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On exponential decay of solutions of Schrödinger and Dirac equations:bounds of eigenfunctions corresponding to energies in the gaps of essential spectrum

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1 Introduction

The motivation for our work comes mainly from the one-electron theory of quantum solids, more exactly from the spectral theory of "perturbed" periodic Schrödinger operators. We shall give below two examples; a more detalied description of other "models of disorder" can be found in [BNN]. Consider a periodic lattice, $\Gamma_p = \{\mathbf{a} = \sum_{i=1}^{3} m_i \mathbf{a}_i \mid m_i \in \mathbf{Z},\ \{\mathbf{a}_i\}_1^3 - basis\ \ in\ \ \mathbf{R}^3\}$, and

$$H_0 = -\Delta + V_{per}(\mathbf{x}) \tag{1.1}$$

where $V_{per}(\mathbf{x}) \in L^2_{loc}(\mathbf{R}^3)$ and

$$V_{per}(\mathbf{x} + \mathbf{a}) = V_{per}(\mathbf{x}), \quad all \quad \mathbf{a} \in \Gamma_p.$$

The hamiltonian H_0 is the basic object of the theory of periodic crystals and its spectral properties are well understood [RS]. Let now Γ be a set in $\mathbf{R}^3$ with the property that

$$\inf_{\mathbf{a},\mathbf{b}\in\Gamma;\ \mathbf{a}\neq\mathbf{b}} \mid \mathbf{a} - \mathbf{b} \mid \geq l > 0 \tag{1.2}$$

and $V(\mathbf{x})$ a rapidly decreasing potential. The "impurity" model of quantum solids is described by the hamiltonian

$$H = H_0 + \sum_{\mathbf{b}\in\Gamma} V(\mathbf{x} - \mathbf{b}) \tag{1.3}$$

(we assume that the decrease of $V(\mathbf{x})$ is sufficiently fast as to assure that $\sum_{\mathbf{b}\in\Gamma} V(\mathbf{x} - \mathbf{b})$ is uniformly locally L^2). If Γ consists of a single point, (1.3) becomes the usual "one-impurity model" hamiltonian:

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$$H_{imp} = H_0 + V(\mathbf{x}) \tag{1.4}$$

whose spectral and scatering theory is again well developed. Consider now for $\lambda > 0$:

$$H_\lambda = H_0 + \sum_{\mathbf{b}\in\Gamma} V(\mathbf{x} - \lambda\mathbf{b}). \tag{1.5}$$

For $\lambda \to \infty$, (1.5) describes the physical situation in which the impurities are far one from each other. At the heuristic level it is "known" that the spectral properties of H_{imp} and H_λ are related; in particular, if $E \in \rho(H_0)$ is an eigenvalue of H_{imp} then in the limit $\lambda \to \infty$, H_λ has a "miniband" arround E with a width which shrinks exponentially as $\lambda \to \infty$. The situation is similar to the one encountered in the usual tight-binding limit in which H_0 is replaced by $-\Delta$. Since the main technical ingredient in the study of the tight binding (as well as semiclassical) limit [D],[C],[HS1-3],[BCD] is the exponential decay of the eigenfunctions of $-\Delta + V(\mathbf{x})$, the first step in the study of the impurity tight binding limit must be a good control of exponential decay of the eigenfunctions of H_{imp} corresponding to energies in $\rho(H_0)$.

Another, interesting from the physical point of view, particular case of (1.3) is the one in which Γ is contained in a plane, say $x_3 = 0$, $(\mathbf{x} = (x_1, x_2, x_3))$. In this case the physical heuristics indicates that the (generalised) eigenfunctions of (1.3) corresponding to energies in $\rho(H_0)$ decay exponentially as $| x_3 |\to \infty$.

One can consider also the same problems when a magnetic field is added i.e. H_0 is replaced by $(\mathbf{P} - \mathbf{a})^2$ or at a higher level of complexity by $(\mathbf{P} - \mathbf{a})^2 + V_{per}(\mathbf{x})$. The simplest question in this context, is to prove the exponential decay of the eigenfunctions of

$$(-i\frac{\partial}{\partial x_1} + \frac{Bx_2}{2})^2 + (-i\frac{\partial}{\partial x_2} - \frac{Bx_1}{2})^2 + V(\mathbf{x}), \quad \mathbf{x} \in \mathbf{R}^2$$

for energies outside the set of the Landau levels.

Following the seminal work of Combes and Thomas [CT] and of Agmon [A] there is an enormous literature on exponential decay of eigenfunctions in the N-body problem and precise results have been obtained (see e.g. [A],[H1],[H2], and references therein; for extensions of Agmon type results to the magnetic field case see [HN],[HS3]). Since we are interested in energies which may belong to the essential spectrum of H and more important are not below the essential spectrum of the "asymptotic" hamiltonians, a direct application of the Combes-Thomas-Agmon analysis is not possible. (The results in [BG],[W],[MP] concerning Dirac operator are for energies in $(-m, m)$ and potentials vanishing at infinity, when one can still apply the Agmon theory to the square of the Dirac operator; see the remark at the end of Section 3.) Moreover due to the fact that the potential does not vanish at infinity, one cannot apply the techniques based on Mourre estimates. In [BNN] an elementary method (covering many cases of physical interest, but not the magnetic field case) to prove exponential decay has been used. The result below is that a Combes-Thomas-Agmon type analysis provides exponential upper bounds under very general conditions. It turns out that one can carry the Agmon analysis to the case at hand by replacing his λ-positivity condition with the strict injectivity of the Combes-Thomas rotated operator (see (2.4),(2.8) below and also [H1]). Exponential decay of eigenfunctions, in some cases when λ-positivity condition is not fulfilled, has been also obtained by Helffer and Sjostrand [HS2] in their deep study of tunelling through nonresonant wells in the semi-classical limit. We obtain only (very likely non optimal) upper bounds. The problem of the lower bounds (see e.g. [FH_3O_2], [H2] and references therein for the N-body case) or of the actual behaviour at infinity of the eigenfunctions seems to be harder and remains open. Detailed proofs and applications will be given elsewhere.

2 The results.

In what follows $\Omega \subset \mathbf{R}^n$ is a domain with (smooth) boundary $\partial\Omega$, and $W^{s,p}(\Omega)$ are the standard Sobolev spaces [GT].

2.1 The Schrödinger case.

Consider in $L^2(\Omega)$ the Schrodinger operator

$$H = (\mathbf{P} - \mathbf{a}(\mathbf{x}))^2 + q(\mathbf{x}), \;\; \mathbf{P} = -i\nabla \tag{2.1}$$

where

$$\mathbf{a} \in (L^p_{loc}(\Omega))^n; \;\; \nabla\mathbf{a} \in L^2_{loc}(\Omega); \;\; p = max\{n, 4\}; \;\; q \in S_n(\Omega) \tag{2.2}$$

(see [CFKS] for the definition of S_n; we recall that for $n \leq 3, q \in S_n(\Omega)$ if and only if
$\sup_{x\in\Omega} \int_{\{|\mathbf{x}-\mathbf{y}|\leq 1\}\bigcap\Omega} \mid q(\mathbf{y}) \mid^2 d\mathbf{y} < \infty$.

As a consequence of (2.2), H is well defined and symmetric (but, in general, not essentially self-adjoint) on $\mathcal{C}_0^\infty(\Omega)$.

Definition 1 (S) *Let $E \in \mathbf{R}$. $\psi(\mathbf{x}) \in W^{1,2}_{loc}(\Omega)$, is said to be a slowly increasing solution of $(H-E)\psi = 0$ in Ω if it is a weak solution, i.e. for all $\varphi(\mathbf{x}) \in \mathcal{C}_0^\infty(\Omega)$ ($(\cdot,\cdot)$ denotes the scalar product in $L^2(\Omega)$)*

$$((H-E)\varphi, \psi) = 0 \tag{2.3}$$

and for all $\delta > 0$, $\exp(-\delta(1+\mid \mathbf{x} \mid^2)^{1/2})\psi(\mathbf{x}) \in L^2(\Omega)$

For $h(\mathbf{x}) : \Omega \to \mathbf{R}, h \in \mathcal{C}^2(\Omega)$, we consider the "rotated" operator

$$H(h) = H - iB(h) - \mid \nabla h \mid^2 = \exp(-h)H\exp(h) \tag{2.4}$$

with

$$B(h) = (\mathbf{P}-\mathbf{a})\cdot\nabla h + \nabla h\cdot(\mathbf{P}-\mathbf{a}) \tag{2.5}$$

defined on $\mathcal{C}_0^\infty(\Omega)$.

For $d > 0$ we set

$$\Omega_d = \{\mathbf{x} \in \Omega \mid dist(\mathbf{x}, \partial\Omega) > d\} \tag{2.6}$$

and for $h(\mathbf{x})$ as before and $\varepsilon, \delta \geq 0$

$$h_{\delta,\varepsilon}(\mathbf{x}) = -\delta(1+\mid \mathbf{x} \mid^2)^{1/2} + h(\mathbf{x})(1+\varepsilon h^2(\mathbf{x}))^{-1}. \tag{2.7}$$

Theorem 1 (S) *Suppose:*

i. $\psi(\mathbf{x})$ is a slowly increasing solution of $(H-E)\psi = 0$ in Ω, $\mid E \mid \leq E_0$.

ii. There exist δ_0, ε_0, $c > 0$ such that for $0 \leq \delta \leq \delta_0$, $0 \leq \varepsilon \leq \varepsilon_0$ and all $\varphi \in \mathcal{C}_0^\infty(\Omega)$

$$\| (H(-h_{\delta,\varepsilon}) - E)\varphi \| \geq c \| \varphi \| . \tag{2.8}$$

Then there exists $K < \infty$ depending upon $\mathbf{a}$, q, d, c and E_0 such that for all $0 \leq \delta \leq \delta_0$

$$\int_{\Omega_{2d}} \mid e^{h_{\delta,0}(\mathbf{x})}\psi(\mathbf{x}) \mid^2 d\mathbf{x} \leq$$
$$K \int_{\Omega\setminus\Omega_{2d}} (1+\mid \nabla h_{\delta,0}(\mathbf{x}) \mid^2) \mid e^{h_{\delta,0}(\mathbf{x})}\psi(\mathbf{x}) \mid^2 d\mathbf{x}. \tag{2.9}$$

2.2 The Dirac case.

Consider now, in $(L^2(\Omega))^4$, the Dirac operator

$$D = \alpha \cdot \mathbf{P} + \beta m + Q(\mathbf{x}), \ Q(\mathbf{x}) = Q_1(\mathbf{x}) + Q_2(\mathbf{x}) \tag{2.10}$$

where $Q_i(\mathbf{x})$ are 4×4 hermitean matrices satisfying:

$$\int_{\{|\mathbf{x}-\mathbf{y}|\leq 1\}\bigcap\Omega} \| Q_1(\mathbf{y}) \|^2 | \mathbf{x} - \mathbf{y} |^{\rho-3} \, d\mathbf{y} < \infty, \ \text{all } \mathbf{x} \in \Omega, \ \ \rho < 2$$

$$\| Q_2(\mathbf{x}) \| \leq C \sum_{\mathbf{a}\in\Gamma} \frac{\exp(- | \mathbf{x} - \mathbf{a} |)}{| \mathbf{x} - \mathbf{a} |}, \ C < 1/2$$

where Γ is a set in Ω such that $\inf_{\mathbf{a}\neq\mathbf{b};\ \mathbf{a},\mathbf{b}\in\Gamma} | \mathbf{a} - \mathbf{b} | > 0$

Definition 2 (D) *Let $E \in \mathbf{R}$. $\Psi(\mathbf{x}) \in (L^2_{loc}(\Omega))^4$ is said to be a slowly increasing solution of $(D - E)\Psi = 0$ in Ω if it is a weak solution, i.e. for all $\Phi(\mathbf{x}) \in (\mathcal{C}_0^\infty(\Omega))^4$ ($< \cdot, \cdot >$ denotes the scalar product in $(L^2(\Omega))^4$)*

$$< (D - E)\Phi, \Psi >= 0 \tag{2.11}$$

and for all $\delta > 0$
$\exp(-\delta(1+ | \mathbf{x} |^2)^{1/2})\Psi(\mathbf{x}) \in (L^2(\Omega))^4$

As in the Schrödinger case, for $h : \Omega \to \mathbf{R}, h \in \mathcal{C}^1(\Omega)$ we consider the rotated operator

$$D(h) = \exp(-h) D \exp(h) = D - i\alpha \cdot \nabla h. \tag{2.12}$$

Theorem 2 (D) *Suppose:*
i. $\Psi(\mathbf{x})$ is a slowly increasing solution of $(D - E)\Psi = 0$ in Ω
ii. There exist $\delta_0, \varepsilon_0 > 0, c > 0$ such that for $0 \leq \delta \leq \delta_0, 0 \leq \epsilon \leq \epsilon_0$ and all $\Phi \in (\mathcal{C}_0^\infty(\Omega))^4$

$$\| (D(-h_{\delta,\varepsilon}) - E)\Phi \| \geq c \| \Phi \| \tag{2.13}$$

Then there exists $K < \infty$ depending upon Q, d, c such that for all $0 \leq \delta \leq \delta_0$

$$\int_{\Omega_{2d}} \sum_{j=1}^{4} | \mathit{exp}(h_{\delta,0}(\mathbf{x}))\Psi_j(\mathbf{x}) |^2 \, d\mathbf{x} \leq K \int_{\Omega\setminus\Omega_{2d}} \sum_{j=1}^{4} | \exp(h_{\delta,0}(\mathbf{x}))\Psi_j(\mathbf{x}) |^2 \, d\mathbf{x} \tag{2.14}$$

2.3 An example.

Let

$$\Omega_{\mathbf{n},R} = \{\mathbf{x} \in \mathbf{R}^3 \mid \mathbf{n} \cdot \mathbf{x} > R, \ \mid \mathbf{n} \mid = 1, \ R > 0\} \subset \mathbf{R}^3 \tag{2.15}$$

$$H = H_0 \mid_{C_0^\infty(\Omega_{\mathbf{n},R})} \tag{2.16}$$

(see Section 1 for H_0)

Suppose $E \in \rho(H_0)$, $\mid E \mid \leq E_0$, $\alpha = dist(E, \sigma(H_0))$ and let ψ be a slowly increasing solution of $(H - E)\psi = 0$ in $\Omega_{\mathbf{n},R}$. Take in Theorem 1S, $h(\mathbf{x})$ of the form

$$h(\mathbf{x}) = \mu(\mathbf{n} \cdot \mathbf{x} - R); \ \mu > 0. \tag{2.17}$$

It turns out that for sufficiently small μ the condition (2.8) is fulfilled. For example, by standard perturbation arguments, (2.8) is fulfilled for all $\mu < \mu_0$ where μ_0 is given by

$$\alpha\mu_0^2 + 2\mu_0 \parallel \mathbf{P} \cdot \mathbf{n}(H_0 - E)^{-1} \parallel = 1. \tag{2.18}$$

Then from (2.9) one obtains for all $\mu < \mu_0$:

$$\int_{\mathbf{n}\cdot\mathbf{x} \geq R+2d} \mid e^{-\delta(1+|\mathbf{x}|^2)^{1/2} + \mu(\mathbf{n}\cdot\mathbf{x} - R)} \psi(\mathbf{x}) \mid^2 d\mathbf{x} \leq$$

$$const. \int_{R+2d \geq \mathbf{n}\cdot\mathbf{x} \geq R} \mid e^{-\delta(1+|\mathbf{x}|^2)^{1/2}} \psi(\mathbf{x}) \mid^2 d\mathbf{x}. \tag{2.19}$$

If in addition one supposes that

$$\sup_{\mathbf{x} \in \Omega_{\mathbf{n},R}} \int_{\{|\mathbf{x}-\mathbf{y}| \leq 1\} \bigcap \Omega_{\mathbf{n},R}} \mid \psi(\mathbf{x}) \mid^2 d\mathbf{y} < \infty \tag{2.20}$$

then one obtains ($\mathbf{y} = z\mathbf{n} + \mathbf{y}_\perp, \ \mathbf{y}_\perp \perp \mathbf{n}$)

$$\sup_{\mathbf{x}_\perp \in \mathbf{R}^2} \int_{z > R+2d; \ |\mathbf{y}_\perp - \mathbf{x}_\perp| \leq 1} \mid e^{\mu z} \psi(z\mathbf{n} + \mathbf{y}_\perp) \mid^2 d\mathbf{y} < \infty. \tag{2.21}$$

The value of μ_0 given by (2.18) is far from being optimal even at the qualitative level. In particular in the limit $\alpha \to 0$ it gives $\mu_0 \sim \alpha$ while, as well known, for $E < inf\sigma(H_O)$ one has $\mu_0 \sim \alpha^{1/2}$. A more carefull analysis shows that the same is true for E in the gaps of H_O:

Theorem 3 *There exists $k > 0$ such that (2.8) is fulfilled for $\mu < k\alpha^{1/2}$.*

The best value of k (very likely it depends upon $\mathbf{n}$) is still to be found.

3 Outline of the proof.

We shall outline the proof in the Schrödinger case; the proof in the Dirac case is similar and much simpler, due to the fact that D is first order. We start with the following "localisation energy lemma", going back implicitely at least to Agmon [A] (I was kindly informed by T. Hoffmann-Ostenhof that it is actually much older) and having a clear physical meaning: it gives the amount of kinetic energy due to localisation by f of the "eigenfunction" ψ. Let for $\phi_1,\ \phi_2 \in W_c^{1,2}(\Omega)$

$$h[\phi_1,\ \phi_2] = \int_\Omega \overline{(\mathbf{P}-\mathbf{a})\phi_1(\mathbf{x})}(\mathbf{P}-\mathbf{a})\phi_2(\mathbf{x})d\mathbf{x} + \int_\Omega \overline{\phi_1(\mathbf{x})}q(\mathbf{x})\phi_2(\mathbf{x})d\mathbf{x}.$$

Lemma 1 *Let ψ be a solution of $(H-E)\psi = 0$ in Ω and $f:\Omega \to \mathbf{R},\ \ f \in C_0^\infty(\Omega)$. Then*

$$h[f\psi, f\psi] - E(f\psi, f\psi) = (\psi, \mid \nabla f \mid^2 \psi)$$

Let $h:\Omega \to \mathbf{R},\ \ h \in C^\infty(\Omega),\ g \in C_0^\infty(\Omega)$. Since for all $\varphi \in C_0^\infty(\Omega)$:

$$0 = ((H-E)\varphi, \psi) = (H(h)-E)e^{-h}\varphi, e^h\psi),$$

$$((H(h)-E)\varphi, e^h g\psi) = ([g, H(h)]\varphi, e^h\psi) = (\varphi, F) \tag{3.1}$$

with

$$F = \{-2i(\mathbf{P}-\mathbf{a})\cdot\nabla g - \Delta g + 2\nabla h \cdot \nabla g\}e^h\psi. \tag{3.2}$$

The next lemma gives (via Lemma 1) the control of (F, F):

Lemma 2 *Suppose supp $g \subset \Omega_d$. Then there exist $a < 1,\ b < \infty$, depending upon $\mathbf{a},\ q,\ d$ such that*

$$(F, F) \le 2(e^h\psi, me^h\psi)$$

with

$$m(\mathbf{x}) = \frac{4n}{1-a}\sum_{i=1}^n m_i(\mathbf{x}) + (-\Delta g + 2\nabla h\cdot\nabla g)^2$$

where

$$m_i(\mathbf{x}) = \mid (\frac{\partial g(\mathbf{x})}{\partial x_i})\nabla h + \nabla(\frac{\partial g(\mathbf{x})}{\partial x_i}) \mid^2 + (\mid E \mid + b)(\frac{\partial g(\mathbf{x})}{\partial x_i})^2$$

The next and the last ingredient is a regularity lemma:

Lemma 3 *Suppose*

$$\sup_{\Omega}(|\nabla h|) + |\Delta h|) \leq M < \infty \tag{3.3}$$

and $g : \Omega \to R, \quad g \in C_0^\infty(\Omega_d)$. *Then* $H(\pm h) |_{C_0^\infty(\Omega_{d/2})}$ *is closable in* $L^2(\Omega_{d/2})$ *and* $e^h g\psi$ *belongs to the domain of its closure.*

¿From (3.1), due to Lemma 3,for h satisfying (3.3) and $g \in C_0^\infty(\Omega_d)$

$$(H(-h) - E)e^h g\psi = F.$$

Suppose now $h_{\delta,\varepsilon}$ satisfies (2.8). Then using again Lemma 3:

$$(e^{h_{\delta,\varepsilon}} g\psi, e^{h_{\delta,\varepsilon}} g\psi)^{1/2} \leq C^{-1}(F,F)^{1/2} \tag{3.4}$$

Let now $g_d(\mathbf{x}) : \Omega \to R, \quad g_d \in C^\infty(\Omega), \quad 0 \leq g_d(\mathbf{x}) \leq 1;$

$$g_d(\mathbf{x}) = \begin{cases} 1 & \text{for } \mathbf{x} \in \Omega_{2d} \\ 0 & \text{for } \mathbf{x} \notin \Omega_d \end{cases}$$

$$\sup_{\mathbf{x}\in\Omega}(|\nabla g_d(\mathbf{x})| + \sum_{i=1}^{n} |\frac{\partial^2 g_d(\mathbf{x})}{\partial x_i^2}|) = G(g_d) < \infty.$$

Take $g_n \in C_0^\infty(\Omega_d)$ satisfying $g_n(\mathbf{x}) \to g_d(\mathbf{x})$ together with the derivatives up to second order and $\sup_n G(g_n) \leq G_d < \infty$. Then from (3.4), Lemma 2 and Lebesgue dominated convergence theorem:

$$\int_{\Omega_{2d}} | e^{h_{\delta,\varepsilon}(\mathbf{x})}\psi(\mathbf{x}) |^2 \, d\mathbf{x} \leq$$
$$K \int_{\Omega\setminus\Omega_{2d}} (1 + |\nabla h_{\delta,\varepsilon}(\mathbf{x})|^2) | e^{h_{\delta,\varepsilon}(\mathbf{x})}\psi(\mathbf{x}) |^2 \, d\mathbf{x}. \tag{3.5}$$

and the result in Theorem 1 follows taking the limit $\varepsilon \to 0$.

Remarks :

i. If for some E, H satisfies the Agmon's λ condition then, as well known, the exponential bound follows directly from Lemma 1: one takes $f = ge^h$ and a removing cut-off procedure as above gives the result.

ii. In the Dirac case (supposing $\Psi \in (W^{1,2}_{loc}(\Omega))^4$) one has instead of Lemma 1:

$$< Df\Psi, Df\Psi > -E^2 < f\Psi, f\Psi > = < \Psi, |\nabla f|^2 \Psi >$$

so for energies for which $D^2 - E^2 \geq \lambda$ the exponential bound comes again directly, la Agmon, without using (2.13) [W],[MP] (see also [BG]).

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