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Sharp condition on the decay of the potential for the absence of a zero-energy ground state of the Schrödinger equation

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Abstract. We prove a sharp criterion on the decay of the potential of a Schrödinger operator on $\Re^3$ that ensures the absence of a zero-energy ground state. This condition complements results due to Simon and Lieb. We also give an improved version of their results which, however, is still not optimal.

1. Introduction

There has been some interest in the last few years in determining conditions on the potential that guarantee the absence of a zero-energy ground state of the Schrödinger operator (see e.g. Simon 1981, Lieb 1981, Ramm 1987, 1988). In this paper we prove a sharp condition on the decay of the potential that guarantees the absence of a zero-energy ground state of the Schrödinger operator in $\Re^3$. This condition becomes necessary and sufficient if one restricts the potential to have an asymptotic power law behaviour. We also give an improved version of a theorem of Simon and Lieb (Simon 1981, Lieb 1981). We point out that the techniques used here do not only work in three but also in more dimensions. We refer the reader to the articles of Knowles (1981) and Agmon (1970) for the existence of zero eigenvalues in the one-dimensional case and in the higher-dimensional case respectively. We refer also to the work of Murata (1986 and references therein) for recent results on the subject.

Here we are concerned with positive solutions (i.e. ground states) of the Schrödinger equation with zero energy,

$$-\Delta u + Vu = 0 \tag{1}$$

in $\Re^3$. For simplicity we assume V to be continuous in the whole $\Re^3$, although this condition can be relaxed (see remark (iii) below theorem 1). For a function h defined on $\Re^3$ we denote by $[h]$ its spherical average (i.e. $[h](r) = \int h(r, \Omega)\, d\Omega$, and $d\Omega$ is the normalised, invariant, spherical measure on the unit ball). We also denote by $h_+ = \max(h, 0)$ the positive part of h. Our main result is the following.

Theorem 1. Let u be a positive solution of (1) with V continuous in $\Re^3$ and such that

$$[V(x)]_+ \leq \frac{3}{4|x|^2} \qquad \text{for all } |x| \geq \alpha, \text{ some } \alpha > 0. \tag{2}$$

Then, $u \notin L^2(\Re^3)$.

Remarks.

(i) The multiplicative constant 3/4 in (2) is optimal, as it is simple to exhibit a potential decaying as $c/|x|^2$ at infinity for any $c > 3/4$, with $u > 0$, $u \in L^2(\mathfrak{R}^3)$. In fact, take

$$u(r) \equiv (r+1)^{-(3/2+\varepsilon)} \qquad \varepsilon > 0$$

which is clearly in $L^2(\mathfrak{R}^3)$ and positive (here $r \equiv |x|$). This is the ground state of the Schrödinger equation for the potential

$$V(r) = \frac{(\frac{3}{2}+\varepsilon)[(\frac{1}{2}+\varepsilon)r-2]}{r(r+1)^2} \approx \frac{(\frac{3}{2}+\varepsilon)(\frac{1}{2}+\varepsilon)}{r^2} \qquad \text{at } \infty$$

with zero energy.

(ii) Theorem 1 complements a theorem of Simon (1981, theorem A.3.1) on the absence of zero-energy ground states for potentials $V \in L^{3/2}(\mathfrak{R}^3)$. Simon's theorem was later improved by Lieb (1981, lemma 7.18).

(iii) The condition on V to be continuous was made only for simplicity of the proof. It is enough to request the potential V to be in L^q_{loc}, with $q > 3/2$. This condition guarantees the existence of Harnack's inequality for u (Gilbarg *et al* 1983), needed in the proof. In that case one should interpret the equations in distributional sense.

(iv) The proof of theorem 1 also works for the weaker condition on V:

$$[V(x)]_+ \leqslant \frac{3}{4r^2} + P(r) \qquad \text{for } r \geqslant \alpha > 0 \tag{3}$$

where $P > 0$ and $\int_\beta^\infty P(r) r \, dr < \infty$ for some $\beta \geqslant \alpha > 0$. See remark (i) below the proof of theorem 2.

(v) Theorem 1 even holds for a condition slightly weaker than (3), namely

$$[V(x)]_+ \leqslant \frac{1}{r^2}\left(\frac{3}{4} + \frac{1}{\ln r}\right) \tag{4}$$

for $r \geqslant \alpha > 0$. The multiplicative constant 1 in front of $1/\ln r$ is optimal.

(vi) Ideas similar to the ones used in the proof of theorem 1 have been recently used (Ashbaugh *et al* 1989) to study the L^2-norm of the positive solution of the Thomas-Fermi-von Weizsäcker equation (Lieb 1981) with exponents $3/2 \leqslant p \leqslant 5/3$.

The rest of this paper is organised as follows: in section 2 we give a proof of theorem 1 in the spherically symmetric case. The general proof follows from that with the help of a technical lemma due to Lieb. In section 3 we give an improved version of a theorem of Lieb and Simon on the non-existence of zero-energy ground states under an integral condition on the potential.

2. Proof of theorem 1

First we prove theorem 1 in the spherically symmetric case. We do so because the proof in this case is technically very simple and at the same time illustrates the general idea. Moreover, the proof of the general case follows from here and the use of a theorem of Lieb (lemma 5, below).

Theorem 2 (spherically symmetric case). Consider the Schrödinger equation (1) with $V(x)=V(|x|)$ and $u(x)=u(|x|)>0$. Assume.

$$V_+(r)\leqslant\frac{3}{4r^2}\qquad \text{for all } r\equiv|x|\geqslant\alpha \tag{5}$$

for some positive α. Then $u\notin L^2(D)$, with $D\equiv\{x\,\|x|\geqslant\alpha\}$.

Proof. In the spherically symmetric case the Schrödinger equation (1) is given by

$$u''+\frac{2}{r}u'=Vu\leqslant\frac{3}{4r^2}u\qquad \text{for } r\geqslant\alpha. \tag{6}$$

Here $'\equiv \mathrm{d}/\mathrm{d}r$. Let $g(r)=1/r^{3/2}$. Then g satisfies

$$g''+\frac{2}{r}g'=\frac{3}{4r^2}g\qquad \text{for } r\neq 0. \tag{7}$$

From (6) and (7) it follows that

$$(u-ag)''+\frac{2}{r}(u-ag)'\leqslant\frac{3}{4r^2}(u-ag)\qquad \text{for all } r\geqslant\alpha \tag{8}$$

and any positive a. Since we are assuming V continuous, $u\in C^2$, therefore $u-ag\in C^2(D)$. Since u and g are both strictly positive, we can choose $a=u(\alpha)/g(\alpha)>0$. Then $(u-ag)(\alpha)=0$ and it is clear from (8) that $u-ag$ cannot have a negative minimum. Therefore, there are two possibilities:

(i) either $(u-ag)(r)\geqslant 0$ for all $r\geqslant\alpha$, or

(ii) $(u-ag)(r)\leqslant 0$ and decreasing (non-increasing) for all $r\geqslant\alpha$.

If case (i) holds the proof is complete, since $g\notin L^2(D)$. If case (ii) holds, $0\geqslant u(r)-ag(r)\geqslant u(s)-ag(s)\geqslant -ag(s)$ for all $s>r$ since $u-ag$ is decreasing (non-increasing) and $u>0$. Taking $s\to\infty$ we get $u(r)-ag(r)\equiv 0$ for all $r\geqslant\alpha$ which again implies $u\notin L^2$. □

Remarks.

(i) The proof of theorem 2 also works if (5) is replaced by

$$V(r)\leqslant\frac{3}{4r^2}+P(r)$$

with $P\geqslant 0$ and $\int_\beta^\infty rP(r)\,\mathrm{d}r<\infty$, for some $\beta\geqslant\alpha$. By theorem 9.1 of Hartman's book (Hartman 1964) this condition on P implies the existence of a positive solution g of

$$\frac{1}{r}(rg)''=\left(\frac{3}{4r^2}+P(r)\right)g$$

that behaves as $1/r^{3/2}$ at infinity.

(ii) One can prove theorem 2 even under the slightly weaker condition

$$V(r)\leqslant\frac{1}{r^2}\left(\frac{3}{4}+\frac{1}{\ln r}\right)$$

by choosing an appropriate g (see the remark after corollary 4). In this condition, the multiplicative constant 1 in front of the $1/\ln r$ term is optimal. Adding more small terms which decay slightly faster than $1/\ln r$ is also possible. It does not seem to be obvious how to describe exhaustively the class of all potentials which do not have zero-energy ground states (except for the statement of corollary 4 below).

Using the same method as in the proof of theorem 2 one can prove the following.

Lemma 3. Let g be a positive radial solution of $\Delta g \geqslant Vg$ on $D \equiv \{x \mid |x| \geqslant \alpha\}$ (with V spherically symmetric), such that $g \to 0$ as $r \to \infty$. Then, there is an $a > 0$ such that $ag \leqslant u$, on D, where u is a positive radial solution of (1).

The previous lemma allows us to give the following extension of theorem 2, which somehow gives an implicit characterisation of the potentials which do not have zero-energy ground states.

Corollary 4. If there is a function g satisfying the hypothesis of lemma 3, and $g \notin L^2(D)$, then $u \notin L^2(D)$, where u is a positive radial solution of (1).

Remark. To illustrate the content of corollary 4, let us show that if $V(r) \leqslant [(3/4) + (1/\ln r)]/r^2$ on D, then $u \notin L^2(D)$. This follows by taking the function $g(r) = 1/(r^{3/2}(\ln r)^{1/2})$, which is positive (choose $\alpha > 1$) on D, it goes to zero at infinity, it is not in $L^2(D)$ and it satisfies $\Delta g \geqslant Vg$ on D. The constant in front of the term $1/\ln r$ is optimal. In fact,

$$u(r) = \frac{1}{(r+2)^{3/2}} \frac{1}{(\ln(r+2))^{(1+\varepsilon)/2}}$$

is in $L^2(\Re^3)$, for any $\varepsilon > 0$, and it is the ground state of the Schrödinger operator with a potential that behaves as

$$V(r) \approx \frac{1}{r^2}\left(\frac{3}{4} + \frac{1+\varepsilon}{\ln r}\right)$$

at infinity.

The proof of theorem 1 is a consequence of theorem 2 and the following result of Lieb (1981, lemma 7.17) which we reproduce here for completeness.

Lemma 5 (Lieb). Let S_R denote the sphere $\{x \mid |x| = R\}$ and let $\mathrm{d}\Omega$ be the normalised, invariant, spherical measure on S_1. For any function h, let $[h](r) = \int h(r, \Omega)\, \mathrm{d}\Omega$ be the spherical average of h. Now suppose $\psi(x) > 0$ is C^2 in a neighbourhood of S_R. Let $f(r) = \exp\{[\ln \psi](r)\}$. Then for all r in some neighbourhood of R,

$$\left[\frac{\Delta\psi}{\psi}\right](r) \geqslant \left(\frac{\Delta f}{f}\right)(r) = \frac{1}{f(r)}\left(\frac{\mathrm{d}^2 f}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}f}{\mathrm{d}r}\right).$$

Proof. Let $p(x) = \ln \psi(x)$. Then $(\Delta\psi/\psi) = \Delta p + (\nabla p)^2$. Clearly $[\Delta p] = \Delta[p]$. Moreover, $(\nabla p)^2 \geqslant \{\partial p(r, \Omega)/\partial r\}^2$, and $[(\partial p/\partial r)^2] \geqslant (\mathrm{d}[p]/\mathrm{d}r)^2$ by the Schwarz inequality. Thus $[\Delta\psi/\psi] \geqslant \Delta[p] + (\nabla[p])^2 = \Delta f/f$. □

To conclude this section we give the following proof.

Proof of theorem 1. Let u be a positive solution of (1) and let $f(r) = \exp\{[\ln u](r)\}$ as in lemma 5. Then f satisfies

$$\frac{1}{r}(rf)'' \leqslant \frac{3}{4r^2} f \qquad \text{for all } r \geqslant \alpha$$

and, because of theorem 2, $f \notin L^2(D)$. By Jensen's inequality $\int f^2 \leqslant \int u^2$, then $u \notin L^2(D)$ (this argument is taken from Lieb (1981, lemma 7.18)). □

3. Improved version of a theorem of Lieb and Simon

Our theorem 1 is a complement to the following theorem of Lieb (1981, lemma 7.18), which is an improvement of an earlier result of Simon (1981, theorem A.3.1).

Theorem 6 (Lieb). Suppose $\psi(x) > 0$ is a C^2 function in a neighbourhood of the domain D and ψ satisfies $(-\Delta + V(x))\psi(x) \geqslant 0$ on D. Suppose $[V]_+ \in L^{3/2}(D)$. Then $\psi \notin L^2(D)$.

In this section we give a theorem (theorem 7 below) that bridges the gap between our theorem 1 and Lieb's theorem. In fact, theorem 7 is an improvement of theorem 6, and its proof is based on the same methods as employed in section 2.

Theorem 7. Let u be a positive solution of the equation

$$-\Delta u + Vu \geqslant 0 \qquad \text{in } D = \{x \,|\, |x| > \alpha\}. \tag{9}$$

Assume that $[V]_+$ satisfies

$$\int_r^\infty [V]_+(s)\,\mathrm{d}s \leqslant \frac{1}{2r} \qquad \text{for } r > \alpha. \tag{10}$$

Then $\psi \notin L^2(D)$.

Proof. Using Lieb's method (i.e. using lemma 5 above), it is enough to prove theorem 6 for V and u spherically symmetric. In the spherically symmetric case, theorem 7 is a consequence of lemma 3 above and an ordinary differential equations existence result which we give in what follows (lemma 8 below). □

Remarks.

(i) The condition (9) on V is weaker than the hypothesis $[V]_+ \in L^{3/2}$ used by Lieb (1981, lemma 7.18). In fact, if $[V]_+ \in L^{3/2}(D)$, using Hölder's inequality we get

$$\int_r^\infty [V]_+(s)\,\mathrm{d}s \leqslant \frac{1}{3^{1/3}r}\left(\int_r^\infty [V]_+^{3/2} s^2\,\mathrm{d}s\right)^{2/3}.$$

Hence, $\int_r^\infty [V]_+(s)\,\mathrm{d}s = \mathrm{o}(1)/r$, for $r \to \infty$.

(ii) The multiplicative constant 1/2 in (10) is not optimal, as is clear from theorem 1.

Lemma 8. Let V be a non-negative, spherically symmetric potential satisfying $\int_r^\infty V(s)\,\mathrm{d}s \leqslant 1/(2r)$ on D. Then there is a positive radial solution of $\Delta g = Vg$, such that $g \to 0$ as $r \to \infty$ and $g \notin L^2(D)$.

Proof. Let $w(r) = rg(r)$. Hence,

$$w''(r) = V(r)w(r) \tag{11}$$

on D. Since $V \geqslant 0$, there are two types of positive solutions of (11) namely, those which are increasing and go to infinity at infinity and those which are decreasing and whose derivative go to zero at infinity (Hartman 1964). We choose here a solution of the second type and we will denote it by w. If $\lim_{r\to\infty} w(r) \neq 0$ we are done, since $g(r) = w(r)/r \notin L^2(D)$. Thus, we can assume $\lim_{r\to\infty} w(r) = 0$. Integrating (11) from r to infinity we have

$$-w'(r) = \int_r^\infty V(s)w(s)\,\mathrm{d}s \leqslant w(r)\int_r^\infty V(s)\,\mathrm{d}s \leqslant \frac{w(r)}{2r} \tag{12}$$

where the second inequality follows from the monotonicity of w and the third follows from the hypothesis on V. Therefore, from (12), we have that $w(r)r^{1/2}$ is non-decreasing, hence $w(r) \geqslant kr^{-1/2}$ and thus $g \notin L^2(D)$. $\square$

To conclude, we point out that if V is such that $\int_r^\infty V(s)\,\mathrm{d}s \leqslant c/r$ in lemma 8, then $g \notin L^p$, for all $1 \leqslant p \leqslant 3/(c+1)$. As we have seen in remark (i) below theorem 7, if $V \in L^{3/2}(D)$, we have that c can be taken arbitrarily small for big enough r and thus g (and therefore u, because of lemma 3) is not in L^p for all $1 \leqslant p < 3$, a result due to Brezis (see the note added in proof after lemma 7.18 in Lieb (1981)).

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