155. *Approximation of Obstacles by High Potentials; Convergence of Eigenvalues*

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§ 1. Introduction.

Let K be a compact subset of R^3 whose boundary is of class C^2 and $\Omega=R^3-K$. Consider the following equation of Schrödinger type in Ω with the Dirichlet boundary condition:

$$\text{(1)} \qquad \begin{cases} -\Delta\varphi(x)+q(x)\varphi(x)=\lambda\varphi(x), \\ \varphi(x)\,|_{\partial K}=0. \end{cases}$$

Furthermore, let us consider the Schrödinger equation of the form

$$\text{(2)} \qquad -\Delta\varphi(x)+q(x)\varphi(x)+n\chi_K(x)\varphi(x)=\lambda\varphi(x)$$

in the whole space R^3, where $\chi_K(x)$ is the characteristic function of K and n is a positive integer.

The purpose of the present paper is to show that the negative eigenvalues of (1) can be obtained as a limit of those of (2) when n tends to infinity. Convergence of eigenfunctions will also be discussed.

The idea of regarding (1) as the limit problem of (2) is closely related to the penalty method (cf. Lions [3]). It may be noted that χ_K in (2) can be replaced by any function f which is measurable, positive and bounded on K and is zero outside K. In a physical sense Problem (1) is sometimes referred to as the hard core model. Thus, as far as eigenvalues and eigenfunctions are concerned, the hard core, i.e. the infinite potential on K, can be approximated by potentials which are strongly repulsive on K. Furthermore, looking in the reverse way, one may use the hard core to approximate such a potential on K.

Among related works we mention those of Titchmarsh [6] and Konno [2]. Titchmarsh obtained the eigenfunction expansions for a finite two-dimensional region by making $q(x)\to\infty$ outside the region considered. Recently Konno considered the same problem as ours and proved the convergence of eigenfunctions belonging to the continuous spectrum.

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§ 2. Statement of results.

Throughout the present paper we always assume that $q(x)$, a real valued function defined on R^3, satisfies the following conditions:

(C.1) $q(x)$ is measurable and bounded except in some neighbourhoods U_i of a finite number of singular points p_i in Ω and satisfies the inequalities

$$|q(x)| \leqq \frac{\text{const.}}{|x-p_i|^{3/2-\varepsilon}}, \quad x \in U_i \text{ and } \varepsilon > 0;$$

(C.2) there exist constants $R>0$, $\alpha>0$ and $C_0>0$ such that

$$|q(x)| \leqq \frac{C_0}{|x|^\alpha}, \quad \text{if } |x| \geq R.$$

Let A be the operator in $L^2(\Omega)$ associated with the exterior Dirichlet problem (1). More precisely A is defined as follows[1]:

$$(3) \qquad \begin{cases} Au = -\Delta u + qu, & u \in D(A), \\ D(A) = \mathcal{D}^1_{L^2}(\Omega) \cap \mathcal{E}^2_{L^2}(\Omega). \end{cases}$$

Let $A_n, n=1,2,\cdots$, be the operator in $L^2(R^3)$ defined as

$$(4) \qquad \begin{cases} A_n u = -\Delta u + qu + n\chi_K u, & u \in D(A_n), \\ D(A_n) = \mathcal{E}^2_{L^2}(R^3). \end{cases}$$

The following properties of A and A_n are known:
(i) they are self-adjoint; (ii) they are bounded below uniformly with respect to n; (iii) the negative part of the spectrum of A_n is discrete, namely, it consists of at most countable number of eigenvalues with finite multiplicity and has no points of accumulation except for zero (cf. Schechter [5]).

(C.1) was assumed to ensure property (ii). Thanks to property (ii), $(A_n+t)^{-1}$ exists and is bounded for all n if $t>0$ is sufficiently large. Now we have the next preliminary theorem.

Theorem 1. (a) *For every sufficiently large $t>0$, the sequence $(A_n+t)^{-1}$ converges strongly as $n\to\infty$ to a bounded self-adjoint operator G in $L^2(R^3)=L^2(K)\oplus L^2(\Omega)$. G is reduced by the subspaces $L^2(K)$ and $L^2(\Omega)$. The part of G in $L^2(K)$ is equal to* 0 *and the part of G in $L^2(\Omega)$ is equal to $(A+t)^{-1}$.* (b) *The negative part of the spectrum of A is discrete.*

Let us enumerate the negative eigenvalues of A_n and A as

$$(5) \qquad \lambda_1^{(n)} \leqq \lambda_2^{(n)} \leqq \cdots,$$

$$(6) \qquad \lambda_1 \leqq \lambda_2 \leqq \cdots,$$

where each eigenvalue is counted repeatedly according to its multiplicity. These series may terminate in finite terms or may even be vacuous. Let s be the number which is equal to the total multiplicity of eigenvalues of A. In other words, $s=0$ if series (6) is vacuous, $s=k$ if (6) terminates at the k-th term, and $s=\infty$ if (6) does not terminate in finite terms. Then, our main result is expressed in the following theorem.

1) $D(T)$ stands for the domain of an operator T.

Theorem 2. *Let s be defined as above. Then, for every $j \leqq s$, each eigenvalue $\lambda_j^{(n)}$ converges to λ_j as $n \to \infty$. For $j > s$, each $\lambda_j^{(n)}$ tends to zero as $n \to \infty$ or the series $\{\lambda_j^{(n)}\}_{n=1,2,\dots}$ terminates in finite terms.*

The next lemma is essential in the proof.

Lemma 3. *For every $\varepsilon > 0$, there exists a constant $r > 0$ independent of λ such that $A_n\varphi = \lambda\varphi, \lambda < 0$ and $\|\varphi\| = 1$ imply*

$$\int_{|x|\geq r} |\varphi|^2 dx < \frac{\varepsilon}{|\lambda|}.$$

Remark 4. Let $\varphi_j^{(n)}$ be the eigenfunction of A_n corresponding to $\lambda_j^{(n)}$. As can be seen from the proof of Theorem 2, a subsequence $\{\varphi_j^{(n')}\}$ converges strongly as $n' \to \infty$ to an eigenfunction φ_j of A corresponding to λ_j. About the convergence of eigenfunction we can actually say more, namely, when λ_j is simple, we can choose the sequence $\{\varphi_j^{(n)}\}_{n=1,2,\dots}$ such that it converges strongly as $n \to \infty$ to φ_j, where φ_j is extended to K by setting $\varphi_j = 0$ there.

§ 3. Proof of Theorems.

Proof of Theorem 1. Let $t > 0$ be sufficiently large. Then the sequence $\{(A_n + t)^{-1}\}$ is monotone decreasing in n and $\{\|(A_n + t)^{-1}\|\}$ is bounded in n. Consequently $(A_n + t)^{-1}$ converges strongly to a bounded self-adjoint operator G in $L^2(R^3)$ (cf. Kato [1]). Thus we have the first statement of Theorem 1. Now, let $u \in L^2(R^3)$ be arbitrarily fixed. Put $(A_n + t)^{-1}u = f_n$ and $Gu = g$. Clearly $f_n \to g$ as $n \to \infty$ strongly in $L^2(R^3)$. Let us express q as $q = q_+ - q_-, q_\pm \geqq 0$. Then using the uniform boundedness of $(A_n + t)^{-1}$ and assumption (C.1) and making t larger if necessary, we can prove that there exist $M > 0, \varepsilon > 0$ and $\beta_\varepsilon > 0$ satisfying $1 - \varepsilon > 0$ and $t - \beta_\varepsilon > 0$ such that

$$(7) \qquad M\|u\|^2 \geqq ((A_n + t)f_n, f_n) \geqq (1-\varepsilon)\||\nabla f_n|\|^2 + (q_+ f_n, f_n) + (t - \beta_\varepsilon)\|f_n\|^2 + n\|\chi_K f_n\|^2, \quad u \in L^2(R^3).$$

It follows from (7) that $\|\chi_K f_n\| \to 0$ as $n \to \infty$ and that $\{f_n\}$ is a bounded sequence in $\mathcal{E}^1_{L^2}(R^3)$. Therefore, since $f_n \to g$ in $L^2(R^3)$, we see that $\nabla f_n \to \nabla g$ weakly in $L^2(R^3)^3$. As $f_n \to 0$ on K, $g = 0$ on K. In other words,[2] $g \in \mathcal{D}^1_{L^2}(\Omega)$. If $u \in L^2(K)$ i.e. $u|_\Omega = 0$, then we can write u as $u = (A_n + t)f_n = \chi_K(A_n + t)f_n$. From property (ii), there is $\gamma > 0$ such that

$$(8) \qquad \|u\|\,\|\chi_K f_n\| \geqq ((A_n + t)f_n, f_n) \geqq \gamma\|f_n\|^2, \quad u \in L^2(K).$$

Therefore f_n tends to zero as $n \to \infty$. Thus we have that G is reduced by $L^2(K)$ and $L^2(\Omega)$. Next we show that if $u \in L^2(\Omega)$ i.e. $u|_K = 0$, then $Gu|_\Omega = (A + t)^{-1}u$ in $L^2(\Omega)$. In fact, for each $\varphi \in C_0^\infty(\Omega)$

2) We sometimes use the same letter to denote a function in R^3 and its restriction to Ω or to K. Furthermore, $L^2(K)$ and $L^2(\Omega)$ are frequently regarded as subspaces of $L^2(R^3) = L^2(K) \oplus L^2(\Omega)$.

$$(u,\varphi)_{L^2(\Omega)}=((A_n+t)f_n,\varphi)_{L^2(\Omega)}$$
$$=(\nabla f_n,\nabla\varphi)_{L^2(\Omega)}+((q+t)f_n,\varphi)_{L^2(\Omega)}.$$

Taking the limit, we have

$$(u,\varphi)_{L^2(\Omega)}=(\nabla g,\nabla\varphi)_{L^2(\Omega)}+((q+t)g,\varphi)_{L^2(\Omega)}.$$

Moreover, we have for each $v\in D(A)=\mathcal{D}^1_{L^2}(\Omega)\cap\mathcal{E}^2_{L^2}(\Omega)$

(9) $$(u,v)_{L^2(\Omega)}=(\nabla g,\nabla v)_{L^2(\Omega)}+((q+t)g,v)_{L^2(\Omega)},\ v\in D(A).$$

Furthermore we have

$$((A+t)^{-1}u,(A+t)v)_{L^2(\Omega)}=(g,(A+t)v)_{L^2(\Omega)},\ v\in D(A).$$

Since the range of $A+t$ is equal to $L^2(\Omega)$, we obtain $g=(A+t)^{-1}u$ in $L^2(\Omega)$. Thus we have proved (a).

Next we show (b). Let E_n and E be the resolutions of identity associated with A_n and A respectively and let $I=[c,d]$ be an arbitrary interval, where $c<\lambda_1^{(1)}<d<0$. By virtue of the minimax principle one has $\lambda_j^{(1)}\leqq\lambda_j^{(2)}\leqq\cdots$. Considering the strong convergence of resolvents and the monotonicity of the sequence $(A_n+t)^{-1}$ in the sense of quadratic forms, we have

(10) $$\dim E_1(I)\geqq\dim E_2(I)\geqq\cdots\geqq\dim E_n(I)\geqq\cdots\geqq\dim E(I).$$

From (10) we can easily see (b).

Proof of Theorem 2. Put $\dim E(I)=s_0$ in (10). Then it can be seen from (10) that for every $j\leqq s_0$ the sequence $\lambda_j^{(n)}$ converges to some number $\mu_j\leqq d<0$ as $n\to\infty$. Now we suppose in the proof that $\{\varphi_j^{(n)}\}$ is already orthonormalized. Hence, there exists a subsequence $\{\varphi_j^{(n')}\}$[3] which converges weakly to some element $\tilde\varphi_j$ of $L^2(R^3)$. According to Lemma 3 and Rellich's theorem, however, we can easily show that the convergence is actually the strong convergence. In the same way as in the proof of Theorem 1 (cf. (7) and (9)), we obtain $\tilde\varphi_j=(A+t)^{-1}(\mu_j+t)\tilde\varphi_j$ in $L^2(\Omega)$. Thus we have $\tilde\varphi_j\in D(A)=\mathcal{D}^1_{L^2}(\Omega)\cap\mathcal{E}^2_{L^2}(\Omega)$ and $A\tilde\varphi_j=\mu_j\tilde\varphi_j$ in $L^2(\Omega)$. Furthermore, since $\varphi_j^{(n')}$ converges strongly, $\{\tilde\varphi_j\}$ is also orthonormalized. Thus we can see that each μ_j is actually equal to λ_j. Therefore the original sequence $\{\lambda_j^{(n)}\}_{n=1,2,\ldots}$ converges as $n\to\infty$ to the eigenvalue λ_j.

§ 4. Proof of Lemma 3.

We show that there exist $r_1>0$ and $C>0$, independent of λ, such that for any $r>r_1$

(11) $$\int_{|x|\geq r}|\varphi|^2dx\leqq\frac{C}{|\lambda|r^\theta},$$

where $\theta=\alpha$ for $0<\alpha<1$ and $\theta=1$ for $1\leqq\alpha$. Since the proof in the case $1\leqq\alpha$ is essentially the same as in the case $0<\alpha<1$, we shall only deal with the case $0<\alpha<1$. Put[4] $\Omega_{a,b}=\{a<|x|<b\}$, $\Omega_a=\{|x|>a\}$ and

3) We can choose numbers $\{n'\}$ in common with respect to all $j\leqq s_0$.

4) We suppose that a is sufficiently large and $\Omega_a\cap K=\phi$.

$S_a=\{|x|=a\}$. Denoting by (,) the innerproduct in R^3, we get by Green's formula

$$\int_{\Omega_{a,b}}|x|^\alpha(|\nabla\varphi|^2-\lambda|\varphi|^2)dx \leqq a^{\alpha-1}\int_{S_a}|(\nabla\varphi, x)\varphi|dS$$
$$+\, b^{\alpha-1}\int_{S_b}|(\nabla\varphi, x)\varphi|dS+\int_{\Omega_{a,b}}|(\nabla\varphi, \alpha x|x|^{\alpha-2})\varphi|dx$$
$$+\int_{\Omega_{a,b}}|x|^\alpha|q||\varphi|^2dx.$$

There exists $r_0>0$ independent of λ such that the fourth term on the right side is not greater than C_0 for any $a\geqq r_0$. We note that $\{\varphi\}$ is bounded in $\mathcal{E}^1_{L^2}(R^3)$ uniformly in $\lambda<0$ by the same estimate as in (7). Let M be a constant such that $\||\nabla\varphi|\|\leqq M$. The third term is majorized by $\alpha\||\nabla\varphi|\|\,\|\varphi\|$ and is bounded by αM. Also we have

(12) $$\|(\nabla\varphi, x|x|^{\alpha-2})\varphi\|_{L^1(\Omega_1)}\leqq M.$$

It follows from (12) that there exists a sequence $\{b(k)\}_{k=1,2,\dots}$ tending to infinity as $k\to\infty$ such that

$$b(k)^{\alpha-1}\int_{S_{b(k)}}|(\nabla\varphi, x)\varphi|dS=b(k)\int_{S_{b(k)}}|(\nabla\varphi, xb(k)^{\alpha-2})\varphi|dS\to 0, \text{ as } k\to\infty.$$

We proceed to the first term. By virtue of (12), there exists some a such that $r_0\leqq a\leqq r_0+1$ and

$$a^{\alpha-1}\int_{S_a}|(\nabla\varphi, x)\varphi|dS\leqq(r_0+1)M.$$

From what was stated above, we see that there exists a constant $M'>0$ independent of λ such that

$$\int_{|x|>r_0+1}|x|^\alpha(|\nabla\varphi|^2-\lambda|\varphi|^2)dx\leqq M'.$$

Hence follows the desired inequality (11).

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