Enhanced Binding in non-relativistic QED

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December 6, 2001

Abstract

We consider a spinless particle coupled to a photon field and prove that even if the Schrödinger operator $p^2 + V$ does not have eigenvalues the system can have a ground state. We describe the coupling by means of the Pauli-Fierz Hamiltonian and our result holds in the case where the coupling constant α is small.

1 INTRODUCTION

In the picture of Quantum electrodynamics (QED) atoms consist of charged particles, which are necessarily coupled to a photon field. If one neglects the radiation effects one obtains the Schrödinger operator. Although the fundamental properties of the one-particle and multi-particle Schrödinger operators have been successfully studied since the middle of the last century, the systematical mathematical study of the non-relativistic QED model was initiated by Bach, Fröhlich, and Sigal in [BFS1, BFS2, BFS3] only a couple of years ago (a comprehensive review of results in non-relativistic QED can be found in [GLL]) and some very fundamental problems are remaining still open. One of these problems is the question of enhanced binding via interaction with a quantized radiation field.

[3]Marie Curie Fellow

Consider a three-dimensional particle in a potential well $\beta V(x)$ with $V(x) \leq 0$. If the potential well is not deep enough, i.e. β is small, the corresponding Schrödinger operator does not have a discrete spectrum and binding does not occur. For a negative potential there exists a critical value β_0 such that for $\beta > \beta_0$ there is at least one bound state whereas for $\beta \leq \beta_0$ no particle can be bound.

In a recent paper Griesemer, Lieb, and Loss ([GLL]) proved that a photon field cannot decrease the binding energy. If the Schrödinger operator with potential βV has an eigenvalue, the corresponding energy operator in non-relativistic QED (Pauli-Fierz Hamiltonian) has a ground state.

However, the physical intuition tells us that interaction with a photon field must increase binding. Leaving the region of the potential the particle produces a photon field and consequently it needs more energy to leave the potential well.

The goal of this paper is to give a mathematical rigorous proof this phenomenon. Previously the enhanced binding was studied in the dipole approximation by Hiroshima and Spohn in [HS]. In this approximation it is assumed that the magnetic vector potential does not depend on the coordinates of the particle. They proved that, if the potential βV is fixed, for sufficiently large values of the coupling parameter α (which is the fine structure constant, see (1)), binding takes place.

Our approach to this problem is different. On the one hand we study the Pauli-Fierz operator without additional restrictions on the magnetic vector potential and on the other hand our results hold for small values of α (recall, that the physical value of α is about $1/137$). We prove that in case of the Pauli-Fierz operator (and for small α enough) binding starts at values of β strictly less than β_0.

2 DEFINITIONS AND MAIN RESULTS

We describe the self-energy of the particle by

$$T = (p + \sqrt{\alpha} A(x))^2 + H_f. \tag{1}$$

The unit of energy is $mc^2/2$, where m is the electron mass, the unit length is $l_c = 2\hbar/mc$, twice the Compton wavelength of the particle, and $\alpha = e^2/\hbar c$ is the *fine structure constant*. The physical value is $\alpha \sim 1/137$. In the present paper α plays the role of a small, dimensionless number. Our results hold for sufficiently small values of α. The charge of the electron is e.

The operator $p = -i\nabla_x$, while A is the magnetic vector potential. The unit of $A(x)^2$ is $mc^2/2l_c$. We fix the gauge $\mathrm{div}A = 0$.

The Hilbert space is

$$\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3) \otimes \mathcal{F}, \tag{2}$$

where $\mathcal{F}$ is the symmetric Fock space for the photon field.

Throughout this paper we denote the position-vector of the particle by x and by ξ_i the position-vectors of the photons. It is also convenient to use the relative coordinates $x - \xi_i$ for the photons. The vector potential is

$$A(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\chi(|k|)}{|k|^{1/2}} [\varepsilon_\lambda a_\lambda(k) e^{ikx} + \varepsilon_\lambda^*(k) a_\lambda^*(k) e^{-ikx}] dk, \tag{3}$$

where the operators a_λ, a_λ^* satisfy the usual commutation relations

$$[a_\nu(k), a_\lambda^*(q)] = \delta(k-q)\delta_{\lambda,\nu}, \quad [a_\lambda(k), a_\nu(q)] = 0, \quad \text{etc.} \tag{4}$$

The vectors $\varepsilon_\lambda(k)$ are the two possible orthonormal polarization vectors perpendicular to k. The units are chosen as in [GLL].

Obviously,

$$A(x) = D(x) + D^*(x), \tag{5}$$

where

$$D(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\chi(|k|)}{|k|^{1/2}} [\varepsilon_\lambda a_\lambda(k) e^{ikx} dk \tag{6}$$

and D^* is the operator adjoint to D.

For $x \in \mathbb{R}^3$ let

$$\vec{G}(x) = \mathcal{F}^{-1}[\hat{\vec{G}}(k)] \equiv \mathcal{F}^{-1}\left[\sum_{\lambda=1,2} \frac{\varepsilon_\lambda(k)\chi(|k|)}{|k|^{1/2}}\right], \tag{7}$$

where $\mathcal{F}$ is the Fourier transform and let $\psi_n(x, \xi_1, ..., \xi_n)$ be the n-photon component of a function $\Psi \in \mathcal{H}$. Obviously,

$$[D\psi_n]_{n-1}(x, \xi, ..., \xi_{n-1}) = \sqrt{n} \int \vec{G}(x - \xi_n)\psi_n(x, \xi_1, ..., \xi_n) d\xi_n. \tag{8}$$

We shall also use the following commutation relation [GLL]

$$[D, D^*] = 4\pi\Lambda^2. \tag{9}$$

The function $\chi(|k|)$ describes the ultraviolet cutoff on the wavenumbers k.

Concerning this cutoff we do not make further assumptions except those that are needed to apply [GLL]. It may be a sharp or a smooth cutoff. Only to ease the understanding of the calculations one can suppose that $\chi(|k|)$ is the characteristic function $\Theta(\Lambda - |k|)$.

The photon field energy H_f is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a_\lambda^*(k) a_\lambda(k) dk. \tag{10}$$

Let again ψ_n be the n-photon component of a function $\Psi \in \mathcal{H}, \psi_n \in H^{1/2}(\mathbb{R}^{3(n+1)})$. Then,

$$(\psi_n, H_f \psi_n) = n(\psi_n, |\nabla_{\xi_1}| \psi_n). \tag{11}$$

To prove existence of enhanced binding in non-relativistic QED we would like to compare binding in the presence of the photon field and without it. To this end let us introduce the Schrödinger operator

$$h_\beta = -\Delta + \beta V(x) \tag{12}$$

with external potential $\beta V(x) \in C(\mathbb{R}^3)$, which we assume to be radial $V(x) = V(|x|)$, non positive $V(x) \leq 0$, and with compact support. It is known that there is a critical value of the parameter $\beta_0 > 0$ such that for $\beta \leq \beta_0$ there is no ground state and the operator (12) has only an essential spectrum and at the same time for all $\beta > \beta_0$ the operator h_β has at least one eigenvalue.

The corresponding operator with a quantized radiation field is

$$\mathbf{H}_\beta = T + \beta V(x). \tag{13}$$

Our goal now is to show that the operator $\mathbf{H}_\beta$ has bound states for values of β smaller h_β. To establish the existence of a ground state of $\mathbf{H}_\beta$ we apply the criterion of [GLL], which says that $\mathbf{H}_\beta$ has a ground state if

$$\text{inf spec } \mathbf{H}_\beta < \text{inf spec } T. \tag{14}$$

However, in contrast to the Schrödinger operator h_β, for which the infimum of the spectrum without potential is always 0, the inf spec T is a complicated function depending on α and Λ. To prove the inequality (14) one needs precise estimates on this function. Our first result is the following asymptotic estimate on $\Sigma_0 = \text{inf spec } T$.

THEOREM 1 (Localization of the spectrum of a free spinless particle). *Let*

$$\mathcal{E}_0 = 2\sum_{\mu,\nu=1,2}\int \frac{(\hat{\vec{G}}_\mu(p)\cdot\hat{\vec{G}}_\nu(q))^2}{[p+q]^2+|p|+|q|}dpdq.^1 \tag{15}$$

Then, for small α,

$$\Sigma_0 = \inf \text{ spec } T = 4\pi\alpha\Lambda^2 - \alpha^2\mathcal{E}_0 + o(\alpha^2). \tag{16}$$

Recall, that the operator h_β has a critical value β_0 of the parameter β such that, for $\beta \le \beta_0$, h_β does not have a bound state. Using Theorem 1 we construct a variational trial function proving for small values of α the following:

THEOREM 2 (Enhanced binding). *For all sufficiently small α there exists a number $\beta_1(\alpha) < \beta_0$, such that for all $\beta > \beta_1(\alpha)$ the operator $\mathbf{H}_\beta$ has a ground state.*

3 PROOF OF THEOREM 1

3.1 Some a-priori estimates

We start this section with an a-priori estimate on Σ_0.

LEMMA 3. *For $\alpha\Lambda$ sufficiently small the inequality*

$$\Sigma_0 \ge 4\pi\alpha\Lambda^2 - \bar{c}\alpha^2\Lambda^3, \tag{17}$$

holds with a constant $\bar{c}$ independent of α. Moreover,

$$T \ge 4\pi\alpha\Lambda^2 - \bar{c}\alpha^2\Lambda^3 + \frac{1}{2}p^2 + \frac{1}{2}H_f \tag{18}$$

in the sense of quadratic forms.

Proof. For Ψ in the form domain of T we have

$$(\Psi, T\Psi) = \|p\Psi\|^2 + 2\sqrt{\alpha}(p\Psi, A(x)\Psi) + \alpha\|A(x)\Psi\|^2 + (\Psi, H_f\Psi). \tag{19}$$

Notice that $A(x) = D(x) + D^*(x)$ and $[p, A(x)] = 0$ imply

$$2\sqrt{\alpha}(p\Psi, A(x)\Psi) = 4\sqrt{\alpha}\Re(p\Psi, D(x)\Psi) \le \sqrt{\alpha\Lambda}\|p\Psi\|^2 + 16\sqrt{\alpha/\Lambda}\|D(x)\Psi\|^2. \tag{20}$$

Moreover, with the commutation relation

$$D(x)D^*(x) = D^*(x)D(x) + 4\pi\Lambda^2 \tag{21}$$

we get

$$\alpha\|A\Psi\|^2 = 4\pi\alpha\Lambda^2\|\Psi\|^2 + 2\alpha(\Psi, D^*D\Psi) + 2\alpha\Re(\Psi, DD\Psi). \tag{22}$$

By Schwarz inequality

$$2\alpha\Re D(x)D(x) \le C^{-1}D^*(x)D(x) + C\alpha^2 D(x)D^*(x) \quad \text{for an arbitrary } C > 0. \tag{23}$$

The relations (19)-(23) together with the estimate [GLL]

$$D^*(x)D(x) \le 8\pi\Lambda H_f \tag{24}$$

imply

$$\begin{aligned}(\Psi, T\Psi) \;\ge\;& (4\pi\alpha\Lambda^3 - 4\pi C\alpha^2\Lambda^2)\|\Psi\|^2 + \tfrac{1}{2}\{\|p\Psi\|^2 + (\Psi, H_f\Psi)\} + \\ &+(\tfrac{1}{2} - \sqrt{\alpha\Lambda})\|p\Psi\|^2 + \left(\tfrac{1}{2} - 8\pi[16\sqrt{\alpha\Lambda} + C^{-1}\Lambda + \alpha^2 C\Lambda]\right)(\Psi, H_f\Psi).\end{aligned} \tag{25}$$

For C large enough and $\alpha\Lambda$ sufficiently small the last two terms in (25) are positive which completes the proof of the Lemma. □

REMARK 4. The inequalities (20) and (24) imply also that

$$\begin{aligned}(\Psi, T\Psi) \;&\ge (1 - \sqrt{\alpha\Lambda})\|p\Psi\|^2 + \alpha\|A\Psi\|^2 + (1 - 128\pi\sqrt{\alpha}\Lambda)(\Psi, H_f\Psi) \\ &\ge 4\pi\alpha\Lambda^2 + (1 - C\sqrt{\alpha})\|p\Psi\|^2 - 2\alpha|\Re(\Psi, DD\Psi)| + (1 - C\sqrt{\alpha})(\Psi, H_f\Psi),\end{aligned} \tag{26}$$

with some constant $C > 0$ independent of α. We will use the last relation (26) for obtaining a sharp lower bound on Σ_0.

REMARK 5. Obviously $\Sigma_0 \le 4\pi\alpha\Lambda^2$. Let Ψ be a state with energy close to Σ_0, i.e. $(\Psi, T\Psi) \le 4\pi\alpha\Lambda^2 + \bar{c}\alpha^2\Lambda^3$. By Lemma 3 we conclude

$$\|\nabla\Psi\|^2 + (\Psi, H_f\Psi) \le 4\bar{c}\alpha^2\Lambda^3\|\Psi\|^2. \tag{27}$$

The last inequality says that for small α no photon can be concentrated in a small region, in particular in a small region near the particle. The state Ψ is mainly supported in the regions where all photons are far away from the particle. This observation plays an important role for estimating Σ_0 and we will make it mathematically precise later.

Another important observation, which we get from the proof of Lemma 3, is that as long as we consider the ground state energy of the "free" Hamiltonian, the term $\sqrt{\alpha}pA$ is irrelevant, because it is relatively bounded by $\varepsilon(p^2 + H_f)$ with some small constant ε.

Consequently, the process of annihilation of *one* photon, which is involved in that term, is not relevant for the estimation of Σ_0.

At the same time the annihilation of two photons, which is represented by the term $2\alpha\Re(\Psi, DD\Psi)$, contributes to the next to leading order of α^2. On this basis one can infer that a function $\Psi \in \mathcal{H}$ containing only two components, a 0-photon part and 2-photon part, can be a good candidate for a minimizer of the quadratic form $(\Psi, T\Psi)$ up to an error of order $o(\alpha^2)$. Additionally, in order to satisfy (27) we shall take the two photon component of Ψ with norm bounded by $C\alpha$.

The presence of a negative external potential V changes the role of the term $\alpha(p\Psi, A\Psi)$ dramatically. The positive term $\|p\Psi\|^2$ can be compensated by the negative term $(\Psi, V\Psi)$ and the term $\alpha(p\Psi, A\Psi)$ can be responsible for shifting the bottom of the spectrum. This observation will be used in the proof of Theorem 2.

3.2 Upper bound for Σ_0

Let

$$\Psi_n = \{f_n(x), 0, \alpha f_n(x)\varphi(\eta_1, \eta_2), 0, 0...\}, \tag{28}$$

with

$$\varphi(\eta_1, \eta_2) = -\sqrt{2}\mathcal{F}^{-1}\left(\frac{\hat{\vec{G}}(p)\cdot\hat{\vec{G}}(q)}{[p+q]^2 + |p| + |q|}\right). \tag{29}$$

We assume $f_n(x)$ to be a real function, with $\|f_n\| = 1$.

Then

$$\begin{aligned}(\Psi_n, T\Psi_n) \quad = \quad & \|\nabla_x f_n(x)\|^2 + \alpha^2(\varphi, [-i\nabla_{\eta_1} - i\nabla_{\eta_2}]^2\varphi) + \alpha^2\|\nabla_x f_n(x)\|^2\|\varphi\|^2 \\ & + \alpha^2 \sum_{i=1,2} \||\nabla_{\eta_i}|^{1/2}\varphi\|^2 + \alpha(\Psi_n, A^2\Psi_n).\end{aligned} \tag{30}$$

Notice, that

$$\alpha(\Psi_n, A^2\Psi_n) = 4\pi\alpha\Lambda^2 + 2\alpha(\Psi_n, D^*D\Psi_n) + 2\alpha^2\Re(f_n(x), DDf_n(x)\varphi(\eta_1, \eta_2)). \tag{31}$$

The first term on the r.h.s. of (31) can be estimated ([GLL]) as

$$2\alpha|(\Psi_n, D^*D\Psi_n)| \le 16\pi\alpha^3\Lambda \sum_{i=1,2} \||\nabla_{\eta_i}|^{1/2}\varphi\|^2, \tag{32}$$

and the last term is

$$2\sqrt{2}\alpha^2 \int \vec{G}(\eta_1) \cdot \vec{G}(\eta_2)\varphi(\eta_1, \eta_2) d\eta_1 d\eta_2, \tag{33}$$

which implies

$$\begin{aligned}(\Psi_n, T\Psi_n) \;\; &\leq \;\; 4\pi\alpha\Lambda^2 + (1 + C\alpha^2)\|\nabla_x f_n(x)\|^2 + \alpha^2\{(\varphi, [(i\nabla_{\eta_1} + i\nabla_{\eta_2})^2 + |\nabla_{\eta_1}| + |\nabla_{\eta_2}|]\varphi) \\ &+2\sqrt{2}\alpha^2 \int \vec{G}(\eta_1) \cdot \vec{G}(\eta_2)\varphi(\eta_1, \eta_2) d\eta_1 d\eta_2\} + O(\alpha^3), \end{aligned} \tag{34}$$

where C is independent of α, Λ, n.

The inequality

$$\|F_1\|^2 + 2(F_1, F_2) \geq -\|F_2\|^2, \tag{35}$$

with

$$F_1 = [(i\nabla_{\eta_1} + i\nabla_{\eta_2})^2 + |\nabla_{\eta_1}| + |\nabla_{\eta_2}|]\varphi(\eta_1, \eta_2) \;\in \mathcal{L}^2(\mathbb{R}^3) \tag{36}$$

and

$$F_2 = \sqrt{2}[(i\nabla_{\eta_1} + i\nabla_{\eta_2})^2 + |\nabla_{\eta_1}| + |\nabla_{\eta_2}|]^{1/2}\vec{G}(\eta_1) \cdot \vec{G}(\eta_2) \tag{37}$$

implies now that

$$(\Psi_n, T\Psi_n) \leq 4\pi\alpha\Lambda^2 - \alpha^2\mathcal{E}_0 + (1 + C\alpha^2)\|\nabla_x f_n(x)\|^2 + O(\alpha^3), \tag{38}$$

with $\mathcal{E}_0$ is given by (15). The upper bound on Σ_0 follows from (38) if we take a sequence $f_n(x)$ with $\|\nabla_x f_n(x)\| \to 0$.

3.3 Lower bound on Σ_0.

3.3.1 Partition of unity for the photon space and field energy estimates

Let ψ_n be the n-photon component of the state Ψ and let a_1 and $\varepsilon > 0$ be some fixed but arbitrary numbers. Let $u_1(\eta)$ and $u_2(\eta)$ be the localization functions defined in Theorem 7 with the above chosen $a_1 > 0$ and $\varepsilon > 0$. Obviously the products

$$u_{k_1 \ldots k_n}(\eta_1, \ldots, \eta_n) := \Pi_{i=1}^n u_{k_i}(\eta_i), \quad k_i = 1, 2 \tag{39}$$

make the partition of unity in $\mathbb{R}^{3n}$ in the sense that $\sum_{k_1,\ldots,k_n=1,2} u^2_{k_1 \ldots k_n} = 1$, where the sum is taken over all possible combinations of $k_i, k_i = 1, 2;\; i = 1, \ldots, n$.

Applying Theorem 7 we immediately arrive at

$$(\psi_n, H_f\psi_n) \geq (1-\varepsilon) \sum_{k_1,\dots,k_n=1,2} (u_{k_1\dots k_n}\psi_n, H_f u_{k_1\dots k_n}\psi_n) \tag{40}$$

The inequality (40) has two important consequences. First, notice that the sum on the r.h.s. of (40) contains $\frac{n(n-1)}{2}$ terms corresponding to the products $u_{k_1\dots k_n}$ in which the function $u_1(\eta_i)$ appears exactly twice. Using the symmetry of ψ_n we derive that for $n \geq 2$

$$(\psi_n, H_f\psi_n) \geq (1-\varepsilon)\frac{n(n-1)}{2}(\psi_n u_{2,n}, H_f\psi_n u_{2,n}), \tag{41}$$

where

$$u_{2,n} = u_1(\eta_1)u_1(\eta_2)u_2(\eta_3)\dots u_2(\eta_n) \tag{42}$$

and

$$(\Psi, H_f\Psi) \geq (1-\varepsilon)\sum_{n\geq 0}\frac{(n+2)(n+1)}{2}(\psi_{n+2}u_{2,n+2}, H_f\psi_{n+2}u_{2,n+2}). \tag{43}$$

Second, denote by γ_0 the lowest eigenvalue of the operator $|\nabla_\eta|^{1/2}$ with the Dirichlet boundary condition at $|\eta| = b_1$. (Recall that $u_1(\eta) = 0$ for $|\eta| \geq b_1$.) Then for all $u_{k_1\dots k_n}$ with $\sum_{i=1}^n k_i < 2n$ (at least one photon is localized near the electron) holds:

$$(\psi_n u_{k_1\dots k_n}, H_f\psi_n u_{k_1\dots k_n}) \geq \gamma_0\|\psi_n u_{k_1\dots k_n}\|^2, \tag{44}$$

which implies

$$(\psi_n, H_f\psi_n) \geq \gamma_0(\|\psi_n\|^2 - \|\psi_n^0\|^2), \tag{45}$$

with $\psi_n^0 = \psi_n\Pi_{i=1}^n u_2(\eta_i)$. Let Ψ^0 be the state with components $\{\psi_0^0, \psi_1^0, \dots, \psi_n^0, \dots\}$. Comparing (45) with (27) we immediately conclude that for all states Ψ, with energy close to Σ_0, holds

$$\|\Psi^0\|^2 \geq (1 - 4\bar{c}\gamma_0^{-1}\alpha^2\Lambda^3)\|\Psi\|^2, \tag{46}$$

which means that for small α the difference between Ψ_0 and Ψ is small. As the last remark for this section notice, that for the operator $p_n^2 = -(\nabla_x + \sum_{i=1}^n \nabla_{\eta_i})^2$ the localization error corresponding to the localization with the functions $u_{k_1\dots k_n}$ is the same as for the operator $-\sum \Delta_{\eta_i}$ and applying Remark 8 to this operator in an analogical way as to (41) we get

$$(\psi_n, p_n^2\psi_n) \geq (1-\varepsilon)\frac{n(n-1)}{2}\|(\nabla_x + \sum_{i=1}^n \nabla_{\eta_i})\psi_n u_{2,n}\|^2 + (1-\varepsilon)\|(\nabla_x + \sum_{i=1}^n \nabla_{\eta_i})\psi_n^0\|^2, \tag{47}$$

which implies

$$(\Psi, p^2\Psi) \geq (1-\varepsilon)\sum_{n=0}^{\infty}\left\{\frac{(n+1)(n+2)}{2}\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\psi_{n+2}u_{2,n+2}\|^2 + \|(\nabla_x + \sum_{i=1}^{n}\nabla_{\eta_i})\psi_n^0\|^2\right\}. \tag{48}$$

Summarizing the inequalities (26), (27) and (48) we conclude that for small α

$$\begin{aligned}(\Psi, T\Psi) \quad \geq \quad & \alpha\|A\Psi\|^2 + \sum_{n=0}^{\infty}(1-2\varepsilon)\left\{\frac{(n+1)(n+2)}{2}(\widetilde{\psi}_{n+2}, H_f\widetilde{\psi}_{n+2}) + \right. \\ & \left. + \|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\widetilde{\psi}_{n+2}\|^2 + \|(\nabla_x + \sum_{i=1}^{n}\nabla_{\eta_i})\psi_n^0\|^2\right\},\end{aligned} \tag{49}$$

with

$$\widetilde{\psi}_{n+2} = \psi_{n+2}u_1(\eta_1)u_1(\eta_2)\prod_{i=3}^{n+2}u_2(\eta_i). \tag{50}$$

3.3.2 Estimate on the $A^2(x)$ term

The inequality (26) shows that the only term which can make the value of the quadratic form $(\Psi, T\Psi)$ less that $4\pi\alpha\Lambda^2$ is $2\alpha\Re(\Psi, DD\Psi)$ coming from $A(x)^2$. Our next goal is to estimate this term precisely.

Obviously

$$\begin{aligned}\alpha(\Psi, DD\Psi) \quad = \quad & \alpha\sum_n\sqrt{(n+2)(n+1)}\int\overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})}\times \\ & \times\psi_n(x,\eta_3,...,\eta_{n+2})dx\prod_{i=1}^{n+2}d\eta_i = \alpha\sum_n(I_{1,n}+I_{2,n}),\end{aligned} \tag{51}$$

with

$$\begin{aligned}I_{1,n} = \sqrt{(n+2)(n+1)}\int & \overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})}\times \\ & \times\psi_n(x,\eta_3,...,\eta_{n+2})\prod_{i=3}^{n+2}u_2(\eta_i)^2dxd\eta\end{aligned} \tag{52}$$

and

$$\begin{aligned}I_{2,n} = \sqrt{(n+2)(n+1)}\int & \overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})}\times \\ & \times\psi_n(x,\eta_3,...,\eta_{n+2})(1-\prod_{i=3}^{n+2}u_2(\eta_i)^2)dxd\eta,\end{aligned} \tag{53}$$

where we used the notation $d\eta = \prod_{i=1}^{n+2} d\eta_i$. Similarly to (23) the bound

$$\begin{aligned}
|\alpha I_{2,n}| &\leq \alpha \|D\psi_{n+2}\| \|D^*\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\| \\
&\leq \alpha\sqrt{8\pi\Lambda}(\psi_{n+2}, H_f\psi_{n+2})^{1/2}\Bigg\{4\pi\Lambda^2\|\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\|^2 + \\
&\quad +\|D\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\|^2\Bigg\}^{1/2} \qquad (54)
\end{aligned}$$

holds. To estimate the last term on the r.h.s. of (54) in terms of $(\psi_n, H_f\psi_n)$ we cannot use directly the inequality [GLL]

$$D^*(x)D(x) \leq 8\pi\Lambda H_f. \qquad (55)$$

However, a very similar estimate, given by Lemma 9 in the Appendix, holds for some constant $C > 0$ independent of ψ_n. Namely

$$\|D\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\|^2 \leq C(\psi_n, H_f\psi_n), \qquad (56)$$

which implies

$$|\alpha I_{2,n}| \leq \alpha 8\pi\Lambda[(\psi_{n+2}, H_f\psi_{n+2}) + (\psi_n, H_f, \psi_n)] + \alpha 4\pi\Lambda^2 C\|\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\|^2, \qquad (57)$$

where C is independent of α. Notice, that

$$\|\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)\|^2 \leq \|\psi_n(1-\prod_{i=1}^{n} u_2(\eta_i)^2)^{1/2}\|^2 = \|\psi_n\|^2 - \|\psi_n^0\|^2. \qquad (58)$$

Applying (46) and summing over all n we arrive at

$$\begin{aligned}
2\sum_n |\alpha I_{2,n}| &\leq 16\pi\Lambda\alpha(\Psi, H_f\Psi) + 4C\bar{c}\gamma_0^{-1}\alpha^3\Lambda^3\|\Psi\|^2 \\
&\leq 16\pi\Lambda\alpha(\Psi, H_f\Psi) + O(\alpha^3)\|\Psi\|^2. \qquad (59)
\end{aligned}$$

Let us now turn to estimating the terms $I_{1,n}$. In these terms we will separate three parts. The first two parts $\bar{I}_{1,n}$ and $\tilde{I}_{1,n}$ correspond to the process of annihilation of two photons very far from the particle or one photon near the particle and the second one far away from the particle. It is intuitively clear that these two parts are small if we compare them to the process of the annihilation of two photons near the particle. We will prove it rigorously and after that we will analyze the main part $I^0_{1,n}$. Let

$$\bar{I}_{1,n} = \sqrt{(n+2)(n+1)} \int \overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})} \times \\ \times \psi_n(x,\eta_3,...,\eta_{n+2}) \prod_{i=1}^{n+2} u_2(\eta_i)^2 dx d\eta, \tag{60}$$

$$\tilde{I}_{1,n} = \sqrt{(n+2)(n+1)} \int \overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})} \times \\ \times \psi_n(x,\eta_3,...,\eta_{n+2}) \prod_{i=2}^{n+2} u_2(\eta_i)^2 u_1(\eta_1)^2 dx d\eta \tag{61}$$

and

$$I^0_{1,n} = \sqrt{(n+2)(n+1)} \int \overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\psi_{n+2}(x,\eta_1,...,\eta_{n+2})} \times \\ \times \psi_n(x,\eta_3,...,\eta_{n+2}) \prod_{i=3}^{n+2} u_2(\eta_i)^2 u_1(\eta_1)^2 u_1(\eta_2)^2 dx d\eta. \tag{62}$$

Obviously

$$I_{1,n} = \bar{I}_{1,n} + 2\tilde{I}_{1,n} + I^0_{1,n}. \tag{63}$$

Let us get the bound for $\tilde{I}_{1,n}$, the term $\bar{I}_{1,n}$ can be evaluated in a similar and simpler way. Define the operators D_1 and D_2 analogously to D replacing the vector function $\vec{G}(\eta)$ by $\vec{G}(\eta)u_1(\eta)^2$ for D_1 and by $\vec{G}(\eta)u_2(\eta)^2$ for D_2. Similar to (21) we have

$$[D_2, D_2^*] = 2\|\vec{G}(\eta)u_2(\eta)\|^2, \tag{64}$$

where the coefficient 2 describes the 2 possible photon polarizations. Notice that if the number a_1 in the definition of the function u_2 grows,

$$\|\vec{G}(\eta)u_2(\eta)^2\| \to 0. \tag{65}$$

Hence

$$\begin{aligned} \alpha|\tilde{I}_{1,n}| &\le \alpha\|D_1\psi_{n+2}\|\|D_2^*\psi_n\prod_{i=1}^n u_2(\eta_i)^2\| \\ &\le \alpha\|D_1\psi_{n+2}\|\left(2\|\vec{G}(\eta)u_2(\eta)\|^2\|\psi_n\|^2 + \|D_2\psi_n\prod_{i=1}^n u_2(\eta_i)^2\|^2\right)^{1/2} \\ &\le \alpha^2\varepsilon(a_1)\nu\|\psi_n\|^2 + \nu^{-1}C(\psi_{n+2}, H_f\psi_{n+2}) + \alpha^2 C\nu(\psi_n, H_f\psi_n), \end{aligned} \tag{66}$$

where ν is an arbitrary number and C is a constant, which does not depend α and Ψ (see Lemma 6). For fixed ε_0 we first choose ν and α such that $\nu^{-1}C + \nu\alpha^2 C < \frac{1}{2}\varepsilon_0$ and then choose a_1 so large that $\varepsilon(a_1)\nu < \frac{1}{2}\varepsilon_0$. Thus we arrive at

$$2\sum_n \alpha|\tilde{I}_{1,n}| \leq \varepsilon_0\alpha^2\|\Psi\|^2 + \varepsilon_0(\Psi, H_f\Psi), \tag{67}$$

which together with the similar estimate for $\bar{I}_{1,n}$ implies

$$2\Re\sum_n \alpha I_{1,n} \geq -2\varepsilon_0\alpha^2\|\Psi\|^2 - 2\varepsilon_0(\Psi, H_f\Psi) + 2\Re\sum_n \alpha I^0_{1,n}. \tag{68}$$

Finally for $\|A\Psi\|^2$ we have

$$\alpha\|A\Psi\|^2 \geq 4\pi\alpha^2\Lambda^2\|\Psi\| - 2\varepsilon_0(\Psi, H_f\Psi) + 2\Re\sum_n \alpha I^0_{1,n} + (2\varepsilon_0\alpha^2 + O(\alpha^3))\|\Psi\|^2. \tag{69}$$

Applying (69) to (49) we get

$$\begin{aligned}(\Psi, T\Psi) \quad \geq \quad & 4\pi\alpha\Lambda^2\|\Psi\|^2 + \sum_{n=0}^{\infty}\Bigg[(1-\varepsilon_1(a_1,\alpha))\Bigg(\frac{(n+1)(n+2)}{2}\Big\{(\widetilde{\psi}_{n+2}, H_f\widetilde{\psi}_{n+2}) + \\ & +\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\widetilde{\psi}_{n+2}\|^2\Big\} + \|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\psi^0_n\|^2\Bigg) + 2\Re\sum_n \alpha I^0_{1,n}\Bigg] \\ & -\varepsilon_1(a_1,\alpha)\alpha^2\|\Psi\|^2,\end{aligned} \tag{70}$$

where $\varepsilon_1(a_1,\alpha) \to 0$ if $a_1 \to \infty$ and $\alpha \to 0$. For the integral $\alpha I^0_{1,n}$ the a-priori estimate

$$|\alpha I^0_{1,n}| \leq \frac{1}{4}(\psi_{n+2}, H_f\psi_{n+2}) + C\alpha^2\|\psi^0_n\|^2 \tag{71}$$

holds, with some constant C independent of α. Assume, that for some $n = \bar{n}$

$$\frac{(\bar{n}+1)(\bar{n}+2)}{2}(\widetilde{\psi}_{\bar{n}+2}, H_f\widetilde{\psi}_{\bar{n}+2}) + \|(\nabla_x + \sum_{i=1}^{n}\nabla_{\eta_i})\psi^0_{\bar{n}}\|^2 \geq C\alpha^2\|\psi^0_{\bar{n}}\|^2. \tag{72}$$

Then the term in the sum (70) corresponding to $\bar{n}$ is positive, thus we can omit it. We replace this sum by the sum $\sum^*$ over all n, for which (72) does not hold.

Notice, that the inequality

$$\frac{(n+1)(n+2)}{4}(\widetilde{\psi}_{n+2}, H_f\widetilde{\psi}_{n+2}) \leq C\alpha^2\|\psi^0_n\|^2 \tag{73}$$

implies

$$\|\widetilde{\psi}_{n+2}\|^2 \leq \frac{C_1(a_1)\alpha^2 4}{(n+1)(n+2)}\|\psi^0_n\|^2. \tag{74}$$

Let us project the function $\widetilde{\psi}_{n+2}$ on ψ_n^0:

$$\widetilde{\psi}_{n+2}(x,\eta_1,...,\eta_{n+2}) = \alpha\gamma_n(\eta_1,\eta_2)\psi_n^0(x,\eta_3,...,\eta_{n+2}) + g_n(\eta_1,...,\eta_{n+2}), \tag{75}$$

where $g_n \perp \psi_n^0$ for all η_1,η_2.

By (74)

$$\|g_n\|^2 \leq \frac{C\alpha^2}{(n+1)(n+2)}\|\psi_n^0\|^2 \tag{76}$$

and

$$\|\gamma_n\|^2 \leq \frac{C}{(n+1)(n+2)}. \tag{77}$$

Our goal is to estimate the term

$$\begin{aligned}
&\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\widetilde{\psi}_{n+2}\|^2 = \\
&= \|\alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n + \alpha\psi_n^0(\nabla_{\eta_1}+\nabla_{\eta_2})\gamma_n + (\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n\|^2 \\
&= \|\alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n + \alpha\psi_n^0(\nabla_{\eta_1}+\nabla_{\eta_2})\gamma_n\|^2 + \|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n\|^2 \\
&\quad +2\Re(\alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n + \alpha\psi_n^0(\nabla_{\eta_1}+\nabla_{\eta_2})\gamma_n, (\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n)
\end{aligned} \tag{78}$$

For the first part of the cross term we have

$$\begin{aligned}
&|((\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n, \alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n)| \leq \\
&\leq \alpha\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n\|^2 + \alpha\|(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\|^2\|\gamma_n\|^2
\end{aligned} \tag{79}$$

and the inequality (77) together with the condition

$$\|(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\|^2 \leq C\alpha^2\|\psi_n^0\|^2 \tag{80}$$

implies that the last term on the r.h.s. of (79) is less than $\frac{C\alpha^3}{(n+1)(n+2)}\|\psi_n^0\|^2$. The second part of the cross term can be evaluated as

$$
\begin{aligned}
&|(\nabla_x + \sum_{i=1}^{n+2} \nabla_{\eta_i}) g_n, \alpha\psi_n^0(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n)| = \\
&\quad = |(g_n, -(\nabla_x + \sum_{i=3}^{n+2} \nabla_{\eta_i})\psi_n^0 \alpha(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n))| \le \\
&\qquad \le \{\alpha\|g_n\|^2 + C\alpha^3\|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2\} \\
&\qquad \le \frac{C\alpha^3}{(n+1)(n+2)}\|\psi_n^0\|^2 + C\alpha^3\|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2.
\end{aligned}
\tag{81}
$$

Summing the inequalities (79) and (81) we obtain

$$
\begin{aligned}
&2\left|\Re\left(\alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n + \alpha\psi_n^0(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n, (\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n\right)\right| \le \\
&\le 2\alpha\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})g_n\|^2 + \|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2 + \frac{C\alpha^3}{(n+1)(n+2)}\|\psi_n^0\|^2.
\end{aligned}
\tag{82}
$$

Let us turn now to the first term on the r.h.s. of (78)

$$
\begin{aligned}
&\|\alpha(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\gamma_n + \alpha\psi_n^0(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2 \ge \\
&\qquad \ge (1-\alpha)\alpha^2\|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2 - \alpha\|(\nabla_x + \sum_{i=3}^{n+2}\nabla_{\eta_i})\psi_n^0\|^2\|\gamma_n\|^2 \ge \\
&\qquad \ge (1-\alpha)\alpha^2\|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2 - \frac{C\alpha^3}{(n+1)(n+2)}\|\psi_n^0\|^2.
\end{aligned}
\tag{83}
$$

Applying (82) and (83) to (78) we arrive at

$$
\begin{aligned}
&\frac{(n+1)(n+2)}{2}\|(\nabla_x + \sum_{i=1}^{n+2}\nabla_{\eta_i})\widetilde{\psi}_{n+2}\|^2 \ge \\
&\quad \frac{(n+1)(n+2)}{2}\alpha^2\|\psi_n^0\|^2\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2(1 - C\alpha) - C\alpha^3\|\psi_n^0\|^2,
\end{aligned}
\tag{84}
$$

which implies

$$
\begin{aligned}
(\Psi, T\Psi) \ \ge\ & 4\pi\alpha\Lambda^2\|\Psi\|^2 + \textstyle\sum_n^* \Big[(1 - \varepsilon_1(a_1,\alpha))\alpha^2\|\psi_n^0\|^2\frac{(n+1)(n+2)}{2}\times \\
& \times\left\{\|(\nabla_{\eta_1} + \nabla_{\eta_2})\gamma_n\|^2 + \||\nabla_{\eta_1}|^{1/2}\gamma_n\|^2 + \||\nabla_{\eta_2}|^{1/2}\gamma_n\|^2\right\} + 2\Re\sum_n \alpha I_{1,n}^0\Big] \\
& -\varepsilon_1(a_1,\alpha)\alpha^2\|\Psi\|^2,
\end{aligned}
\tag{85}
$$

Finally, we turn to the estimation of $I_{1,n}^0$.

Notice, that $\sqrt{(n+1)(n+2)}\|\gamma_n(\eta_1,\eta_2)\| \le C$ which implies

$$\begin{aligned}
\alpha\Re I^0_{1,n} &= \alpha^2\sqrt{(n+1)(n+2)}\|\psi^0_n\|^2\Re\int\overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)}u_1(\eta_1)u_1(\eta_2)\overline{\gamma_n(\eta_1,\eta_2)}d\eta_1 d\eta_2 \ge \\
&\ge \alpha^2\sqrt{(n+1)(n+2)}\|\psi^0_n\|^2\Re\int\overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\gamma_n(\eta_1,\eta_2)}d\eta_1 d\eta_2 - \\
&\qquad -\alpha^2 C\|\psi^0_n\|^2\|\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\sqrt{1-u_1(\eta_1)u_1(\eta_2)}\|^2 \qquad (86)
\end{aligned}$$

The last term in (86) can be estimated as $\varepsilon(a_1,\alpha)\alpha^2$ as $a_1\to\infty$. Finally, using the inequality

$$\|f\|^2 + 2\Re(f,h) \ge -\|h\|^2, \qquad f,h\in\mathcal{L}^2, \qquad (87)$$

we arrive at

$$\begin{aligned}
&(1-\varepsilon_1(a_1,\alpha))\frac{(n+1)(n+2)}{2}\left\{\|(\nabla_{\eta_1}+\nabla_{\eta_2})\gamma_n\|^2 + \||\nabla_{\eta_1}|^{1/2}\gamma_n\|^2 + \||\nabla_{\eta_2}|^{1/2}\gamma_n\|^2\right\} - \\
&\quad -\sqrt{(n+1)(n+2)}2\Re\int\overline{\vec{G}(\eta_1)\cdot\vec{G}(\eta_2)\gamma_n(\eta_1,\eta_2)}d\eta_1 d\eta_2 \ge \\
&\quad\ge -\frac{1}{1-\varepsilon_1(a_1,\alpha)}\mathcal{E}_0, \qquad (88)
\end{aligned}$$

with $\varepsilon_1(a_1,\alpha)$ arbitrarily small, which completes the proof of the Theorem.

4 PROOF OF THEOREM 2

Proof of Theorem 2. To prove the Theorem we will check the binding condition of [GLL] for $\beta=\beta_0$. Namely, we will show that

$$\inf \text{spec } \mathbf{H}_{\beta_0} < \Sigma_0 - \delta\alpha^2 + o(\alpha^2). \qquad (89)$$

The binding for all $\beta\in(\beta_1,\beta_0]$ with some $\beta_1>\beta_0$ follows from (89) and the continuity of the quadratic form in β. In the proof of Theorem 1 we have seen that the sequence

$$\Psi_n = \{f_n(x), 0, \alpha f_n(x)\varphi(x-\xi_1,x-\xi_2), 0, 0, ..\}, \qquad (90)$$

with $\|f_n(x)\|=1, \lim_{n\to\infty}\|\nabla f_n(x)\|=0$ and φ is the function given by (29), is a minimizing sequence up to the order α^2 for the quadratic form $(\Psi_n, T\Psi_n)$. More precisely, according to (38), $\|\nabla f_n\|^2\le O(\alpha)\|f_n\|^2$ yields

$$(\Psi_n, T\Psi_n) \le \|\nabla f_n\|^2 + (\Sigma_0 + o(\alpha^2))\|\Psi_n\|^2. \qquad (91)$$

Our next goal is to modify this sequence in such a way that for the modified function Ψ_0

$$(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \le (\Sigma_0 - \delta\alpha^2 + o(\alpha^2))\|\Psi_0\|^2, \qquad (92)$$

with some $\delta > 0$. To this end we will make a special choice of the function $f(x)$ and additionally add a one photon term, which leads to

$$\Psi^0 = \{f(x), i\sqrt{\alpha} d\nabla f(x) \cdot \vec{G}(\eta), \alpha f(x)\varphi(x-\xi_1, x-\xi_2), 0, 0, ...\}, \tag{93}$$

where d is a parameter to be chosen later. We assume $f(x) \in C_0^2(\mathbb{R}^3)$ to be a real, spherically symmetric function and to fulfill the condition

$$\|\Delta f(x)\| \le C_1 \|\nabla f(x)\| \le C_2 \sqrt{\alpha} \|f(x)\|, \tag{94}$$

with some constants $C_{1,2}$. Next, let us turn to the estimate of the quadratic form $(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0)$. The negativity of the terms $(\psi_1, V\psi_1)$ and $(\psi_2, V\psi_2)$ together with (38) implies

$$\begin{aligned}(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \ \le\ & (\Sigma_0 + o(\alpha^2))\|\Psi_0\|^2 + \|\nabla f(x)\|^2 + \beta_0(f, V(x)f) \\ & + 4\sqrt{\alpha}\Re\{(p\psi_1, D\psi_2) + (p\psi_0, D\psi_1)\} + \|(\nabla_x + \nabla_\eta)\psi_1\|^2 + \||\nabla_\eta|^{1/2}\psi_1\|^2,\end{aligned} \tag{95}$$

where $\psi_0 = f(x), \psi_1, \psi_2$ are the three non vanishing components of Ψ^0. Since we assumed $f(x)$ to be real and spherically symmetric we derive

$$\begin{aligned}\|(\nabla_x + \nabla_\eta)\psi_1\|^2 \ =\ & -(\psi_1, \Delta_x\psi_1) - (\psi_1, \Delta_\eta\psi_1) \\ \le\ & \alpha d^2 \left\{ \int |\vec{G}(\eta)|^2 d\eta \int \left[\left(\frac{\partial^2 f}{\partial x_1^2}\right)^2 + 2\left(\frac{\partial^2 f}{\partial x_1 \partial x_2}\right)^2 \right] dx \right. \\ & \left. + \int \left(\frac{\partial f}{\partial x_1}\right)^2 dx \int \sum_{i,k=1}^{3} \left(\frac{\partial G_i(\eta)}{\partial \eta_k}\right)^2 d\eta \right\},\end{aligned} \tag{96}$$

where G_i are the components of $\vec{G}$. Applying (94) we arrive at

$$\|(\nabla_x + \nabla_\eta)\psi_1\|^2 \le C\alpha d^2 \|\nabla f\|^2, \tag{97}$$

with C depending only on C_1 of (94).

Obviously

$$\||\nabla_\eta|^{1/2}\psi_1\|^2 = \alpha d^2 \sum_{i=1}^{3} \int \left(\frac{\partial f}{\partial x_i}\right)^2 dx \||\nabla_\eta|^{1/2} G_i\|^2 \le C\alpha d^2 \|\nabla f(x)\|^2. \tag{98}$$

Substituting (97) and (98) into (95) we arrive at

$$\begin{aligned}(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \ \le\ & (\Sigma_0 + o(\alpha^2))\|\Psi_0\|^2 + \|\nabla f(x)\|^2 + \beta_0(f, V(x)f) \\ & + 4\sqrt{\alpha}\Re\{(p\psi_1, D\psi_2) + (p\psi_0, D\psi_1)\} + C\alpha d^2 \|\nabla f\|^2.\end{aligned} \tag{99}$$

Next, we estimate the term $\sqrt{\alpha}(p\psi_1, D\psi_2)$. By Schwarz inequality and condition (94)

$$|\sqrt{\alpha}(p\psi_1, D\psi_2)| \le \sqrt{\alpha}d\|D\psi_2\|^2 + \sqrt{\alpha}d^{-1}\|p\psi_1\|^2 \le Cd[\alpha^{5/2}\|f\|^2 + \alpha^{1/2}d^{-1}\|p\psi_1\|^2] \le C_1\alpha^{5/2}d\|f\|^2. \tag{100}$$

By (99) and (100) we get

$$\begin{aligned}(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \quad \le \quad & (\Sigma_0 + o(\alpha^2))\|\Psi_0\|^2 + \|\nabla f(x)\|^2 + \beta_0(f, V(x)f) \\ & +4\sqrt{\alpha}\Re(p\psi_0, D\psi_1) + C\alpha d^2\|\nabla f(x)\|^2, \end{aligned} \tag{101}$$

where C is independent of α.

Notice that

$$\sqrt{\alpha}\Re(p\psi_0, D\psi_1) = -\alpha d \int \left(\frac{\partial f}{\partial x_1}\right)^2 dx \int |\vec{G}(\eta)|^2 d\eta = -\frac{1}{3}\alpha d\|\nabla f\|^2 4\pi\Lambda^2 = -\frac{4\pi}{3}\alpha\Lambda^2 d\|\nabla f\|^2, \tag{102}$$

which implies

$$(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \le (1 - \frac{16\pi}{3}\alpha\Lambda^2 d + C\alpha d^2)\|\nabla f\|^2 + \beta_0(f, Vf) + (\Sigma_0 + o(\alpha^2))\|\Psi_0\|^2. \tag{103}$$

As the next step we choose $d < \frac{8\pi\Lambda^2}{3C}$ which gives

$$(\Psi^0, \mathbf{H}_{\beta_0}\Psi^0) \le (1 - \nu\alpha)\|\nabla f\|^2 + \beta_0(f, Vf) + (\Sigma_0 + o(\alpha^2))\|\Psi_0\|^2, \tag{104}$$

where

$$\nu = \frac{64}{3C}\Lambda^2\pi^2. \tag{105}$$

Due to our choice of β_0, obviously the operator

$$-(1 - \nu\alpha)\Delta + \beta_0 V(x) \tag{106}$$

has at least one negative eigenvalue. However, the r.h.s. of (104) contains the terms which are of order $o(\alpha^2)$ and to prove Theorem 2 we have to provide more precise estimates on the negative eigenvalues of (106).

The following Lemma completes the proof of Theorem 1.

LEMMA 6. *Let β_0 be the critical value (the maximal value of the constant β, for which the Schrödinger operator with the potential βV does not have a discrete spectrum). Then*

$$\inf \text{ spec } \{-(1 - \nu\alpha)\Delta + \beta_0 V(|x|)\} < -\delta\alpha^2, \tag{107}$$

for some $\delta > 0$ and α small enough.

Moreover, there exists a function $f_\alpha(x)$, real, spherical symmetric and satisfying condition (94), with constants $C_{1,2}$ independent of α, such that

$$(1-\nu\alpha)\|\nabla f_\alpha\|^2 + \beta_0(f_\alpha, V(|x|)f_\alpha) < -\delta\alpha^2\|f_\alpha\|^2. \tag{108}$$

□

The proof of Lemma 6 is given in Appendix B.

A APPENDIX: Localization error for the relativistic kinetic energy

THEOREM 7. *For arbitrary numbers $a > 0, \varepsilon > 0$ there exists a parameter $b > 0$ and functions $u_1(|x|), u_2(|x|) \in C^2(\mathbb{R}^3)$ such that*

i) $u_1(|x|)^2 + u_2(|x|)^2 = 1$;

ii) $u_1(|x|) = 1$ for $|x| \le a$ and

$u_1(|x|) = 0$ for $|x| \ge b$;

iii) $|(\psi, |\nabla|\psi) - (\psi u_1, |\nabla|\psi u_1) - (\psi u_2, |\nabla|\psi u_2)| \le \varepsilon\||x|^{-1/2}\psi\|^2,\ \psi \in W^{1,2}(\mathbb{R}^3)$ (109)

Proof. According to [LY] the localization error for the operator $|\nabla|$ is

$$\frac{1}{4\pi^2}\sum_{i=1}^{2}\int \frac{\psi(x)\psi(y)}{|x-y|^4}(u_i(x)-u_i(y))^2 dxdy. \tag{110}$$

Our goal is to show that the functions $u_1(x), u_2(x)$ and the number b can be chosen such that the r.h.s. of (109) is greater than (110) for all $\psi \in W^{1,2}(\mathbb{R}^3)$. Therefore we take $u_1(|x|)$ and choose it on some interval $[a \le |x| \le a+\delta]$, $\delta > 0$, strictly decreasing and such that

$$\lim_{|x|\to a+0}\frac{u_1'(x)^2}{1-u_1(x)^2} = 0. \tag{111}$$

For fixed ε_1 we pick a number $\delta > 0$ so small, that for $|x| \in [a, a+\delta]$

$$u_1'(x)^2 + u_2'(x)^2 \le u_1'(x)^2 + \frac{u_1'(x)^2}{1-u_1(x)^2} < \varepsilon_1. \tag{112}$$

Because of symmetry in x and y we can write

$$\sum_{i=1}^{2}\int \frac{\psi(x)\psi(y)}{|x-y|^4}(u_i(x)-u_i(y))^2 dxdy = 2\sum_{i=1}^{2}\int_{|x|\le|y|}\frac{\psi(x)\psi(y)}{|x-y|^4}(u_i(x)-u_i(y))^2 dxdy \le 2(I_1+I_2), \tag{113}$$

where I_1 is the integral over the region $\{(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3 \,||x| \leq |y|, |y| \leq a+\delta\}$ and I_2 over the region $\{(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3 \,||x| \leq |y|, |y| > a+\delta\}$.

Let us estimate I_1. For $|x| < |y| \leq a+\delta$

$$\sum_{i=1}^{2}(u_i(x)-u_i(y))^2 \leq \max_{|y|\leq a+\delta}\{u_1'(y)^2 + \frac{u_1'(y)^2}{1-u_1(y)^2}\}|x-y|^2, \tag{114}$$

which implies

$$\begin{aligned} |I_1| \;\; &\leq \;\; \varepsilon_1 \int_{|y|\leq a+\delta, |x|\leq|y|} \frac{|\psi(x)||\psi(y)|}{|x-y|^2} dxdy \leq 2\varepsilon_1 \int_{|x|\leq 2a} |\psi(x)|^2 dx \int_{|x-y|\leq 3a} |x-y|^{-2} d(x-y) \\ &\leq 2\varepsilon_1 \|\psi(x)\|^2_{|x|\leq 2a} 4\pi 3a \leq 48\pi\varepsilon_1 a^2 \|\psi(x)|x|^{-1/2}\|^2. \end{aligned} \tag{115}$$

Taking $\varepsilon < \varepsilon_1(48\pi a^2)^{-1}$ we arrive at

$$|I_1| < \varepsilon\|\psi(x)|x|^{-1/2}\|^2. \tag{116}$$

Notice that $u_1(a+\delta) < 1$ and for $|y| \geq a+\delta, |y| > |x|$

$$\begin{aligned} &(u_2(x)-u_2(y))^2 = \left((1-u_1(x)^2)^{1/2} - ((1-u_1(y)^2)^{1/2}\right)^2 = \\ &= \frac{(u_1(x)-u_1(y))^2(u_1(x)+u_1(y))^2}{\left((1-u_1(x)^2)^{1/2} + ((1-u_1(y)^2)^{1/2}\right)^2} \leq \\ &\quad \leq 4(u_1(x)-u_1(y))^2(1-u_1(a+\delta)^2)^{-1} = C_0(u_1(x)-u_1(y))^2 \end{aligned} \tag{117}$$

holds. The last inequality implies

$$|I_2| \leq (C_0+1)\int_{|x|<|y|, |y|\geq a+\delta} |\psi(x)||\psi(y)||x-y|^{-4}((u_1(x)-u_1(y))^2 dxdy. \tag{118}$$

Now we define for $|x| \in [a+\delta, b]$

$$u_1(|x|) = \ln\left[\frac{|x|}{b}\right]\ln^{-1}\left[\frac{a+\delta}{b}\right]u_1(a+\delta). \tag{119}$$

It is easy to see that

$$|u_1(x)-u_1(y)| \leq \ln^{-1}\left[\frac{b}{a+\delta}\right]|\ln\left[\frac{|x|}{|y|}\right]| \leq \ln^{-1}\left[\frac{b}{a+\delta}\right]\frac{|y-x|}{|x|}. \tag{120}$$

Let $C > 0$ be a constant, which we specify later. First, we estimate the part of I_2 corresponding to the region where $|x-y| > C|x|$. Let

$$\Omega_1 = \{(x,y)||x| < |y|, \; |y| > a+\delta, \; |x-y| > C|x|\}, \tag{121}$$

then

$$\int_{\Omega_1} \frac{|\psi(x)||\psi(y)|}{|x-y|^4}(u_1(x)-u_1(y))^2 dxdy \le 2\int_{\Omega_1} \frac{\psi(x)\psi(y)}{|x-y|^4}dxdy \le$$
$$\le 2\left(\int \frac{|\psi(x)|^2}{|x-y|^4}dxdy\right)^{1/2}\left(\int \frac{|\psi(y)|^2}{|x-y|^4}dxdy\right)^{1/2}. \tag{122}$$

Notice that

$$\int_{\Omega_1} \frac{|\psi(x)|^2}{|x-y|^4}dxdy \le \int_{\mathbb{R}^3} |\psi(x)|^2 dx \int_{|x-y|>C|x|,|x|<|y|} |x-y|^{-4}dy \le \frac{4\pi}{C}\|\psi(x)|x|^{-1/2}\|^2. \tag{123}$$

The second integral on the r.h.s. of (122) can be estimated as

$$\int_{\Omega_1} \frac{|\psi(y)|^2}{|x-y|^4}dxdy \le \int_{\mathbb{R}^3} |\psi(y)|^2 dy \int_{|x-y|\ge C|x|,|x|<|y|} |x-y|^{-4}dx \le 4\pi\sqrt{\frac{(C-1)}{C(C-2)}}\|\psi(x)|x|^{-1/2}\|^2. \tag{124}$$

For the region

$$\Omega_2 = \{(x,y)||x|<|y|,\, |y|>a+\delta,\, |x-y|<C|x|\} \tag{125}$$

we have

$$\begin{aligned} \int_{\Omega_2} \frac{|\psi(x)||\psi(y)|}{|x-y|^4}dxdy &\le \ln^{-2}\left[\frac{b}{a+\delta}\right]\left(\int_{\Omega_2}\frac{|\psi(x)|^2}{|x-y|^2|x|^2}dxdy\right)^{1/2}\left(\int_{\Omega_2}\frac{|\psi(y)|^2}{|x-y|^2|x|^2}dxdy\right)^{1/2} \\ &\le \ln^{-2}\left[\frac{b}{a+\delta}\right](4\pi C)^{1/2}\|\psi(x)|x|^{-1/2}\|(4\pi C)^{1/2}(C+1)\|\psi(y)|y|^{-1/2}\| \\ &\le 4\pi C(C+1)\ln^{-2}\left[\frac{b}{a+\delta}\right]\|\psi(x)|x|^{-1/2}\|^2. \end{aligned} \tag{126}$$

Now we take C large enough to fulfill the inequality

$$[4(1-u_1(a+\delta)^2)^{-1}+1]4\pi(C-1)^{1/2}[C(C-2)]^{-1/2} < \varepsilon \tag{127}$$

and then for fixed C we choose b so large that

$$4\pi C(C+1)\ln^{-2}\left[\frac{b}{a+\delta}\right][4(1-u_1(a+\delta)^2)^{-1}+1] < \varepsilon \tag{128}$$

which together with (110) and (116) implies *iii*). To complete the proof of the Theorem it suffices to notice that the functions u_1 and u_2 can easily be approximated with some function in $C^2(\mathbb{R}^3)$ satisfying *iii*). □

REMARK 8. With the same functions u_1 and u_2 as in Theorem 7 one has (see [VZ2])

$$|(\psi,-\Delta\psi)-(\psi u_1,-\Delta\psi u_1)-(\psi u_2,-\Delta\psi u_2)| \le \varepsilon\||x|^{-1}\psi\|^2. \tag{129}$$

The last inequality will be used in the proof of Theorem 1

B APPENDIX: Proof of Lemma 6

Proof of Lemma 6. Let us start recalling some properties of the operator

$$h_\beta = -\Delta + \beta V(x), \tag{130}$$

$V(x)$ negative, radial and compactly supported, with critical value $\beta = \beta_0$. For $\beta = \beta_0$ the operator h_β has a so-called virtual level or zero-resonance. It means that the equation

$$-\Delta\psi + \beta_0 V(x)\psi = 0 \tag{131}$$

has a generalized spherical symmetric solution $\tilde{\psi}$ with the following properties [VZ1]:

(i) Let $\mathcal{B}$ be a closure of the space $C_0^\infty(\mathbb{R}^3)$ in the norm $\|\psi\|_B = \|\nabla\psi\|$. Then $\tilde{\psi} \in \mathcal{B}$. From this point we assume that $\tilde{\psi}$ is a normalized solution in the sense that $\|\tilde{\psi}\|_B = 1$. Notice, that $\tilde{\psi} \in \mathcal{L}^2_{\text{loc}}(\mathbb{R}^3)$, but $\tilde{\psi} \notin \mathcal{L}^2(\mathbb{R}^3)$.

(ii) $-\Delta\tilde{\psi} \in \mathcal{L}^2(\mathbb{R}^3)$ and $V(x)\tilde{\psi} \in \mathcal{L}^2(\mathbb{R}^3)$.

(iii) Outside the support of $V(x)$ holds

$$\tilde{\psi}(x) = C|x|^{-1}. \tag{132}$$

The last property follows immediately from the fact that outside the support of $V(x)$ the solutions of (131) can be written as $C_1|x|^{-1} + C_2$, and $\tilde{\psi} \in \mathcal{B}$ implies $C_2 = 0$.

Now we proceed directly to the proof Lemma 6. Let

$$u \in C_0^2(\mathbb{R}^3),\ u(x) \leq 1,\ u(x) = 1 \text{ for } |x| \leq 1,\ u(x) = 0 \text{ for } |x| \geq 2 \tag{133}$$

and set

$$f_n(x) = \tilde{\psi}(x)u(|x|\alpha n^{-1})\|\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^{-1}. \tag{134}$$

Obviously $\|f_n(x)\| = 1$ and for large n

$$\begin{aligned} \|\nabla f_n(x)\| &\leq \|\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^{-1}\{\|\nabla\tilde{\psi}\|_{|x|\leq 2\alpha^{-1}n} + \|C|x|^{-1}\|_{\alpha^{-1}n\leq|x|\leq 2\alpha^{-1}n}\max[|\nabla u(|x|\alpha n^{-1})|]\} \\ &\leq \|\nabla\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^{-1}\{\|\nabla\tilde{\psi}\| + C_1(\alpha^{-1}n)^{1/2}\alpha n^{-1}\} \leq 2\|\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^{-1}. \end{aligned} \tag{135}$$

Assume $V(x)$ is supported in a ball of radius a_0. Then $\tilde{\psi}(x) = C|x|^{-1}$ for $|x| \geq a_0$ and

$$\|\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^2 \geq 4\pi\int_{a_0\leq|x|\leq 2\alpha^{-1}n}|x|^{-2}dx = 4\pi(\alpha^{-1}n - a_0) \geq 2\pi\alpha^{-1}n \tag{136}$$

for $n \geq \frac{2a_0}{\alpha}$.

The inequalities (135) and (136) imply the second relation in (94). To check the first inequality in (94) let us estimate

$$\|\Delta\left(\tilde{\psi}(x)u(|x|\alpha n^{-1})\right)\| \leq \|\Delta\tilde{\psi}\| + \left(\sum_{i=1}^{3}\int\left(\frac{\partial\tilde{\psi}}{\partial x_i}\right)^2\left(\frac{\partial u}{\partial x_i}\right)^2 dx\right)^{\frac{1}{2}} + \left(\int\frac{C}{|x|^2}\Delta u(|x|\alpha n^{-1})dx\right)^{\frac{1}{2}}. \tag{137}$$

According to (ii) the first term on the r.h.s. of (137) is bounded. The second term is also bounded, since $|\nabla u(|x|\alpha n^{-1})| \leq$ const., (recall that $\|\nabla\tilde{\psi}\| = 1$) and the last term is also bounded by a constant for $n \geq \frac{2a_0}{\alpha}$. Finally we arrive at

$$\|\Delta\left(\tilde{\psi}(x)u(|x|\alpha n^{-1})\right)\| \leq C\|\nabla\tilde{\psi}(x)\|, \tag{138}$$

which implies

$$\|\Delta f_n(x)\| \leq C\|\nabla f_n(x)\|. \tag{139}$$

To prove the Lemma it suffices now to show that for large n

$$(1-\nu\alpha)\|\nabla f_n\|^2 + \beta_0(f_n, Vf_n) \leq -\delta\alpha^2\|f_n\|^2, \tag{140}$$

with some $\delta > 0$ independent of α. This is equivalent to

$$(1-\nu\alpha)\|\nabla(\tilde{\psi}(x)u(|x|\alpha n^{-1}))\|^2 + \beta_0(\tilde{\psi}, V\tilde{\psi}) \leq -\delta\alpha^2\|\tilde{\psi}(x)u(|x|\alpha n^{-1})\|^2. \tag{141}$$

Recall that

$$\|\tilde{\psi}u(|x|\alpha n^{-1})\|^2 \leq C_1 + 8\pi C^2\int_{a_0}^{2\alpha^{-1}n} d|x| \leq 2C_2\alpha^{-1}n, \tag{142}$$

for large n, and

$$\|\nabla\tilde{\psi}\|^2 + \beta_0(\tilde{\psi}, V\tilde{\psi}) = 0, \tag{143}$$

which implies

$$\begin{aligned}
&(1-\nu\alpha)\|\nabla(\tilde{\psi}(x)u(|x|\alpha n^{-1}))\|^2 + \beta_0(\tilde{\psi}, V\tilde{\psi}) \leq \\
&\quad \leq -\nu\alpha[\|(\nabla\tilde{\psi})u\| - \|\tilde{\psi}\nabla u\|]^2 + [\|\nabla\tilde{\psi}\|^2 - \|\nabla(\tilde{\psi}u)\|^2] \\
&\quad \leq -\nu\alpha\left[\frac{1}{2}\|\nabla\tilde{\psi}\| - C\alpha^{1/2}n^{-1/2}\right]^2 + 2\|\nabla\tilde{\psi}\|^2_{|x|\geq\alpha^{-1}n} + \|\tilde{\psi}|\nabla u|\|^2_{\alpha^{-1}n\leq|x|\leq 2\alpha^{-1}n}.
\end{aligned} \tag{144}$$

For n large we have

$$i)\quad \|\nabla\tilde{\psi}\|^2_{|x|\geq\alpha^{-1}n} = 4\pi C^2\int_{\alpha^{-1}n}^{\infty}|x|^{-2}dx = C^2\alpha n^{-1},$$

$$ii)\quad \|\tilde{\psi}|\nabla u|\|^2_{\alpha^{-1}n\leq|x|\leq 2\alpha^{-1}n} \leq C_1\alpha^2 n^{-2}4\pi\int_{\alpha^{-1}n}^{2\alpha^{-1}n}dr = C_3\alpha n^{-1}, \tag{145}$$

$$iii)\quad C_3\alpha^{1/2}n^{-1/2} < \frac{1}{4} = \frac{1}{4}\|\nabla\tilde{\psi}\|, \tag{146}$$

which implies together with (144)

$$-(1-\nu\alpha)\|\nabla(\tilde{\psi}(x)u(|x|\alpha n^{-1}))\|^2 + \beta_0(\tilde{\psi}, V\tilde{\psi}) \leq -\nu\alpha/16 \leq -\frac{\nu\alpha^2}{32C_2 n}\|\tilde{\psi}u(|x|\alpha n^{-1}))\|^2. \tag{147}$$

To complete the proof of the Lemma it suffices now to choose n so large that (146) holds (notice, that it can be done uniformly in α for $\alpha \leq 1$) and for this n take $\delta = \frac{1}{32}\nu C_2^{-1}n^{-1}$, where C_2 is the constant in (142), which depends on the zero-resonance solution $\tilde{\psi}$ only. $\square$

LEMMA 9. *Let D_1 and D_2 be the operators defined in Section 5.3. Then*

$$\|D_1\Psi\|^2 \leq \frac{8\pi\Lambda^2}{(1-\varepsilon)^2}(\Psi, H_f\Psi), \quad \|D_2\Psi\|^2 \leq \frac{8\pi\Lambda^2}{(1-\varepsilon)^2}(\Psi, H_f\Psi), \tag{148}$$

where ε is chosen as in Lemma 7, corresponding to the functions u_1 and u_2 in the definition of D_1 and D_2.

Proof. Our goal is to estimate the term

$$\|D_1\psi_n\|^2 = n\int|\int\vec{G}(\eta_1)u_1(\eta_1)^2\psi_n(\eta_1,...,\eta_n)d\eta_1|^2 d\eta_2...d\eta_n. \tag{149}$$

For fixed values of $\eta_2,...,\eta_n$ we get according to [GLL] Lemma A.4

$$|\int\vec{G}(\eta_1)u_1(\eta_1)^2\psi_n(\eta_1,...,\eta_n)d\eta_1|^2 \leq$$
$$8\pi\Lambda^2\int||\nabla_{\eta_1}|^{1/2}u_1(\eta_1)^2\psi_n(\eta_1,...,\eta_n)|^2 d\eta_1. \tag{150}$$

By the Localization Theorem

$$\||\nabla|^{1/2}\varphi\|^2 \geq (1-\varepsilon)\||\nabla|^{1/2}\varphi u_1\|^2 + (1-\varepsilon)\||\nabla|^{1/2}\varphi u_2\|^2 \geq (1-\varepsilon)\||\nabla|^{1/2}\varphi u_1\|^2 \tag{151}$$

for $\varphi \in C_0^2(\mathbb{R}^3)$. Applying (151) twice, first with $\varphi = \psi_n u_1$ and then with $\varphi = \psi_n$ we arrive at

$$\|D_1\Psi\|^2 \leq \frac{8\pi\Lambda^2 n}{(1-\varepsilon)^2}\||\nabla_\eta|^{1/2}\psi_n\|^2 = \frac{8\pi\Lambda^2}{(1-\varepsilon)^2}(\Psi, H_f\Psi). \tag{152}$$

An analogical estimate holds for D_2. $\square$

Acknowledgment: The work was partially supported by the European Union through its Training, Research, and Mobility program FMRX-CT 96-0001. C. Hainzl has been supported by a Marie Curie Fellowship of the European Community programme "Improving Human Research Potential and the Socio-economic Knowledge Base" under contract number HPMFCT-2000-00660. C. H. and S.-A. V. thank Robert Seiringer for many valuable comments.

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