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Some remarks on double-wells in one and three dimensions

by

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ABSTRACT. — We obtain uniformly convergent asymptotic expansions for the energies of certain double-well Hamiltonians in the limit as the spacing (R) goes to infinity. In one dimension some further results are proved. In particular, we discover R-independent eigenvalues.

In an appendix we deal with the convergence of eigenvalues as $R \to \infty$ in any dimension and merely assuming that potentials are relatively form compact.

1. INTRODUCTION

On $L^2(\mathbb{R}^\nu)$ ($\nu = 1$ or 3) we consider the Schroedinger operator

$$H_R(V, W) = -\Delta + V(\underline{x}) + W_R(\underline{x}) \tag{1.1}$$

where $W_R(\underline{x}) = W(\underline{R} - \underline{x})$ and V, W have compact support and lie in L^p ($p = 3/2$ for $\nu = 3$, $p = 1$ for $\nu = 1$). Our results are:

$\nu = 1$. — Without loss we can suppose that supp V and supp $W(R - x)$ ($R \geqslant 0$) are disjoint if and only if $R > 0$. Then

THEOREM (1.1). — *i)* Suppose $E_0 < 0$ is a common eigenvalue of $H_0 + V$ and $H_0 + W$. Then $H_R(V, W)$ has two eigenvalues $E_\pm(R)$ ($E_-(R) < E_0 < E_+(R)$)

which converge to E_0 and, for sufficiently large R, obey a *uniformly* convergent expansion of the form $(\alpha_0^2 = -E_0)$

$$E_\pm(R) - E_0 = \sum_{\substack{n=1\\m=0}}^{\infty} c_{nm}^{\pm}(e^{-\alpha_0 R})^n\,(Re^{-\alpha_0 R})^m \tag{1.2}$$

where $c_{1,0}^{\pm} \neq 0$ and $c_{1,1}^{\pm} \neq 0$. Moreover $E'_-(R) > 0$ for all $R \geq 0$ and $E'_+(R) < 0$ for all R such that $E_+(R) < 0$.

ii) Suppose E_0 is eigenvalue of $H_0 + V$ but not of $H_0 + W$. Then only one eigenvalue E(R) approaches E_0 and we have (R large enough) the uniformly convergent expansion

$$E(R) - E_0 = \sum_{\substack{n=1\\m=0}}^{\infty} c_{nm}(e^{-2\alpha_0 R})^n\,(Re^{-2\alpha_0 R})^m. \tag{1.3}$$

Either $c_{1,0} \neq 0$ or *all* $c_{n,m} = 0$. $E'(R) > 0$ (if $c_{1,0} > 0$) or $E'(R) < 0$ ($c_{1,0} < 0$) as long as $E(R) < 0$.

In case *i*) and *ii*) the energies are real analytic functions of R, $R > 0$.

THEOREM (1.2). — Suppose E_0 is a negative eigenvalue of $H_0 + V$ and W is not non negative. Then there exists an unbounded sequence of numbers σ_i such that E_0 is an (R-independent) eigenvalue of $H_0 + V + \sigma_i W_R$ for all $R \geqq 0$. If $W \leqq 0$ the coupling constants for which E_0 is eigenvalue of $H_0 + \sigma W$ and the σ_i interlace.

Let $n(V)$ denote the number of negative eigenvalues of $H_0 + V$. V is called *critical* if $n((1 + \varepsilon)V) > n(V)$ for any $\varepsilon > 0$.

THEOREM (1.3). — *i*) Suppose at least one of V or W is critical. Then $n(V + W_R) = n(V) + n(W)$ for all $R \geqq 0$.

ii) Suppose neither V nor W is critical. Then $n(V + W_R) = n(V) + n(W)$ for R sufficiently large. Moreover,

$$n(V) + n(W) - 1 \leqq n(V + W_R) \leqq n(V) + n(W), \qquad R > 0,$$

and $n(V + W_R)$ can change at most once.

$\nu = 3$.

THEOREM (1.4). — Let E_0 denote the ground state of $H_0 + V$ and for simplicity suppose that $V = W$. Then for sufficiently large R the two eigenvalues $E_\pm(R)$ which converge to E_0 obey

$$E_\pm(R) - E_0 = \sum_{\substack{n=1\\m=1}}^{\infty} c_{nm}^{\pm}(e^{-\alpha_0 R})^n\,R^{-m} \tag{1.4}$$

where the series is uniformly convergent and $c_{1,1}^{+} = -c_{1,1}^{-} \neq 0$.

In this paper we use ideas of [*1*] to study the large R asymptotics of the eigenvalues of $H_R(V, W)$. It happened that independent of the present author, I. Sigal and B. Simon became aware of this possibility at about the same time, when listening to a talk by E. M. Harrell about his recent work on this subject [*2*]. We consented that it be left up to the present author to write a paper. In fact he had also realized that one can derive an implicit equation ((2.2) ($\nu = 1$) and (3.10) ($\nu = 3$)) for the double-well energies.

Let us comment on some of the main results in this paper.

The point behind the asymptotic expansions in Theorem (1.1) and Theorem (1.4) is that they tell us in terms of which functions of R one has to expand. Other approaches (e. g. [*2*]) might allow us to expand as well but the problem is to predict the analytic form of the terms that might eventually emerge. Moreover, under certain assumptions we can rule out the possibility that the first term in the expansion is zero. This partly answers the question of « miraculous cancellations » alluded to by Harrell [*2*].

Theorem (1.2) and Theorem (1.3) are by-products of our investigations. Theorem (1.2) shows that in one dimension an eigenvalue may stay at the same place as R varies. This result surprised us, and so did Theorem (1.3). In fact, on the basis of [*1*] we were convinced that two critical negative wells would have at least one extra bound state near E = 0 which would eventually enter the continuum as $R \to \infty$. Our attempts to localize it failed, which led us to Theorem (1.3).

If the potentials do not have compact support our method is still able to answer certain general questions. To illustrate this we have added an appendix where we prove a well-known large R result. To the best of our knowledge the assumptions are weaker than those in previous works (see e. g. [*2*]). In particular, we do not need results about the fall-off of eigenfunctions. To get explicit asymptotic expansions (like e. g. for H_2^+) the setting described in the appendix is not suitable, though in principle it would be possible. There exist more effective methods (see J. Morgan and B. Simon [*3*]).

Of course, we could also handle two dimensions but we have not worked out the details.

2. $\nu = 1$

2.1. **An implicit equation**

We recall that any negative bound state E of $H_0 + q$ ($H_0 = - d^2/dx^2$) is determined by the condition that

$$K(\alpha, q) = |q|^{1/2}(H_0 + \alpha^2)^{-1} q^{1/2} (q^{1/2} = |q|^{1/2} \operatorname{sgn} q, E = -\alpha^2)$$

have eigenvalue -1. This is the well-known Birman-Schwinger principle. In our case $q(x) = V(x) + W(R - x)$ and $(H_0 + \alpha^2)^{-1}$ has kernel

$$G_\alpha(x, y) = (2\alpha)^{-1} \exp(-\alpha|x - y|).$$

Following [1] we may view $K(\alpha, q)$ as a two-by-two matrix operator with kernel

$$L_\alpha = \begin{pmatrix} |V(x)|^{1/2}G_\alpha(x, y)V(y)^{1/2} & |V(x)|^{1/2}G_\alpha(x, -y+R)W(y)^{1/2} \\ |W(x)|^{1/2}G_\alpha(x, -y+R)V(y)^{1/2} & |W(x)|^{1/2}G_\alpha(x, y)W(y)^{1/2} \end{pmatrix} \tag{2.1}$$

We observe that $G_\alpha(x, -y + R) = (2\alpha)^{-1}\exp(-\alpha R)\exp(\alpha x)\exp(\alpha y)$ is rank one. Therefore, the eigenvalue problem $L_\alpha\phi = -\phi$ where $\phi = (\phi_1, \phi_2)$ is easily converted into a system of two linear equations in the two unknowns $(V^{1/2}, \phi_1)$ and $(W^{1/2}, \phi_2)$. Setting the determinant equal to zero gives

$$1 = \frac{e^{-2\alpha R}}{4\alpha^2} g(\alpha, V)g(\alpha, W) \tag{2.2}$$

where

$$g(\alpha, V) = (f_{\alpha,V}, (1 + K(\alpha, V))^{-1} | f_{\alpha,V}|) \tag{2.3}$$

and

$$f_{\alpha,V}(x) = V^{1/2}(x)e^{\alpha x} \tag{2.4}$$

Eq. (2.2) is an implicit equation for $\alpha(R)$ where $-\alpha(R)^2$ is a bound state of $H_R(V, W)$.

2.2. Properties of $g(\alpha, V)$

Suppose $H_0 + V$ has n eigenvalues $E_0 < E_1 < \ldots < E_n < 0$. Put $\alpha_i^2 = -E_i$, $i = 1, \ldots, n$. Then we have

LEMMA (2.1). — $g(\alpha, V) \to \infty$ (resp. $-\infty$) as $\alpha \uparrow \alpha_k$ (resp. $\alpha \downarrow \alpha_k$).

Proof. — Fix $k = 1 \ldots n$. Let $\mu_k(\alpha)$ denote the unique eigenvalue of $K(\alpha, V)$ which tends to -1 as $\alpha \to \alpha_k$. Then

$$\mu_k(\alpha) = -1 + c(\alpha - \alpha_k) + 0((\alpha - \alpha_k)^2) \tag{2.5}$$

with $c > 0$. Suppose χ_k obeys $K(\alpha_k, V)\chi_k = -\chi_k$. Then $\chi_k = |V|^{1/2}\psi_k$ where ψ_k satisfies $(H_0 + V)\psi_k = E_k\psi_k$. Now the (non orthogonal) eigen projection associated with χ_k is $d\chi_k((\text{sgn } V)\chi_k, .)$ with $1/d = (\psi_k, V\psi_k)$. Thus

$$g(\alpha, V) = \frac{d}{c(\alpha - \alpha_k)}(Ve^{\alpha_k x}, \psi_k)^2 + 0(1) \tag{2.6}$$

and Lemma (2.1) follows provided $(Ve^{\alpha_k x}, \psi_k) \neq 0$. Since ψ_k obeys

$$\int G_{\alpha_k}(x, y)\psi_k(y)dy = -\psi(x)$$

we see that for x positive and large

$$- \psi(x) = \frac{1}{2\alpha_k} e^{-\alpha_k x}(\mathrm{V} e^{\alpha_k x}, \psi_k)\,. \tag{2.7}$$

Hence $(\mathrm{V}e^{\alpha_k x}, \psi) \neq 0$, for ψ does not vanish identically.

Remark. — The constant c in (2.5) can be expressed as

$$c = -\frac{2\alpha_k \|\psi_k\|^2}{(\psi_k, \mathrm{V}\psi_k)} \tag{2.8}$$

and thus $c > 0$, for $(\psi_k, \mathrm{V}\psi_k) < 0$. (2.8) follows from the observation that the eigenvalue $\mathrm{E}_k(\lambda)$ of $\mathrm{H}_0 + \lambda \mathrm{V}$ which approaches $\mathrm{E}_k(1) = -\alpha_k^2$ as $\lambda \to 1$ also obeys $\lambda\mu_k(\sqrt{-\mathrm{E}_k(\lambda)}) = 1$ which relates c to the first order perturbation of $\mathrm{E}_k(\lambda)$.

Next we consider $g(\alpha, \lambda\mathrm{V})$ as function of $\lambda > 0$. Suppose λ_1 and $\lambda_2 (\lambda_2 > \lambda_1 > 0)$ are two consecutive coupling constants for which $\mathrm{H}_0 + \lambda\mathrm{V}$ has eigenvalue $\mathrm{E} = -\alpha^2$. Then we have

LEMMA (2.2). — $g(\alpha, \lambda\mathrm{V}) \to -\infty$ (resp. $+\infty$) as $\lambda \uparrow \lambda_2$ (resp. $\lambda \downarrow \lambda_1$) and $g(\alpha, \lambda\mathrm{V})$ has at least one and not more than finitely many zeroes on (λ_1, λ_2). If in addition $\mathrm{V} \leq 0$ then $\lambda^{-1}g(x, \lambda\mathrm{V})$ is strictly monotonically decreasing and $g(\alpha, \lambda\mathrm{V})$ has exactly one zero on (λ_1, λ_2).

Proof. — As $\lambda \uparrow \lambda_2$ (resp. $\lambda \downarrow \lambda_1$) an eigenvalue of $\mathrm{K}(\alpha, \lambda\mathrm{V}) = \lambda\mathrm{K}(\alpha, \mathrm{V})$ converges to -1 from above (resp. below). If χ denotes an eigenvector belonging to any nonzero eigenvalue of $\mathrm{K}(\alpha, \mathrm{V})$ then $(f_{\alpha,\mathrm{V}}, \chi) \neq 0$ for we can argue as in (2.6) (2.7) noting that $\chi = |\mathrm{V}|^{1/2}\psi$ where $(\mathrm{H}_0 + \mathrm{V})\psi = \mathrm{E}\psi$ and λ is chosen suitably. This shows that $g(\alpha, \lambda\mathrm{V}) \to -\infty$ (resp. $+\infty$) as $\lambda \uparrow \lambda_2$ (resp. $\lambda \downarrow \lambda_1$). An application of the intermediate value theorem along with analyticity in λ proves the first part of Lemma (2.2).

The second part follows from the (trivial) monotonicity in λ of the eigenvalues of $\mathrm{K}(\alpha, \lambda\mathrm{V})$ (which are all negative).

2.3. **Proofs of Theorems** (1.1.)-(1.3.)

We begin by proving Theorem (1.2).

Let $\mathrm{E}_0 = -\alpha_0^2$ be an eigenvalue of $\mathrm{H}_0 + \mathrm{V}$. By Lemma (2.2), $g(\alpha_0, \sigma\mathrm{W}) = 0$ for $0 < \sigma_1 < \sigma_2 < \ldots$ where $\sigma_i \to \infty$ since the σ_i lie between the coupling constants for which E_0 is eigenvalue of $\mathrm{H}_0 + \sigma\mathrm{W}$. Let

$$\chi_{\mathrm{R},i} = (\mathrm{H}_0 + \sigma_i \mathrm{W}_\mathrm{R} - \mathrm{E}_0)^{-1}\mathrm{V}\psi \tag{2.9}$$

where

$$(H_0 + V)\psi = E_0\psi \tag{2.10}$$

We claim that

$$(H_0 + V + \sigma_i W_R)\chi_{R,i} = E_0\chi_{R,i} \tag{2.11}$$

for *all* $R \geq 0$.

To verify (2.11) we need only prove $V\chi_{R,i} = - V\psi$ and to this end we write

$$\begin{aligned}(H_0 + \sigma_i W_R - E_0)^{-1} &= (H_0 - E_0)^{-1} \\ &- \sigma_i(H_0 - E_0)^{-1}W_R^{1/2}(1 + K(\alpha_0, \sigma_i W_R))^{-1} \mid W_R \mid^{1/2}(H_0 - E_0)^{-1}\end{aligned} \tag{2.12}$$

which is permitted since E_0 is not eigenvalue of $H_0 + \sigma_i W$. Since

$$(H_0 - E_0)^{-1}V\psi = - \psi$$

it suffices to prove that

$$\sigma_i V(H_0 - E_0)^{-1}W_R^{1/2}(1 + K(\alpha_0, \sigma_i W_R))^{-1} \mid W_R \mid^{1/2}(H_0 - E_0)^{-1}V\psi = 0 \tag{2.13}$$

Now

$$U_R W_R^{1/2}(1 + K(\alpha_0, \sigma_i W_R))^{-1} \mid W_R \mid^{1/2} U_R^{-1} = W^{1/2}(1 + K(\alpha_0, \sigma_i W))^{-1} \mid W \mid^{1/2}$$

where $(U_R f)(x) = f(R - x)$. The kernel of $\mid W \mid^{1/2} U_R(H_0 - E)^{-1}V$ is

$$\frac{e^{-\alpha R_0}}{2\alpha_0} \mid W(x) \mid^{1/2} e^{\alpha_0 x} e^{\alpha_0 y} V(y) \tag{2.14}$$

(remembering that $x + y \leq 0$ by our initial assumptions on supp V and supp W).

Thus the l. h. s. of (2.13) equals

$$\frac{e^{-2\alpha_0 R}}{4\alpha_0^2} (V^{1/2}, f(\alpha_0, V))g(\alpha_0, \sigma_i W)V^{1/2}(x)e^{\alpha_0 x} \tag{2.15}$$

which is zero by construction of σ_i. This proves the main part of Theorem (1.2). The rest follows from the second half of Lemma (2.2).

Remark. — The function $\chi_{R,i}$ has been found as follows. We observe that the zero of $g(\alpha, \sigma_i W)$ at $\alpha = \alpha_0$ (which is at least $0(\alpha - \alpha_0)$ owing to analyticity) cancels the singularity of $g(\alpha, V)$. Thus (2.2) cannot possibly have a solution near α_0 if R is sufficiently large. Thus there does not exist a bound state different from but near $E_0 = - \alpha_0^2$. Now E_0 is a bound state of $H_0 + V$ which implies the existence of E(R) (an eigenvalue of (1.1)) approaching E_0 as $R \to \infty$. Thus $E(R) = E_0$ at least for large enough R. Inspection of the equation $L_{\alpha_0}\Phi = - \Phi$ where $\Phi = (\phi_1, \phi_2)$ shows that ϕ_1 is independent of R and obeys $K(\alpha_0, V)\phi_1 = - \phi_1$ and

$$\phi_2 = c(1 + K(\alpha_0, \sigma_i W))^{-1} \mid f_{\alpha_0 W} \mid$$

where $c = -\sqrt{\sigma_i}(e^{-\alpha_0 R}/2\alpha_0)(f_{\alpha_0,V}, \phi_1)$. Now ϕ is nothing but $\chi_{R,i}$ expressed in component form.

Proof of Theorem (1.1). — *i)* Combining (2.2), (2.6) and (2.8) yields

$$\alpha - \alpha_0 = \pm e^{-\alpha R} h(\alpha) \tag{2.16}$$

where $h(\alpha)$ is analytic near $\alpha = \alpha_0$ and

$$h(\alpha_0) = c_V c_W \tag{2.17}$$

with

$$c_V = (2\alpha_0)^{-1} \int V(x) e^{\alpha x} \psi_V(x) dx . \tag{2.18}$$

ψ_V obeys $(H_0 + V)\psi_V = E_0 \psi_V$, $\| \psi_V \| = 1$. Pick now the $+$ sign in (2.16) and set

$$\alpha - \alpha_0 = \tau(1 + z) \tag{2.19}$$

$$\tau = e^{-\alpha_0 R} h(\alpha_0) \tag{2.20}$$

$$\rho = R\tau \tag{2.21}$$

and insert (2.19) into (2.16). We get a relation of the form $F(z, \tau, \rho) = 0$ where

$$F(z, \tau, \rho) = 1 + z - \frac{h(\alpha_0 + \tau(1 + z))}{h(\alpha_0)} e^{-\rho(1+z)} \tag{2.22}$$

Now F is analytic in all three variables and vanishes at $z = \tau = \rho = 0$. Moreover, $\partial F/\partial z$ $(0, 0, 0) = 1$. Thus by the implicit function theorem for several variables we may solve for z an express it by a uniformly convergent power series in the variables τ and ρ. We obtain

$$\alpha - \alpha_0 = \sum_{\substack{n=1 \\ m=0}}^{\infty} d_{nm} (e^{-\alpha_0 R})^n \, (R e^{-\alpha_0 R})^m \tag{2.23}$$

where by inspection (solving (2.23) by iteration) $d_{1,0} = h(\alpha_0)$, $d_{1,1} = -h^2(\alpha_0)$. For the $-$ sign in (2.16) we would get $d_{1,0} = -h(\alpha_0)$. (2.23) is readily converted into (1.2) with the explicit coefficients $c^{\pm}_{1,0} = \mp 2\alpha_0 h(\alpha_0)$, $c^{\pm}_{1,1} = -2\alpha_0 h(\alpha_0)^2$.

The monotonicity properties also follow directly from eq. (2.2), which can immediately be solved for $R = R(\alpha)$. Let I denote the largest (open) interval with left endpoint α_0 such that $R(\alpha) > 0$ for all $\alpha \in I$. On I, $R'(\alpha) \leq 0$ since $R(\alpha) \to +\infty$ as $\alpha \downarrow \alpha_0$ ($u(\alpha) \to +\infty$) and $R(\alpha)$ can not have a local minimum. If it had one at $\alpha = \alpha^*$, say, then as $R \downarrow R(\alpha^*)$ two solutions of $R = R(\alpha)$ would converge to α^* so that $-(\alpha^*)^2$ were a two-fold eigenvalue of $H_R(V, W)$ which is impossible (also, the eigenvalues would suddenly disappear as R drops slightly below $R(\alpha^*)$. Thus $R = R(\alpha)$ has a unique solution $\alpha(R) = (-E_-(R))^{1/2}$ and $E'_-(R) \geq 0$. But $E'_-(R) = 0$ can be excluded since $R'(\alpha)$ is finite on I. $E_+(R)$ is handled similarly (choosing I with right endpoint α_0).

ii) The expansion (1.3) is derived in a similar way as (1.2). As to the alternative for $c_{n,m}$ we note that $c_{1,0}$ is proportional to $g(\alpha_0, W)$ and thus is zero if and only if the latter is. Then the claim follows from Theorem (1.2). The statement about $E'(R)$ follows as in *i*).

The last fact comes from the joint analyticity in α and R of the Kernel (2.1) which we write as $L(\alpha, R)$. Suppose $-\alpha_0^2$ is a bound state of $H_{R_0}(V, W)$ and hence $L(\alpha_0, R_0)$ has eigenvalue -1. Then $L(\alpha, R)$ has eigenvalue

$$\mu(\alpha, R) = -1 + c(\alpha - \alpha_0) + d(R - R_0) + \dots,$$

analytic at $\alpha = \alpha_0$ and $R = R_0$. Since c is nonzero by (2.8), the equation $\mu(\alpha, R) = -1$ has an analytic solution $\alpha(R) = (-E(R))^{1/2}$ near $R = R_0$. Thus $E(R)$ is analytic, too.

This proves Theorem (1.1).

Remark. — Suppose that $V = W \leq 0$ and $V(-x) = V(x)$ and let us concentrate on the ground state. One can work out the coefficient d in the expansion for $\mu(\alpha, R)$ (using the Lippmann-Schwinger equation at some point) and then gets a remarkable equation for $E'(R)$, namely

$$E'(R) = (-E(R)/\| \psi \|^2)\psi^2(R/2)$$

where ψ denotes the ground state of $H_R(V, V)$. We have explicitly verified this formula for $V = -\delta$. For the proof of Theorem (1.3) we need two lemmas.

LEMMA (2.3). — $n(V) = \#(\psi) \equiv$ number of zeroes of ψ where ψ obeys $(H_0 + V)\psi = 0$ and $\psi(a) = 1$, $\psi'(a) = 0$ with $a = \inf\{ x \mid x \text{ supp } V \}$.

Remark. — This lemma should be well known, however we do not know of any reference.

Proof. — Let superscript D, x (resp. N, x) refer to the operator $H_0 + V$ with a Dirichlet (resp. Neumann) boundary condition at $x \in \mathbb{R}$. Let ψ_ε obey $\psi_\varepsilon(a) = 1$, $\psi'_\varepsilon(a) = \varepsilon > 0$. For small enough ε, $\#(\psi_\varepsilon) > \#(\psi)$ since there is certainly an additional zero at some $x_0 < a$. Recall that $\psi_\varepsilon(x) = \varepsilon(x - a) + 1$ for $x \leq a$. By a familiar result [*4*] $\#(\psi_\varepsilon) = n^{D,x_0}(V) + 1$. Similarly $\#(\psi) = n^{N,x_0}(V)$ since ψ obeys Neumann b. c. at x_0. Hence by D/N bracketing [*4*],

$$\#(\psi) \geq n(V) \geq \#(\psi_\varepsilon) - 1 \geq \#(\psi).$$

Thus $n(V) = \#(\psi)$, proving Lemma (4.1).

LEMMA (2.4). — If V is critical there exists $\psi \in L^\infty$ obeying $(H_0 + V)\psi = 0$.

Remark. — Lemma (2.4) has a converse which, however, we do not need.

Proof. — Let ψ_λ satisfy $(H_0 + V)\psi_\lambda = 0$, $\psi_\lambda(a) = 1$ and $\psi'_\lambda(a) = 0$. Then

$\psi_\lambda(x)$ is continuos in λ uniformly on compact sets of the variable x. For x to the right of and outside supp V: $\psi_\lambda(x) = cx + d$. Suppose $c \neq 0$ and $\lambda = 1$. Then $\#(\psi_1) = \#(\psi_{1+\varepsilon})$ for small enough ε by continuity in λ. This contradicts the criticality of V. Thus $c = 0$ and $\psi \in L^\infty$.

Proof of Theorem (1.3). — *i)* Suppose V is critical and let ψ be the zero energy solution in L^∞ with $\psi(a) = 1$, $\psi'(a) = 0$. Let ψ_R be the unique solution of $H_R(V, W)\psi_R = 0$ which is identical to ψ for $x \leq a$. ψ_R is obtained by matching ψ and that solution χ_R of $(H_0 + W_R)\chi_R = 0$ which is constant for large negative x. Clearly, $\chi_R(x) = \chi_0(-R + x)$ and therefore

$$\#(\psi_R) = \#(\psi) + \#(\chi_0)$$

for all $R \geq 0$. Now we can appeal to Lemma (2.3) and conclude that

$$\#(\psi_R) = n(V + W_R) = n(V) + n(W_0).$$

But $n(W_0) = n(W(-x)) = n(W)$ completing the proof of part *i*).

ii) Choose $\lambda_0 > 1$ and $\mu_0 > 1$ to be the smallest coupling constants for which $\lambda_0 V$ and $\mu_0 W$ are critical. Then

$$n(V + W_R) \leq n(\lambda_0 V + \mu_0 W_R) = n(\lambda_0 V) + n(\mu_0 W) = n(V) + n(W)$$

for all $R \geq 0$ while for R large enough: $n(V + W_R) \geq n(V) + n(W)$ by Theorem (1.1) (or Theorem (A.1)). This proves the first claim.

The last inequality of the second assertion has just been proved. Thus we are left proving $n(V) + n(W) - 1 \leq n(V + W_R)$. We observe that the number of negative eigenvalues can only change if an eigenvalues enters or leaves the negative half line at $E = 0$. Since the function $R(\alpha)$ given by (2.2) is single-valued this can happen at most once. More precisely, there exists at most one *finite* R_0 ($R_0 = \infty$ is not possible by *i*)) at which an eigenvalue either enters or leaves $(-\infty, 0)$ as R increases from $R_0 - \varepsilon$ to $R_0 + \varepsilon$. Now an eigenvalue cannot leave the interval since this would imply $n(V + W_{R_0 - \varepsilon}) > n(V) + n(W)$, contradicting what we learned above. Hence at most one eigenvalue can enter $(-\infty, 0)$, proving *ii*).

Remark. — Suppose a negative potential well is so shallow that it has exactly one bound state. Cut the well in two parts and move one of them off to infinity. Then the number of eigenvalues increases by one.

3. $\nu = 3$

$(-\Delta + \alpha^2)^{-1}$ has kernel

$$G_\alpha(\underline{x}, \underline{y}) = \frac{1}{4\pi} \frac{e^{-\alpha|\underline{x} - \underline{y}|}}{|\underline{x} - \underline{y}|} \tag{3.1}$$

with the consequence that the off-diagonal terms in the three-dimensional analog of (2.1) are not rank one. However they are asymptotically rank one, namely

$$G_\alpha(\underline{x}, -\underline{y} + \underline{R}) \simeq \frac{e^{-\alpha R}}{4\pi R} e^{\alpha \hat{R} \underline{x}} e^{\alpha \hat{R} \underline{y}} \tag{3.2}$$

for large R where $\hat{\underline{R}} = \underline{R}/R$, $R = |\underline{R}|$. This suggests we should try to derive an implicit equation as we did for $\nu = 1$. For simplicity we put $V = W$ and restrict ourselves to the ground state. Then there is an additional simplification in that L_α (2.1) has two invariant orthogonal subspaces spanned by vectors of the form $\Phi = (\phi_+, \phi_+)$ or $\Phi = (\phi_-, -\phi_-)$. Then $L_\alpha \Phi = -\Phi$ if and only if

$$K(\alpha, V)\phi_\pm \pm |V(\underline{x})|^{1/2} \int G_\alpha(\underline{x}, -\underline{y} + \underline{R}) V(\underline{y})^{1/2} \phi_\pm(\underline{y}) d^3y = -\phi_\pm \tag{3.3}$$

Now

$$G_\alpha(\underline{x}, -\underline{y} + \underline{R}) = P_\alpha(\underline{x}, \underline{y}) + R_\alpha(\underline{x}, \underline{y}) \tag{3.4}$$

where

$$P_\alpha(\underline{x}, \underline{y}) = \frac{e^{-\alpha R}}{4\pi R} |V(\underline{x})|^{1/2} e^{\alpha \hat{R} x} e^{\alpha \hat{R} y} V(\underline{y})^{1/2} \tag{3.5}$$

and

$$R_\alpha(\underline{x}, \underline{y}) = P_\alpha(\underline{x}, \underline{y}) [e^{-\alpha h(x, y\, R)}(1 + Rg(\underline{x}, \underline{y}; \underline{R})) - 1] \tag{3.6}$$

with h and g given by

$$|\underline{x} + \underline{y} - \underline{R}| = R - (\underline{x} + \underline{y})\hat{\underline{R}} + h(\underline{x}, \underline{y}; \underline{R}) \tag{3.7}$$

$$|\underline{x} + \underline{y} - \underline{R}|^{-1} = R^{-1} - g(\underline{x}, \underline{y}; \underline{R}) \tag{3.8}$$

h and g are analytic in $1/R$ and $|h(\underline{x}, \underline{y}; \underline{R})| \leq c/R$, $|g(\underline{x}, \underline{y}; \underline{R})| \leq d/R^2$ uniformly for $\underline{x}, \underline{y} \in \text{supp } V$.

Choosing the + sign and putting $\phi = \phi_+$ (3.3) is equivalent to

$$(1 + K_\alpha + R_\alpha)^{-1} P_\alpha \phi = -\phi \tag{3.9}$$

provided the inverse exists. Using (3.5) we obtain

$$\frac{e^{-\alpha R}}{4\pi R}(u_\alpha, (1 + K_\alpha + R_\alpha)^{-1} |u_\alpha|) = -1 \tag{3.10}$$

where $u_\alpha(\underline{x}) = V(\underline{x})^{1/2} e^{\alpha \hat{R} x}$. (3.10) replaces (2.2), but R_α depends here also on R. We shall prove the existence of a solution $\alpha(R)$ of (3.10) which obeys $\alpha(R) - \alpha_0 = 0(e^{-\alpha_0 R}/R)$ where $-\alpha_0^2$ is the ground state of $H_0 + V$. This also justifies taking the inverse of $1 + K_\alpha + R_\alpha$, for K_α has an eigenvalue $\mu(\alpha) = -1 + c(\alpha - \alpha_0)$ $(c \neq 0)$ and R_α has norm of order $e^{-\alpha_0 R}/R^2$. In other words, in the α – region where the eigenvalue lies R_α is a small perturbation of P_α. Indeed, neglecting the R_α term and exploiting (3.10) as in the one-dimensional case we see that

$$\alpha - \alpha_0 \simeq a \frac{e^{-\alpha_0 R}}{R} \tag{3.11}$$

where

$$a = \frac{1}{8\pi\alpha_0}\left(\int V(\underline{x})e^{\alpha_0\hat{R}x}\psi(\underline{x})d^3x\right)^2 \tag{3.12}$$

and ψ obeys $(-\Delta + V)\psi = -\alpha_0^2\psi$, $\|\psi\| = 1$. $a \neq 0$ if and only if

$$e^{\alpha_0|x|}\psi = 0(|x|^{-1})$$

by expanding $-\psi = (-\Delta + \alpha_0^2)^{-1}V\psi$ for large $|\underline{x}|$. For the ground state $a \neq 0$ follows from:

LEMMA (3.1). — Let ψ obey $(-\Delta + V)\psi = E_0\psi$ where $E_0 < 0$ is the ground state. Then

$$|\psi(\underline{x})| \geq c\frac{e^{-\alpha_0|\underline{x}|}}{|\underline{x}|}, \qquad -\alpha_0^2 = E_0,\ c > 0$$

Proof. — The proof is a straightforward generalization of Theorem (10.1) in [5], replacing $-\Delta$ by $-\Delta + \alpha^2$.

We now turn to the proof of Theorem (1.4). Since $\|(1+K_\alpha)^{-1}R_\alpha\| = 0(1/R)$ we may expand $(1 + K_\alpha + R_\alpha)^{-1} = (1 + (1 + K_\alpha)^{-1}R_\alpha)^{-1}(1 + K_\alpha)^{-1}$ into a Neumann series. Upon separating off the contribution from the (first order) pole of $(1 + K_\alpha)^{-1}$, (3.10) becomes

$$\alpha - \alpha_0 = a\frac{e^{-\alpha R}}{R}h(\alpha, R) \tag{3.13}$$

where a is given by (3.12) and $h(\alpha, R)$ is analytic in α and R at $\alpha = \alpha_0$ and $R = \infty$. Moreover, $h(\alpha_0, \infty) = 1$ in accordance with (3.11). We introduce now τ, σ and η by

$$\tau = e^{-\alpha_0 R} \tag{3.14}$$

$$\sigma = 1/R \tag{3.15}$$

$$a\tau(1 + \eta) = (\alpha - \alpha_0)R \tag{3.16}$$

and substitute them into (3.13). We obtain

$$1 + \eta = \tilde{h}(\tau, \sigma, \eta) \tag{3.17}$$

where $\tilde{h}$ is analytic in all three variables and $\tilde{h}(0,0,0) = 1$. Thus (3.17) can be solved for η with η being analytic in τ and σ, provided $(\partial/\partial\eta F)(0,0,0) \neq 0$ where $F(\tau, \sigma, \eta) = 1 + \eta - \tilde{h}(\tau, \sigma, \eta)$. Now one can show that $(\partial\tilde{h}/\partial\eta)(0,0,0) = 0$. Since $\partial/\partial\eta = a\tau\sigma\,\partial/\partial\alpha$ we need only worry about terms with singular α-derivative. These come from $(1 + K_\alpha)^{-1}R_\alpha$ and are in essence of the form $(\alpha - \alpha_0)^{-1}R_\alpha$. By inspection, using (3.5) and the substitutions (3.14)-(3.16), the η-derivative is seen to be zero at (0, 0, 0). This proves Theorem (1.4).

APPENDIX

LARGE R DECOUPLING

For any self-adjoint operator A let P (A) denote the spectral projection associated with the Borel set Ω. On $L^2(\mathbb{R}^\nu)$ $(\nu \geq 1)$ we have ($\underline{R} = (R, 0, \ldots, 0)$).

THEOREM (A.1). — Let V and W be Δ-form compact. Let $(a, b) \in (-\infty, 0)$ and

$$a, b \in \rho(H_0 + V) \cap \rho(H_0 + W).$$

Then

$$\dim P_{(a,b)}(-\Delta + V + W_R) = \dim P_{(a,b)}(-\Delta + V) + \dim P_{(a,b)}(-\Delta + W) \quad (A.1)$$

for R sufficiently large (depending on a, b).

Proof. — Let $q_R = V + W_R$ and $K(\alpha, q_R) \mid q_R \mid^{1/2} R_0(E) q_R^{1/2}$ where $R_0(E) = (H_0 - E)^{-1}$, $H_0 = -\Delta$, $E \in \rho(H_0)$, $\alpha = (-E)^{1/2}$. Let $\chi_R(\bar{\chi}_R = 1 - \chi_R)$ denote the characteristic function of the set $\{ \underline{x} \mid x_1 < R/2 \}$. Let $(T_R f)(\underline{x}) = f(\underline{R} - \underline{x})$. By $U_R : f \to (\chi_R f, T_R \bar{\chi}_R f)$ we define an isometry from $L^2(\mathbb{R}^\nu)$ onto $\mathscr{H}_R = L^2(x_1 < R/2) \oplus L^2(x_1 < R/2)$. Then operators on $\mathscr{H}_R$ can be thought of as being matrix operators. For instance

$$U_R K(\alpha, q_R) U_R^{-1} = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \quad (A.2)$$

where

$$K_{11} = \chi_R K(\alpha, q_R)\chi_R,\ K_{12} = \chi_R K(\alpha, q_R)\bar{\chi}_R T_R,\ K_{21} = T_R \bar{\chi}_R K(\alpha, q_R)\chi_R,\ K_{22} = T_R \bar{\chi}_R K(\alpha, q_R)\bar{\chi}_R T_R.$$

Of course, $\mathscr{H}_R$ is naturally imbedded in $\mathscr{H}_\infty = L^2(\mathbb{R}^\nu) \oplus L^2(\mathbb{R}^\nu)$ and operators on $\mathscr{H}_R$ can be extended to $\mathscr{H}_\infty$ such that their spectrum remains unchanged except for the null space. Now we claim that $\| K_{12} \| \to 0$ and $\| K_{21} \| \to 0$ as $R \to \infty$. Our argument is based on the fact [*6*] that for bounded operators: $A_n B$ (resp. BA_n) $\to AB$ (resp. BA) in *norm* if $A_n \to A$ (resp. $A_n^* \to A^*$) strongly and B is compact. Using

$$\mid q_R \mid^{1/2} \leq \mid V \mid^{1/2} + \mid W_R \mid^{1/2}$$

the kernel K_{12} is seen to be bounded by the sum of four terms:

$$\chi_R \mid V \mid^{1/2} R_0(E) \mid W_R \mid^{1/2} \bar{\chi}_R T_R,\ \chi_R \mid V \mid^{1/2} . R_0(E) \mid V \mid^{1/2} \bar{\chi}_R T_R,\ \chi_R \mid W_R \mid^{1/2} R_0(E) \mid V \mid^{1/2} \bar{\chi}_R T_R$$

and

$$\chi_R \mid W_R \mid^{1/2} R_0(E) \mid W_R \mid^{1/2} \bar{\chi}_R T_R .$$

In the first term use that $\mid V \mid^{1/2} \mid R_0(E) \mid^{1/2}$ is compact and that

$$(\mid R_0(E) \mid^{1/2} . \mid W_R \mid^{1/2} \bar{\chi}_R T_R)^* = T_R \bar{\chi}_R \mid W_R \mid^{1/2} \mid R_0(E) \mid^{1/2} = \chi_R \mid W \mid^{1/2} \mid R_0(E) \mid^{1/2} T_R$$

tends to 0 strongly ($T_R \to 0$ weakly). In the second and third term simply use that $\bar{\chi}_R \to 0$ strongly. The forth term is unitarily equivalent (under T_R) to $\bar{\chi}_R \mid W \mid^{1/2} R_0(E) \mid W \mid^{1/2} \chi_R$ and thus tends to zero in norm also.

K_{21} is discussed in the same way. Next we claim that $K_{11} \to K(\alpha, V)$ and $K_{22} \to K(\alpha, W)$ in norm as $R \to \infty$. For the first this follows from

$$\| K_{11} - K(\alpha, V) \| \leq \| K_{11} - \chi_R K(\alpha, V)\chi_R \| + \| \chi_R K(\alpha, V)\chi_R - K(\alpha, V) \| .$$

Again, $\bar{\chi}_R \to 0$ strongly shows that the last term vanishes as $R \to \infty$. The first term is handled with the aid of the elementary estimate $|(V + W_R)^{1/2} - V^{1/2}| \leq c\,|W_R|^{1/2}$, $c > 0$, and appealing to the above arguments. The statement about K_{22} is proved similarly. Also

$$U_R R_0(E) q_R^{1/2} U_R^{-1} \to \begin{pmatrix} R_0(E)V^{1/2} & 0 \\ 0 & R_0(E)W^{1/2} \end{pmatrix} \tag{A.3}$$

and similarly for $|q_R|^{1/2} R_0(E)$. Thus as $R \to \infty$, the second term on the r. h. s. of the resolvent formula (2.12) converges in norm to a direct sum of corresponding single well operators, provided $E \in \rho(H_0 + V) \cap \rho(H_0 + W)$. Now Theorem (A.1) follows from norm convergence of spectral projections which are obtained by integrating the resolvent of $H_0 + V + W_R$ along a suitable loop enclosing (a, b), noting that the free resolvent in (2.12) gives no contribution.

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