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Section A :
Physique théorique.

Binding of Schrödinger Particles Through Conspiracy of Potential Wells

by

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ABSTRACT. — We study the ground state energy E(R) for

$$-\Delta + V(\underset{\sim}{x}) + W(R - \underset{\sim}{x})$$

when V and W are negative with compact support. In particular, in dimension 3, when $-\Delta + V$ and $-\Delta + W$ *both* have no bound states but both have zero energy resonances, we prove that $E(R) \sim -\beta R^{-2}$ for R large with $\beta = .321651512\ldots$

In this note we want to discuss some properties of the ground state energy, $E(\underset{\sim}{R})$, of the Schrödinger operator on $L^2(\mathbb{R}^\nu)$

$$-\Delta + V(\underset{\sim}{x}) + W(\underset{\sim}{R} - \underset{\sim}{x})$$

where V and W have compact support and lie in $L^p\left(p = \frac{\nu}{2}\right.$ for $\nu \geq 3$, $p = 1$ for $\nu = 1$, $p > 1$ for $\nu = 2$) and

$$R \equiv |\underset{\sim}{R}| > R_0 = \sup \{ |\underset{\sim}{x} + \underset{\sim}{y}| \mid x \in \text{supp } V, y \in \text{supp } W \}$$

so that $V(\underset{\sim}{x})$ and $W(\underset{\sim}{R} - \underset{\sim}{x})$ have disjoint supports. Our first result is (all proofs deferred until later):

THEOREM 1. — Let V, W be negative. In the region $R > R_0$, $|E(\underset{\sim}{R})|$ decreases as $\underset{\sim}{R}$ increases, i. e.

$$(\underset{\sim}{R} \cdot \nabla_{\underset{\sim}{R}} E) \geq 0 . \tag{1}$$

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Remarks. — 1. This is to be compared with the results of Lieb-Simon [*2*] who prove (1) when V and W are spherically symmetric and increasing *but without the restriction of disjoint supports.*

2. It is fairly obvious that this will not be true if V and W are sometime positive. For example, if $\nu = 1$ and V consists of a negative well and W a positive well, then $E(\underset{\sim}{R}) > E(\infty)$.

Our remaining results are only of interest in $\nu \geq 3$ dimensions and concern a rather specialized situation. Our interest was stimulated by work of I. Sigal [*4*] on the Effimov effort who found the results we describe below for V = W spherical potentials. Our proofs in addition to being more general have some degree of greater simplicity and elegance.

DEFINITION. — A potential q on $\mathbb{R}^\nu$ (in $L^p(\mathbb{R}^\nu)$ as above) is called *subcritical* if and only if $-\Delta + \lambda q \geq 0$ for $0 \leq \lambda \leq 1 + \varepsilon$. It is called *critical* if and only if $-\Delta + q \geq 0$ but $-\Delta + \lambda q$ has a negative eigenvalue for any $\lambda > 1$. It is called supercritical if $-\Delta + q$ has negative eigenvalues.

THEOREM 2. — Let $\nu \geq 3$. If V and W are both subcritical, then $E(\underset{\sim}{R}) = 0$ for R sufficiently large.

Remark. — There is an alternative proof [*5*] of this fact using hitting probabilities for Brownian paths and one that yields fairly explicit lower bounds on how large R needs to be. This proof depends on the fact [*5*] that q is subcritical if and only if

$$\sup_t \| \exp(-t(-\Delta + q)) \|_{\infty,\infty} < \infty$$

where $\| \cdot \|_{\infty,\infty}$ is the norm as a map from L^∞ to L^∞.

THEOREM 3. — Let $\nu = 3$. If V is subcritical and W is critical, then $E(\underset{\sim}{R}) = 0(R^{-4(\nu-2)})$ at infinity.

THEOREM 4. — Let $\nu = 3$. If V and W are both negative and critical, then $R^2 E(\underset{\sim}{R}) \to -\beta$ as $R \to \infty$ where $\beta = \alpha^2$ and α is the unique solution of

$$e^{-\alpha} = \alpha \tag{2}$$

Remarks. — 1. The fixed point (2) is easily seen to be stable so that α can be computed by iteration easily on a calculator. 24 iterations on an SR-56 leads to the stable value $\alpha = .5671432904$ and $\beta = .321651512\ldots$

2. If $\nu \geq 3$, $E(\underset{\sim}{R})R^{2(\nu-2)}$ has a limit but unlike the case $\nu = 3$, the limit is V and W dependent and *not* universal.

3. The R^{-2} falloff and the related fact that thus $-(2M)^{-1}\Delta_R + E(R)$ will have an infinity of bound states for suitable M are critical to Sigal's proof of the Effimov effect [*4*].

THEOREM 5. — If either V or W is supercritical then $E(\infty) = \lim_{R\to\infty} E(\underset{\sim}{R})$ exists and $E(\underset{\sim}{R}) - E(\infty) = o(e^{-aR})$ for suitable $a > 0$.

Remarks. — 1. In fact, $E(\infty) = \min(\inf \sigma(-\Delta + V), \inf \sigma(-\Delta + W)$.

2. Using the methods of [3], one easily obtains that $E(\underset{\sim}{R}) - E(\infty) = o(R^n)$ for all n.

We now turn to the method of proof of these results. The same method of proof has been used by one of us [1] to analyze the question of defining self-adjoint Dirac Hamiltonians where one has potentials with several singularities.

For simplicity, we suppose that V and W are non-positive, treating the more general case in remarks following the formal proofs. The basic fact that we exploit is that for $q \leq 0$ in L^p, the ground state energy $E(q)$ of $-\Delta + q$ is determined by the condition that $K_q \equiv |q|^{1/2}(-\Delta - E)^{-1}|q|^{1/2}$ have norm 1; equivalently since K_q is a positive compact operator, 1 is its (simple) largest eigenvalue; equivalently since K_q has a positive integral kernel, it has a pointwise, non-negative eigenvector with eigenvalue 1.

Now if $K_q\eta = \eta$ and $q(\underset{\sim}{x}) = V(\underset{\sim}{x}) + W(\underset{\sim}{R} - \underset{\sim}{x})$, then $\eta = \tilde{\eta}_1 + \tilde{\eta}_2$ with η_1 having support in supp (V) and η_2 in support of $W(\underset{\sim}{R} - \underset{\sim}{x})$. If V and $W(\underset{\sim}{R} - \underset{\sim}{x})$ has disjoint supports, then this decomposition is unique. Writing $\eta(x) = \eta_1(\underset{\sim}{x}) + \eta_2(\underset{\sim}{R} - \underset{\sim}{x})$ we see that $K_q\eta = \eta$ is equivalent to $L\Phi = \Phi$ where Φ is the two-component vector $\Phi = (\eta_1, \eta_2)$ and L is the two-by-two matrix operator with integral kernel:

$$L = \begin{pmatrix} |V(\underset{\sim}{x})|^{1/2} G_0(\underset{\sim}{x} - \underset{\sim}{y}; E) |V(\underset{\sim}{y})|^{1/2} & |V(\underset{\sim}{x})|^{1/2} G_0(\underset{\sim}{x} + \underset{\sim}{y} - \underset{\sim}{R}; E) |W(\underset{\sim}{y})|^{1/2} \\ |W(\underset{\sim}{x})|^{1/2} G_0(\underset{\sim}{x} + \underset{\sim}{y} - \underset{\sim}{R}; E) |V(\underset{\sim}{y})|^{1/2} & |W(\underset{\sim}{x})|^{1/2} G_0(\underset{\sim}{x} - \underset{\sim}{y}; E) |W(\underset{\sim}{y})|^{1/2} \end{pmatrix}$$

where $G_0(\underset{\sim}{x} - \underset{\sim}{y}, E)$ is the kernel of $(-\Delta - E)^{-1}$.

To summarize, E(R) is determined in the region $E(R) < 0$ by the condition $\| L(E, R) \| = 1$. Since K and hence L is monotone decreasing as E decreases, we see that if $\| L(E_0, R) \| \leq 1$ (resp ≥ 1), then $E(R) \geq E_0$ (resp $\leq E_0$).

Proof of Theorem 1. — Since $R \geq R_0$, for each $\underset{\sim}{x}$, $\underset{\sim}{y}$ with $\underset{\sim}{x} \in \text{supp } V$, $\underset{\sim}{y} \in \text{supp } W$, $G_0(\underset{\sim}{x} + \underset{\sim}{y} - \lambda\underset{\sim}{R}, E) < G_0(\underset{\sim}{x} + \underset{\sim}{y} - \underset{\sim}{R}, E)$ for any $E < 0$ and any $\lambda > 1$. It follows that, for any $\eta \geq 0$, $(\eta \neq 0)$,

$$(\eta, L(E, \lambda\underset{\sim}{R})\eta) < (\eta, L(E, \underset{\sim}{R})\eta) \tag{3}$$

so, since L has a positive integral kernel, $\| L(E, \lambda\underset{\sim}{R}) \| \leq \| L(E, \underset{\sim}{R}) \|$ proving the result.

Remark. — By the strict inequality in (3) and the compactness of L, we have actually proven that $E(\lambda\underset{\sim}{R}) > E(\underset{\sim}{R})$ for $R \geq R_0$, $\lambda > 1$ and $E(\underset{\sim}{R}) < 0$.

Proof of Theorem 2. — Write $L = L_D + L_0$ with L_D diagonal and L_0 off diagonal. Since $G(x, 0) = c|x|^{-(\nu-2)}$ and $V, W \in L^1$,

$$\| L_0(0, R) \|_{HS} \leq C|R - R_0|^{-(\nu-2)} \qquad \text{for} \quad R > R_0 .$$

Since V, W, are subcritical, $\| L_D(0, R) \| < 1$ ($L_D(0, R)$ is R independent). Thus, for $R \geq [C(1 - \| L_D \|)^{-1}]^{1/(\nu-2)} + R_0$ we have that $E(\underset{\sim}{R}) = 0$.

Remark. — If $\| L \|$ and $\| L_D \|$ (but not $\| L_0 \|_{HS}$) are replaced by max $\sigma(L)$ and max $\sigma(L_D)$, the proof extends to the case where V and W are not necessarily negative.

Proof of Theorem 3. — Make the decomposition $L = L_D + L_0$ as in the proof of Theorem 2. $L_D(0)$ has 1 as a simple discrete eigenvalue by hypothesis and all other eigenvalues are strictly smaller. Write

$$L(E, R) = L_D(0) + \delta L$$

where $\delta L = [L_D(E) - L_D(0)] + L_0(E, R) \equiv \delta L_1 + \delta L_2$. As above, for $R > R_0$, $\| L_0(E, R) \| \leq CR^{-(\nu-2)}$ independently of E. Using $E = k^2$:

$$G_0(\underset{\sim}{x} - \underset{\sim}{y}, E) - G_0(\underset{\sim}{x} - \underset{\sim}{y}, 0) = c_1 k \,|\, \underset{\sim}{x} - \underset{\sim}{y} \,|^{-(\nu-3)} + 0(k^2 \,|\, \underset{\sim}{x} - \underset{\sim}{y} \,|^{-(\nu-4)})$$

we see that $\| \delta L_1 - kA_1 \| \leq Dk^2$ with A_1 the 2×2 matrix operator which is zero off-diagonal and $c_1 V^{1/2} \,|\, \underset{\sim}{x} - \underset{\sim}{y} \,|^{-(\nu-3)} V^{1/2}$ and $C_1 W^{1/2} \,|\, \underset{\sim}{x} - \underset{\sim}{y} \,|^{-(\nu-3)} W^{1/2}$ on-diagonal.

We now use perturbation theory. The largest eigenvalue $\lambda_0(E, R)$ of $L(E, R)$ is determined by

$$\int_{|\lambda-1|=\varepsilon} (\Phi, (L(E, R) - \lambda)^{-1}\Phi)\lambda d\lambda = \lambda_0 \int (\Phi, (L(E, R) - \lambda)^{-1}) d\lambda \qquad (4)$$

where $\Phi = (\eta, 0)$ is the normalized vector with $L_D(0)\Phi = \Phi$. Expanding

$$\begin{aligned}(L(E, R) - \lambda)^{-1} &= (L_D(0) - \lambda)^{-1} - (L_D(0) - \lambda)^{-1}\delta L(L_D(0) - \lambda)^{-1} \\ &+ (L_D(0) - \lambda)^{-1}\delta L(L_D(0) - \lambda)^{-1}\delta L(L(E, R) - \lambda)^{-1}\end{aligned}$$

(4) becomes:

$$1 + (\eta, \delta L_1^{(11)}\eta) + 0(k^2) + 0(R^{-2(\nu-2)}) = \lambda_0(1 + 0(k^2) + 0(R^{-2(\nu-2)}))$$

Since $(\eta, \delta L_1^{(11)}\eta) = ck + 0(k^2)$ with $c \neq 0$, the condition $\lambda_0 = 1$ becomes $k = 0(R^{-2(\nu-2)})$ or $E = 0(R^{-4(\nu-2)})$.

Remark. — By carrying on the calculations explicitly to second order, one can show that $ER^{4(\nu-2)}$ converges to an explicit V, W dependent constant as $R \to \infty$.

Proof of Theorem 4. — For simplicity, consider first the case $V = W$. Then L leaves the subspace $\{ \Phi = (\eta, \pm \eta) \}$ invariant. The largest eigenvalue of L is on the (η, η) subspace. On this subspace, 1 is a simple discrete eigenvalue of $L_D(0)$. Using first order as above we obtain the equation:

$$\begin{aligned}1 + |(\eta, W^{1/2})|^2(4\pi)^{-1}[- k + e^{-kR}/R] + 0(k^2) + 0(R^{-2}) + 0(k/R) \\ = 1 + 0(k^2) + 0(R^{-2})\end{aligned}$$

Since $\eta > 0$, $(\eta, W^{1/2}) \neq 0$ and thus

$$k = e^{-kR}/R + 0(k^2) + 0(R^{-2}) \qquad (5)$$

so $kR \to \alpha_0$ and $- k^2 = + E \sim - \alpha_0^2/R^2$.

For the general case, $V \neq W$, $L_D(0)$ has 1 as a degenerate eigenvalue.

So we need to use degenerate perturbation theory. The first order terms then become:

$$(4\pi)^{-1}\begin{pmatrix} -ka^2 & R^{-1}e^{-kR}ab \\ R^{-1}e^{-kR}ab & -kb^2 \end{pmatrix} = F$$

where $a = (\eta, |V|^{1/2})$, $b = (\tilde{\eta}, |W|^{1/2})$ with $\eta(\tilde{\eta})$ the normalized eigenvalue of $|V|^{1/2}G_0|V|^{1/2}$ (resp. $|W|^{1/2}G_0|W|^{1/2}$). The condition that F have a zero eigenvalue is det $F = 0$ or using $a, b \neq 0$, $k = e^{-kR}/R$. Thus (5) still holds.

Remark. — If $\nu > 3$, and $V = W$ (for simplicity only), then the first order terms are

$$-kc\int(\eta|V|^{1/2})(\underset{\sim}{x})|\underset{\sim}{x}-\underset{\sim}{y}|^{-(\nu-3)}(\eta|V|^{1/2})(\underset{\sim}{y}) + (\eta, |V|^{1/2})^2G_0(R, k^2)$$

Since $G_0(R, k^2) \leq dR^{-(\nu-2)}$, we see that $kR \to 0$ and thus $G_0(R, k^2) \to dR^{-(\nu-2)}$ so that we get $E = -k^2 \sim a^2R^{-2(\nu-2)}$ with a explicitly V dependent.

Proof of Theorem 5. — This follows the proof of Theorem 3, except that since one of V, W is supercritical, the off diagonal terms are $0(e^{-aR})$.

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