum_{n=0}^{\infty} \frac{f^{\otimes n}}{\sqrt{n!}},$$

where Ω stands for the Fock vacuum. Coherent states are eigenvectors of the annihilation operators in the sense that for all $f, h \in \mathfrak{h}$,

$$a(h)\Psi_f = \langle h, f\rangle_{\mathfrak{h}}\, \Psi_f\,.$$

This in turn leads to the following equalities :

$$\langle \Psi_f, \Phi(h)\Psi_f\rangle_{\mathfrak{F}_s(\mathfrak{h})} = 2\mathfrak{Re}\,\langle h, f\rangle_{\mathfrak{h}}\,, \quad \langle \Psi_f, \mathrm{d}\Gamma(\omega)\Psi_f\rangle_{\mathfrak{F}_s(\mathfrak{h})} = \langle f, \omega\, f\rangle_{\mathfrak{h}}\,. \tag{3.72}$$

We recall the following estimates, which holds for any non-negative operator ω on $\mathfrak{h}$, h in the domain of $\omega^{-1/2}$ and Ψ in the domain of $\mathrm{d}\Gamma(\omega)^{1/2}$:

$$\|a(h)\Psi\| \le \|\omega^{-\frac{1}{2}} h\|_{\mathfrak{h}}^2 \|\mathrm{d}\Gamma(\omega)^{\frac{1}{2}}\Psi\|_{\mathfrak{F}_s(\mathfrak{h})}^2, \tag{3.73}$$

$$\|a^*(h)\Psi\| \le \|\omega^{-\frac{1}{2}} h\|_{\mathfrak{h}}^2 \|\mathrm{d}\Gamma(\omega)^{\frac{1}{2}}\Psi\|_{\mathfrak{F}_s(\mathfrak{h})}^2 + \|f\|_{\mathfrak{h}}^2 \|\Psi\|_{\mathfrak{F}_s(\mathfrak{h})}^2. \tag{3.74}$$

The next proposition establishes the self-adjointness of the Pauli-Fierz Hamiltonian $\mathbb{H}$ of the standard model of non-relativistic QED (see (3.9)) under our assumptions. We recall a proof for the convenience of the reader.

Proposition 3.4.1 (Self-adjointness of $\mathbb{H}$)**.** *Suppose that $V = V_+ - V_-$ belongs to $L^1_{\text{loc}}(\mathbb{R}^3;\mathbb{R}^+)$ and that V_- is infinitesimally small with respect to $-\Delta$ in the sense of quadratic forms on $H^1(\mathbb{R}^3)$. Suppose in addition that $\chi : \mathbb{R}^3 \to \mathbb{R}$ is such that both $|k|^{-1/2}\chi$ and $|k|^{-1}\chi$ are in $L^2(\mathbb{R}^3)$. Then the Pauli-Fierz hamiltonian $\mathbb{H}$ is a self-adjoint operator with form domain*

$$\mathcal{Q}(\mathbb{H}) = \mathcal{Q}\left(H_{V_+} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\text{f}} + \mathbf{I}_{\text{el}} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathrm{d}\Gamma(|k|)\right) .$$

Proof. Let $\mathcal{Q}_+ := \mathcal{Q}\left(H_{V_+} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\text{f}} + \mathbf{I}_{\text{el}} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathrm{d}\Gamma(|k|)\right)$. We claim that the following form is closed on $\mathcal{Q}_+$:

$$\begin{aligned} q_+(\Psi_1,\Psi_2) := &\left\langle \vec{\sigma}\cdot(-i\vec{\nabla}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}} - \vec{\mathbb{A}}(\vec{m}_x))\Psi_1, \vec{\sigma}\cdot(-i\vec{\nabla}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}} - \vec{\mathbb{A}}(\vec{m}_x))\Psi_2 \right\rangle_{\mathcal{H}} \\ &+ \left\langle (V_+^{1/2}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_1, (V_+^{1/2}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_2 \right\rangle_{\mathcal{H}} \\ &+ \left\langle (\mathbf{I}_{\text{el}}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbb{H}_f^{1/2})\Psi_1, (\mathbf{I}_{\text{el}}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbb{H}_f^{1/2})\Psi_2 \right\rangle_{\mathcal{H}} . \end{aligned}$$

Let $(\Psi_n)_{n\in\mathbb{N}}$ in $\mathcal{Q}_+^{\mathbb{N}}$ be such that $\Psi_n \xrightarrow[n\to\infty]{\mathcal{H}} \Psi$ and $(q_+(\Psi_n,\Psi_n))_{n\in\mathbb{N}}$ converges. We show that Ψ is in $\mathcal{Q}_+$ and that $q_+(\Psi_n-\Psi,\Psi_n-\Psi) \underset{n\to\infty}{\longrightarrow} 0$. Considering the closed form on $\mathcal{Q}_+$ defined by

$$\begin{aligned} q_0(\Psi_1,\Psi_2) := &\left\langle (-i\vec{\nabla}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_1, (-i\vec{\nabla}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_2 \right\rangle_{\mathcal{H}} \\ &+ \left\langle (V_+^{1/2}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_1, (V_+^{1/2}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbf{I}_{\text{f}})\Psi_2 \right\rangle_{\mathcal{H}} \\ &+ \left\langle (\mathbf{I}_{\text{el}}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbb{H}_f^{1/2})\Psi_1, (\mathbf{I}_{\text{el}}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbb{H}_f^{1/2})\Psi_2 \right\rangle_{\mathcal{H}} , \end{aligned}$$

it is not difficult to verify, using (3.73)–(3.74), that there exists a positive constant C such that, for all $\varepsilon > 0$, for all Ψ in $\mathcal{Q}_+$,

$$(1-C\varepsilon)q_0(\Psi,\Psi) \le q_+(\Psi,\Psi) + C\varepsilon\left(\left\|(\mathbf{I}_{\text{el}}\otimes\mathbf{I}_{\mathbb{C}^2}\otimes\mathbb{H}_f^{1/2})\Psi\right\|_{\mathcal{H}}^2 + \|\Psi\|_{\mathcal{H}}^2\right) . \tag{3.75}$$

This implies that $(q_0(\Psi_n,\Psi_n))_{n\in\mathbb{N}}$ is a Cauchy sequence and hence, since q_0 is closed on $\mathcal{Q}_+$, we deduce that $\Psi \in \mathcal{Q}_+$. Finally, since, similarly as for (3.75), we have

$$q_+(\Psi,\Psi) \le (1-C\varepsilon)q_0(\Psi,\Psi),$$

we conclude that

$$q_+(\Psi_n-\Psi,\Psi_n-\Psi) \underset{n\to\infty}{\longrightarrow} 0.$$

We have shown that the quadratic form q_+ is positive and closed on $\mathcal{Q}_+$. In particular (see e.g. [78, Chap. 6, Thm. 2.1]), this ensures that there exists a positive self-adjoint operator H_+ such that, for all $\Psi_1,\Psi_2 \in \mathcal{Q}_+$, $q_+(\Psi_1,\Psi_2) = \langle H_+^{1/2}\Psi_1, H_+^{1/2}\Psi_2\rangle_{\mathcal{H}}$. Since V_- is infinitesimally form bounded with respect to $-\Delta$, one easily deduces that it is also infinitesimally form bounded with respect to H_+. The KLMN theorem then allows us to conclude that $\mathbb{H}$ identifies to a self-adjoint operator with form domain

$$\mathcal{Q}(\mathbb{H}) = \mathcal{Q}_+ = \mathcal{Q}\left(H_{V_+} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathbf{I}_{\mathrm{f}} + \mathbf{I}_{\mathrm{el}} \otimes \mathbf{I}_{\mathbb{C}^2} \otimes \mathrm{d}\Gamma(|k|)\right) .$$

This concludes the proof. □

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Abstract

In this thesis, we study quantum field theory models that describe the interactions between a non-relativistic particle and a quantized radiation field. In particular, we focus on the minimization of the quasi-classical energy of the considered models, i.e. the energy of the system when the field is in a coherent state. A first result concerns the Spin-boson model. It is a simple (but non-trivial) model where the non-relativistic particle is described by a finite dimensional system and is linearly coupled to a quantized scalar field. We obtain an explicit expression for the quasi-classical ground state energy and the set of minimizers for this model, for any values of the coupling constant. We also prove that the set of minimizers is trivial when the coupling constant is below a critical value. We also obtain the existence of a ground state for the energy when the field is in a superposition of two coherent states. Next, we consider models where the non-relativistic particle is described by a Schrödinger operator. In the case where the coupling between the particle and the field is linear in the creation and annihilation operators (Nelson model, polaron model for instance), we show the existence and uniqueness of a quasi-classical ground state associated with the quasi-classical energy, up to a phase symmetry. We consider a general external potential, either bindind or confining, and do not impose an ultraviolet cutoff in the definition of the energy functional. Then, we obtain an asymptotic expansion of the quasi-classical ground state energy as the coupling parameter goes to 0. Finally, by making the energy depend on the ultraviolet parameter, we prove that the ground states and associated ground state energies converge in the ultraviolet limit. In the case of the standard model of non-relativistic quantum electrodynamics with a spin, under similar assumptions, we show the existence of a quasi-classical ground state. We also obtain an asymptotic expansion as the coupling parameter tends to 0 and the convergence of the ground state energies in the ultraviolet limit.

Résumé

Dans cette thèse, on s'intéresse à des modèles de théorie quantique des champs décrivant les interactions entre une particule non relativiste et un champ de radiation quantifié. En particulier, on s'intéresse à la minimisation de l'énergie quasi-classique des modèles considérés, c'est-à-dire l'énergie du système lorsque le champ se trouve dans un état cohérent. Un premier résultat concerne le modèle spin-boson, c'est un modèle simple (mais non trivial) où la particule non relativiste est décrite par un système de dimension finie et est couplée linéairement à un champ quantifié scalaire. On obtient pour ce modèle une expression explicite de l'énergie fondamentale quasi-classique et de l'ensemble des minimiseurs, pour toute valeur de la constante de couplage. On montre également que l'ensemble des minimiseurs est trivial si la constante de couplage est inférieure à une valeur critique. D'autre part, on obtient l'existence d'un état fondamental pour l'énergie lorsque le champ se trouve dans une superposition de deux états cohérents. On considère ensuite des modèles pour lesquels la particule non relativiste est décrite par un opérateur de Schrödinger. Dans le cas où le couplage entre la particule et le champ est linéaire en les opérateurs de création et d'annihilation (modèle de Nelson, modèle du Polaron), on montre l'existence et l'unicité d'un état fondamental quasi-classique associé à l'énergie quasi-classique, à symétrie de phase près. On suppose le potentiel extérieur confinant ou liant et nous n'imposons pas de troncature ultraviolette dans la définition de la fonctionnelle d'énergie. Nous obtenons ensuite un développement asymptotique de l'énergie fondamentale quasi-classique lorsque le paramètre de couplage tend vers 0. Enfin, en faisant dépendre l'énergie du paramètre ultraviolet, on montre que les états fondamentaux, ainsi que les énergies fondamentales associées convergent dans la limite ultraviolette. Dans le cas du modèle standard de l'électrodynamique quantique non relativiste, sous des hypothèses similaires, on montre l'existence d'un état fondamental quasi-classique. Nous obtenons aussi un développement asymptotique lorsque le paramètre de couplage tend vers 0 et la convergence dans la limite ultraviolette de l'énergie fondamentale.