сообщения
объединенного
института
ядерных
исследований
дубна

E2-84-49

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IMPROVED ROSEN'S CONDITIONS ON BOUND STATES OF SCHRÖDINGER OPERATORS

1984

1. Introduction

Various qualitative methods for analyzing the discrete spectrum of Schrödinger operators have been elaborated during the last three decades - for a review see Ref.1, Section XIII.3 . They are of a great physical interest, especially because they can provide us with an information about $\sigma_{disc}(H)$ for the few-body and many-body Hamiltonians, for which the quantitative methods are usually difficult to be applied. It is not strange, therefore, that new results of this type continue to appear.

Recently, Rosen[2] employed a Sobolev inequality to deduce a necessary condition for existence of bound states of a Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$, and a lower bound to the ground-state energy of H . These results are formulated in terms of integrals of certain powers of $|V|$, and no symmetry of the potential is required. On the other hand, convergence of the mentioned integrals demands $|V|$ to decrease rapidly enough at infinity, excluding thus many physically interesting cases. In this note, we are going to give an improvement which makes it possible to relax this restriction. At the same time, we present extension of the results to any dimension $d \geq 3$ of the configuration space.

2. The Main Result

We shall be concerned with the Schrödinger operators $H = -\Delta + V$ on $\mathcal{H} = L^2(\mathbb{R}^d)$, $d \geq 3$. For a given ε , we denote

$$V_-(\varepsilon, x) := \max\{0, \varepsilon - V(x)\} . \tag{1}$$

The functions $V_-(\varepsilon, .)$ are essential in formulation of our result :

Theorem : Suppose that H is self-adjoint on $D(H) = D(-\Delta)\cap D(V)$.
(a) Let $V_-(\varepsilon,.)\in L^{d/2}(\mathbb{R}^d)$, then the condition

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx > K_d^d = \frac{\pi^{1/2}(\pi d(d-2))^{d/2}}{2^{d-1}\,\Gamma\left(\frac{d+1}{2}\right)} \qquad (2)$$

is necessary for the operator H to have an eigenvalue below ε .
(b) Let $V_-(\varepsilon,.)\in L^{\gamma d/2}(\mathbb{R}^d)$ for some ε and $\gamma > 1$, then any eigenvalue E of H fulfils the inequality

$$E \geq \varepsilon - (1-\gamma^{-1})\left(\gamma^{-d/2}\,K_d^{-d}\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\,dx\right)^{2/d(\gamma-1)} . \qquad (3)$$

In particular, this is true for the ground-state energy E_0 .

Proof : Since the improvements of Rosen's arguments follow the same line, we limit ourselves with sketching the proof of the assertion (b) ; the details will be given in a forthcoming paper. The starting point is the Sobolev inequality

$$\|\nabla\psi\|_2 \geq K_d\|\psi\|_q \quad , \qquad (4)$$

where $q = 2d/(d-2)$ and K_d is given by (2). It is the best constant for the inequality (4) whose value was found by Talenti[3], and earlier by Rosen[4] for $d = 3$. If ψ is a normalized eigenvector, $\|\psi\|_2 = 1$, corresponding to E , then

$$E = \|\nabla\psi\|_2^2 + \int_{\mathbb{R}^d} V(x)|\psi(x)|^2\,dx \geq$$

$$\geq \|\nabla\psi\|_2^2 + \varepsilon - \int_{\mathbb{R}^d} V_-(\varepsilon,x)|\psi(x)|^2\,dx$$

so the inequality (4) gives

$$E \geq \varepsilon + K_d^2\|\psi\|_q^2 - \int_{\mathbb{R}^d} V_-(\varepsilon,x)|\psi(x)|^2\,dx \quad . \qquad (5a)$$

Next one has to estimate the last term on the r.h.s. using twice the Hölder inequality

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)|\psi(x)|^2\,dx \leq$$

$$\leq \left(\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\,dx\right)^{2/\gamma d}\|\psi\|_2^{2(\gamma-1)/\gamma}\,\|\psi\|_q^{2/\gamma} . \qquad (5b)$$

Finally, one has to maximize the expression following from the inequalities (5) over $\|\psi\|_q$ to get the desired result.

3. Examples and Remarks

(i) The Rosen's results are recovered if $d = 3$, $\varepsilon = 0$ and the potential V is non-positive. In particular, he treated the spherically symmetric exponential well, $V(r) = -V_0\exp(-r/a)$. Here the necessary condition given by (2) differs by 0.6% from the critical value of V_0a^2 . Furthermore, the inequality (3) for $V_0a^2 >> 1$ and $\gamma \approx 1.7262\,(V_0a^2)^{1/3}$ gives

$$E_0 \geq -V_0\left[1 - 1.73791(V_0a^2)^{-1/3} + O((V_0a^2)^{-2/3})\right] ,$$

while the exact value is easily found to be

$$E_0 = -V_0\left[1 - 2.33810(V_0a^2)^{-1/3} + 1.45779(V_0a^2)^{-2/3} + O(V_0^{-1}a^{-2})\right] .$$

(ii) Another simple three-dimensional example concerns the spherically symmetric square well, $V(r) = -V_0\,\Theta(a-r)$. In this case, the necessary condition following from (2) is about 15% from the critical value of V_0a^2 . The best lower bound from (3),

$$E_0 \geq -V_0\left[1 - 2.10809(V_0a^2)^{-1}\right] ,$$

is now achieved with a non-zero ε , and it is independent of γ .

(iii) The assertion (a) can be regarded also as a consequence of Cwikel-Lieb-Rosenbljum theorem (see Ref.1, Theorem XIII.12, and Ref.5) except for the value of the constant. Moreover, the latter can be obtained from another Sobolev-inequality argument (cf. Ref.6, or Ref.7, Section III.9). The Rosen-type proof is, however, much more simple and straightforward. Notice also that for $d = 3$ and $\varepsilon = 0$, (2) becomes a particular case of the GMGT-condition (see Ref.6, or Ref.1, Theorem XIII.9) with $p = 3/2$.

(iv) In order to illustrate how powerfull the obtained conditions might be, we present two d-dimensional examples concerning the following exactly solvable problems :

harmonic oscillator : $V(r) = \omega^2r^2$ (6a)

hydrogen-like atom : $V(r) = 2\alpha/r,$ (6b) where $r^2 = \sum_{j=1}^{d} x_j^2$. In both cases, the inequality (3) yields the best lower bound for a non-zero $\mathcal{E}$; in the limit $\mu \to 1+$ we get

$$E_0 \geq 2^{1/d}(d(d-2))^{1/2}\omega \quad , \tag{7a}$$

$$E_0 \geq -4\alpha^2/d(d-2) \quad , \tag{7b}$$

respectively (for details see the forthcoming paper mentioned above). Since the ground-state energies are $E_0 = \omega d$ for the oscillator, and $E_0 = -4\alpha^2/(d-1)^2$ for the hydrogen-like atom /8/, we see that both the lower bounds (7) are asymptotically exact with $d \to \infty$.

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Received by Publishing Department
on January 30,1984

Экснер П. E2-84-49
Улучшенные условия Розена на связанные состояния операторов Шредингера

Выводится необходимое условие для того, чтобы оператор Шредингера $H = -\Delta + V$ на $L^2(\mathbb{R}^d)$, $d \geq 3$, имел связанное состояние ниже заданной энергии ϵ, а также оценка снизу на энергию основного состояния оператора H. Эти условия выражаются только в терминах потенциала V и обобщают недавние результаты Розена на случаи размерности $d > 3$ и для потенциалов, которые не должны быстро убывать на бесконечность.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1984

Exner P. E2-84-49
Improved Rosen's Conditions on Bound States of Schrödinger Operators

We derive a necessary condition on a Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^d)$, $d \geq 3$ to have a bound state below a given energy ϵ, and a lower bound to the ground-state energy of H. These conditions are expressed in terms of the potential V alone, and generalize the recent results of Rosen to the dimensions $d > 3$ and to the potentials that are not necessarily rapidly decreasing. Some examples are given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1984