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Section A :
*Physique théorique.*

# On the double-well problem for Dirac operators

by

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ABSTRACT. — We show that the eigenvalues of a Dirac Hamiltonian with two centers of force converge to those of the Hamiltonians with only one center of force in the limit as the spacing goes to infinity. We discuss perturbation theory and show how to estimate the spread of asymptotically degenerate sets of eigenvalues. The methods are for the most part not special to Dirac operators.

RÉSUMÉ. — On montre que les valeurs propres d'un Hamiltonien de Dirac avec deux centres d'interaction tendent vers celles des deux Hamiltoniens ayant seulement un centre d'interaction quand la distance de ces centres tend vers l'infini. On étudie la théorie des perturbations et on montre comment on peut estimer l'étalement de familles de valeurs propres asymptotiquement dégénérées. L'essentiel des méthodes n'est pas particulier aux opérateurs de Dirac.

## I. INTRODUCTION

Consider the operator

$$T_0 + Q \equiv \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta + Q \tag{1.1}$$

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on $\mathscr{H} = [L^2(\mathbb{R}^3)]^4$, where $T_0$ is known as the free Dirac operator, Q is multiplication (in all spinorial components) by a real-valued, measurable potential function $Q(x)$, and $\alpha_1, \alpha_2, \alpha_3$, and $\alpha_4 \equiv \beta$ are the Dirac matrices, satisfying the commutation relations $\alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij}$, $i = 1, 2, 3, 4$. The vectors $\boldsymbol{\alpha}$ and $\boldsymbol{p}$ stand for $(\alpha_1, \alpha_2, \alpha_3)$ and $-i(\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$. In this note $Q(\boldsymbol{x})$ is of the form

$$Q(\boldsymbol{x}) = V(\boldsymbol{x} - \mathbf{R}) + W(\boldsymbol{x} + \mathbf{R}), \tag{1.2}$$

where $\mathbf{R} = (0, 0, R)$. The Hamiltonian (1.1) models the motion of an electron in the field of two nuclei or positive ions after separation of the time variable, provided that V and W are predominantly negative near $x_3 = 0$, fall off at infinity, and are otherwise reasonable. Some conditions will be placed on V and W below. We shall denote the operator (1.1) with Q as in (1.2) as T(R); various aspects of T(R) have been studied previously [*1*] [*2*] [*3*], and in particular [*2*] contains a comprehensive list of further references. Part of the motivation for this note is that in these references some conclusions about the spectral behavior of T(R) as $R \to 0$ or $R \to \infty$ are based on intuition alone and need to be put on a rigorous basis. In addition we lay the foundations of a general perturbation theory in Section III for the limit $R \to \infty$ and control eigenvalue gaps in Section IV. We normalize so that $m = 1$, making the mass gap of T(R) the interval $(-1.1)$.

II. The main issue in this paper is the behavior of the discrete eigenvalues of T(R) as $R \to \infty$. The nature of the limit is described by Theorems II.2 and II.3. The restriction to one particle and two centers of force is largely for convenience; we believe that analogues of most of the theory of Morgan and Simon for Schrödinger operators hold for Dirac operators as well, given the techniques described below. Morgan and Simon [*5*] have shown that nonrelativistic molecular energy levels in the Born-Oppenheimer approximation converge to the constituent energy levels as the nuclear spacing increases to infinity. They rely on the min-max principle, which restricts them to operators bounded below, which Dirac operators are not, but we shall replace min-max with a simple lemma in spectral theory due to Weinhold [*6*] [*7*], which applies to a discrete eigenvalue of any self-adjoint operator, whether bounded below or not. Moreover, we shall be able to make simpler commutator arguments because the Dirac differential operator is only of the first order.

LEMMA II.1. — (Weinhold): *If* A *is self-adjoint and* $\Phi \in D(A)$, $\|\Phi\| = 1$, *then* A *has spectrum in the interval*

$$[\langle \Phi | A\Phi \rangle - \Delta_\Phi A, \langle \Phi | A\Phi \rangle + \Delta_\Phi A], \tag{2.1}$$

*where*

$$(\Delta_\Phi A)^2 \equiv \| A\Phi \|^2 - \langle \Phi | A\Phi \rangle^2 = \| [A - \langle \Phi | A\Phi \rangle]\Phi \|^2. \quad (2.2)$$

The idea is that the eigenfunctions of the two-center problem can be used to estimate those of either one-center problem and *vice-versa*, so Lemma II.1 will imply that the eigenvalues of the two operators are paired up within some small interval, which has vanishingly small width in the limit. We remark that given $n$ orthonormal trial functions, a simple generalization of Weinhold's lemma guarantees that the eigenspace associated with the interval (2.2) is at least $n$-dimensional; this is clear since the proof of the lemma uses min-max applied to the operator $[A - \langle \Phi | A\Phi \rangle]^2$.

THEOREM II.2. — *Let* V *and* W *be compact relative to* $T_0$ *and suppose that*

$$\lim_{R\to\infty} \| \chi_{\{|x|>R\}} V \|_{op} = \lim_{R\to\infty} \| \chi_{\{|x|>R\}} W \|_{op} = 0,$$

*where* $\chi$ *is the characteristic function of the subscripted set. Then the pure-point part of the spectrum of* T(R) *consists of continuous functions* $E_i(R)$ *of* R; *for any discrete eigenvalue* $\lambda$ *of* $T_0 + V(x)$ *or* $T_0 + W(x)$ *there exist eigenvalues* $E_i(R)$ *such that* $\lim_{R\to\infty} E_i(R) = \lambda$. *There are no accumulation points of the discrete point spectra of* T(R) *as* $R \to \infty$ *other than the points of* $\sigma_{pp}(T_0 + V) \cup \sigma_{pp}(T_0 + W)$, *possibly also including the edges of the essential spectrum. The number of functions* $E_i(R)$, *counting multiplicities, equals the multiplicity of the limit* $\lambda$ *if it is in only one of the point spectra* $\sigma_{pp}(T_0+V)$ *and* $\sigma_{pp}(T_0 + W)$, *and otherwise equals the sum of the multiplicities of* $\lambda$ *in both point spectra.*

*Remarks.* — 1. The choices open to a discrete eigenvalue of T(R) are to converge to an eigenvalue of one of the one-center problems; to drop into the essential spectrum at finite R; or to drop into the essential spectrum asymptotically. It can not, for example, approach the wrong value, wiggle around with no limit, or make an infinite number of passages from one piece of the essential spectrum to the other (the essential spectrum, as is well known, consists of the whole real line outside an interval, the mass-gap, in which there may be bound states).

2. There is nothing special about two centers of force here, except that we wish to avoid the detailed symmetry analysis of [*5*] for this paper.

3. Relative compactness allows local singularities in V or W so long as they are $L^3$. The Coulomb potential just misses this condition, but the conclusion of the theorem still holds. In (2.5) below we argue that

$$\| W\Omega_{2R} \| \to 0$$

(the subscript op will not be written on operator norms when no confusion will result from its omission) due to compactness of $WT_0^{-1}$, but it also follows from the fall-off of the unperturbed eigenfunctions as $|x| \to \infty$.

*Proof.* — Continuity: Write

$$T_0 + V(\boldsymbol{x} - \mathbf{R}) + W(\boldsymbol{x} + \mathbf{R}) - E$$
$$= (1 + W(\boldsymbol{x} + \mathbf{R})(T_0 + V(\boldsymbol{x} - \mathbf{R}) - E)^{-1})(T_0 + V(\boldsymbol{x} - \mathbf{R}) - E), \quad (2.3)$$

which is unitarily equivalent to

$$T_0 + V(\boldsymbol{x}) + W(\boldsymbol{x} + 2\mathbf{R}) - E$$
$$= (1 + W(\boldsymbol{x} + 2\mathbf{R})(T_0 + V(\boldsymbol{x}) - E)^{-1})(T_0 + V(\boldsymbol{x}) - E), \quad (2.4)$$

and thus has the same eigenvalues. Given any $\varepsilon > 0$, E can be chosen complex and large enough that $\| W(\boldsymbol{x} + 2\mathbf{R})(T_0 - E)^{-1} \| < \varepsilon$, and since $\| T_0(T_0 + V - E)^{-1} \|$ is bounded as $| E | \to \infty$, we can also arrange that

$$\| W(\boldsymbol{x} + 2\mathbf{R})(T_0 - E)^{-1} \| \; \| (T_0 - E)(T_0 + V - E)^{-1} \| < 1$$

by choosing $| E |$ large enough. Now let $Z_R$ denote the unitary translation of vectors of $\mathscr{H}$ by the amount-R in the coordinate $x_3$, i. e. $(Z_R f)(x) = f(x+R)$, so that $W(\boldsymbol{x} + 2\mathbf{R}) = Z_{2R} W(\boldsymbol{x}) Z_{2R}{}^{-1}$. The operator

$$W(\boldsymbol{x} + 2\mathbf{R})(T_0 - E)^{-1} = Z_{2R} W(\boldsymbol{x})(T_0 - E)^{-1} Z_{2R}^{-1}$$

is then norm continuous in R, for $Z_R$ is strongly continuous and $W(\boldsymbol{x})(T_0 - E)^{-1}$ is compact. Hence the inverse of (2.4),

$$(T_0 + V(\boldsymbol{x}) + W(\boldsymbol{x} + 2\mathbf{R}) - E)^{-1},$$

is norm continuous, which means that its eigenvalues vary continuously, and so do those of (2.3).

*Remark.* — In the case of the Coulomb potential, by scaling

$$T_0 + \mu/| \boldsymbol{x} - \mathbf{R} | + \sigma/| \boldsymbol{x} + \mathbf{R} |$$

and translation it is equivalent to consider

$$\frac{1}{2R}(\boldsymbol{\alpha}.\boldsymbol{p} + 2R\beta + \mu/ | \boldsymbol{x} | + \sigma/ | \boldsymbol{x} + \mathbf{R}/\mathbf{R} |),$$

and $\mathbf{R}/R$ is just a unit vector and $2R\beta$ is a continuous perturbation; thus the eigenvalues are still continuous.

*Convergence:* Since $\| A\Phi \| < \varepsilon$ implies $| \langle \Phi | A\Phi \rangle | < \varepsilon$ and $\Delta_\Phi A < \varepsilon^2$, it suffices to apply Lemma II.1 to

*a*) Any eigenvalue $\lambda \in \sigma_{pp}(T_0 + V) \cup \sigma_{pp}(T_0 + W)$, for which we must find a family of trial functions $\Omega(R)$, $\| \Omega(R) \| = 1$, such that $(T_0 + Q - \lambda)\Omega(R) \to 0$; and

*b*) Any of the functions $E_i(R)$, for which we must find a family of trial functions $T(R)$, $\| T(R) \| = 1$, such that either $(T_0 + V(\boldsymbol{x}) - E_i(R))\Upsilon(R) \to 0$ or $(T_0 + W(\boldsymbol{x}) - E_i(R))\Upsilon(R) \to 0$.

*a*) For brevity let $f_R$ denote the translate $Z_R f$ for any vector $f \in \mathscr{H}$ and let $B_R$ denote $Z_R B Z_R^{-1}$ for any operator B on $\mathscr{H}$. Suppose that $(T_0+V)\Omega=\lambda\Omega$, $\|\Omega\|=1$; then we take $\Omega(R)=\Omega_{-R}$. The relevant computation is

$$\|(T(R)-\lambda)\Omega_{-R}\| = \|W_R\Omega_{-R}\| = \|W\Omega_{-2R}\| \\ = \|W(T_0-i)^{-1}(T_0-i)\Omega_{-2R}\| \to 0 \qquad (2.5)$$

by the relative compactness of W and the weak convergence of

$$(T_0-i)\Omega_{-2R} = [(T_0-i)\Omega]_{-2R} \quad \text{to} \quad 0.$$

The argument for $\lambda\in\sigma_{pp}(T_0+W)$ is the same, *mutatis mutandis.*

*b*) Let $J\in C^1(\mathbb{R}^3)$ (and depending on R) be such that

$$0\le J\le 1, \ \|\nabla J\|_\infty \le KR^{-1/2}$$

and

$$J = \begin{cases} +1, & x_3 > R^{1/2} \\ 0, & x_3 < -R^{1/2}. \end{cases}$$

Then if $T(R)\Phi(R)=E(R)\Phi(R)$,

$$(T_0+V_{-R}-E(R))J\Phi(R) = [T_0, J]\Phi + J(T_0+V_{-R}-E(R))\Phi \\ = [T_0, J]\Phi - JW_R\Phi.$$

The first term is $0(R^{-1/2})$ and the second $\to 0$ by assumption, so

$$(T_0+V_{-R}-E(R))J\Phi(R) \to 0.$$

A similar calculation shows that

$$(T_0+W_R-E(R))(1-J)\Phi(R) \to 0.$$

By the triangle inequality, for any value of R, the norm of either $J\Phi(R)$ or $(1-J)\Phi(R)$ is at least 1/2. Hence, passing to a subsequence in R if necessary, we may take $\Upsilon(R)$ to be either $\left(\frac{J\Phi(R)}{\|J\Phi(R)\|_R}\right)$ or $\left(\frac{(1-J)\Phi(R)}{\|(1-J)\Phi(R)\|}\right)_{-R}$, whichever has a denominator bounded away from zero.

If E(R) had an accumulation point other than an eigenvalue of $T_0+V$ or $T_0+W$, then the argument just made, applied to another subsequence so that $E(R_i)$ had the accumulation point as a limit, would produce a contradiction. The multiplicities add up correctly, because one can make the same arguments with the *n*-fold generalization of Weinhold's lemma, using an exhaustive finite set of orthonormal trial functions for each of the (only finitely degenerate) eigenvalues $\lambda$ and $E_i(R)$; in essence one shows that the total dimensionality of the perturbed problem is at least the sum of the dimensionalities of the unperturbed problem, and *vice-versa.*

We have thus established that the eigenvalues of T(R) have a kind of stability allowing possible coalescence and change of multiplicity at $R=\infty$. The spectral projections fail to converge in norm; however, since

$$Z_R T(R) Z_{-R} = T_0 + V + W_{2R}$$

and

$$Z_{-R}T(R)Z_R = T_0 + V_{-2R} + W$$

clearly converge on the functions of $D(T_0)$ to $T_0 + V$ and $T_0 + W$ respectively, and the resolvents are bounded uniformly as $R \to \infty$ for $z \notin \sigma(T_0 + V) \cup \sigma(T_0 + W)$ by our stability result and the spectral theorem, a theorem of [9] gives strong resolvent convergence,

$$(T_0 + V + W_{2R} - z)^{-1} \xrightarrow{s} (T_0 + V - z)^{-1} ,$$
$$(T_0 + V_{-2R}TW - z)^{-1} \xrightarrow{s} (T_0 + W - z)^{-1},$$

and consequently strong convergence of the spectral projections. Indeed, the double-well problem furnishes an ideal illustration of the distinction between strong and norm resolvent convergence and their relationship to eigenvalue stability.

It is possible, on the other hand, to identify a sense in which the projections converge in norm. Namely, we shall see that if P(R) is the spectral projection onto some piece of the mass gap for

$$(T + V_{-R} + W_R - z),$$

then $\| P(R) - P(R)^X \| \to 0$, where $P(R)^X$ has an additional boundary condition on the plane $\{ x_3 = 0 \}$ analogous to a Dirichlet or Neumann boundary condition in the Schrödinger case. Of course, P(R) and $P(R)^X$ do not converge separately in norm. We shall develop this idea for use in Section IV, concerning the case where V and W are symmetric, though the perturbation theory of Section III will be independent of it. It shows how the asymptotic eigenvalue degeneracy of, for instance, relativistic $H_2^+$ corresponds to asymptotic behavior of the symmetry subspaces.

Different choices are available for the boundary conditions. The most natural choice takes parity into account, but as a consequence treats different spinorial components differently. Let $\mathscr{R}$ denote reflection in $x_3$:

$$[\mathscr{R}f](x_1, x_2, x_3) = f(x_1, x_2, -x_3),$$

and choose the matrices $\alpha_i$ so that

$$T_0 = \begin{pmatrix} 1 & 0 & p_3 & p_1 - ip_2 \\ 0 & 1 & p_1 + ip_2 & -p_3 \\ p_3 & p_1 - ip_2 & -1 & 0 \\ p_1 + ip_2 & -p_3 & 0 & -1 \end{pmatrix}$$

if

$$U = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

then the parity symmetry is expressed as

$$T_0 U\mathscr{R} = U\mathscr{R}T_0 .$$

Now we impose (in a sense to be made precise below) Dirichlet conditions on $\{ x_3 = 0 \}$ for the first and fourth spinorial components and Neumann conditions for the second and third (or *vice versa*).

The precise operator-theoretic definition of the Dirac operator with this boundary condition is as follows. The Green matrix for $T_0 : (T_0 - z)G = \delta$ is explicitly known,

$$G(\boldsymbol{x}, \boldsymbol{y}; z) = (\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta + Z) \frac{e^{-\sqrt{1-Z^2}|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi |\boldsymbol{x} - \boldsymbol{y}|},$$

so the Green matrix for $T_0^X$ can be defined by the method of images as

$$G^X_{(\boldsymbol{x},\boldsymbol{y};E)} = \chi_{\{x_3 \geq 0\}}(G(\boldsymbol{x} - \boldsymbol{y}; E) \pm G(\boldsymbol{x} - \boldsymbol{y}; E)UR_y)\chi_{\{y_3 \geq 0\}} + \chi_{\{x_3 \leq 0\}}(G(\boldsymbol{x} - \boldsymbol{y}; E) \pm G(\boldsymbol{x} - \boldsymbol{y}; E)UR_y)\chi_{\{y_3 \leq 0\}} .$$

This construction is meant to be conceptually similar to that of the Dirichle and Neumann Laplacians in [*10*], but the use of a symmetry plane makes it technically simpler. We let $T_0^X$ be the self-adjoint operator with this Green matrix and observe:

*i*) By comparison with the free operator $T_0$ and its Green's function, it is easy to see that the Green's function $G^X$ defines a bounded, normal operator when $Z \notin (-\infty, -1] \cup [1, \infty)$, which is self-adjoint for Z real.

*ii*) $G^X$ has decoupled action on the half-spaces $I_+ = \{ x_3 > 0 \}$ and $I_- = \{ x_3 < 0 \}$.

*iii*) Denoting the operator corresponding to $G^X$ formally as $(T_0^X - Z)^{-1}$, the usual resolvent equation

$$(T_0^X - Z_1)^{-1} - (T_0^X - Z_2)^{-1} = (Z_1 - Z_2)(T_0^X - Z_1)^{-1}(T_0^X - Z_2)^{-1}$$

follows from the observations that $URG = GUR$, $U^2 = \mathscr{R}^2 = \mathbb{1}$, $[U, R] = 0$, and $\chi_{\{X_3 < 0\}}R = R\chi_{\{X_3 > 0\}}$.

*iv*) V, W, and $Q = V_{-R} + W_R$ are still compact relative to $T_0^X$, i. e. their products with $(T_0^X - 1)^{-1}$ are compact.

*v*) To justify regarding $(T_0^X - Z)^{-1}$ as the resolvent of an operator $T_0$, it needs to be shown that $\operatorname{Ker}((T_0^X - Z)^{-1} \restriction I_\pm) = \{ 0 \}$ [*9*]. But if $f \in \operatorname{Ker}((T_0^X - Z)^{-1} \restriction I_+)$, say, then $g = (T_0 - Z)^{-1}(1 + UR)\chi_{\{X_3 > 0\}}f = 0$ for $X_3 > 0$. Since $g \in \mathscr{D}(T_0)$, $T_0 g = (1 + UR)\chi_{\{X_3 > 0\}}f = 0$ for $X_3 > 0$, and therefore $\chi_{\{X_3 > 0\}}f = 0$. The argument for $I_-$ is similar.

*vi*) $T_0^X$ is thus a well-defined self-adjoint extension of the minimal operator $T_0 \restriction [C_0^\infty(\mathbb{R}^3 \backslash \{ X_3 = 0 \})]^4$, which, however, is not essentially self-adjoint.

Let D be the operator $(T^0 - z)^{-1} - (T_0^X - z)^{-1}$. Then a straightforward exercise in noncommutative algebra yields an iterated resolvent equation for $z \notin \sigma(T_0 + Q) \cup \sigma(T_0^X + Q)$:

$$\begin{aligned}(T_0 + Q - z)^{-1} = (T_0^X + Q - z)^{-1} + D \\ - DQ(T_0^X + Q - z)^{-1} - (T_0 + Q - z)^{-1}QD \\ + (T_0 + Q - z)^{-1}QDQ(T_0^X + Q - z)^{-1}. \quad (2.6)\end{aligned}$$

It is easy to see that $\lim_{R\to\infty} \| Q(R)D \| = 0$, by using the exponential fall-off of the G's. Now let $\mathscr{C}$ be a contour encircling an interval in the mass-gap, avoiding the points of $\sigma(T_0 + V) \cup \sigma(T_0 + W)$. A slight variant of Theorem II.2 shows that the eigenvalues of $T_0^X + Q$ have the same convergence properties and limits as those of $T_0 + Q$, so as $R \to \infty$ the contour will avoid $\sigma(T_0 + Q) \cup \sigma(T_0^X + Q)$. Then

$$\begin{aligned}P(R) &= \frac{-1}{2\pi i}\oint_{\mathscr{C}} (T_0 + Q(R) - z)^{-1}dz \\ &= \frac{-1}{2\pi i}\oint_{\mathscr{C}} (T_0^X + Q(R) - z)^{-1}dz + \text{four other terms}.\end{aligned}$$

The term explicitly written is the spectral projection $P(R)^X$ of $T_0^X + Q(R)$. One of the remaining terms is

$$-\frac{1}{2\pi i}\oint_{\mathscr{C}} D(z)dz = 0,$$

because $T_0$ and $T_0^X$ have no eigenvalues in the mass-gap. The other three integrands are products of bounded operators and $Q(R)D$, which goes to zero in norm. This proves the norm convergence:

THEOREM II.3. — $\| P(R) - P(R)^X \| \to 0$ as $R \to \infty$.

## III. PERTURBATION THEORY

In this section we show that the perturbation theory of T(R) is up to errors $O(e^{-aR})$ for some $a > 0$ identical to that of a pair of independent single-well Dirac Hamiltonians with well-behaved perturbations. This procedure is an alternative to the more common argument of performing perturbation theory directly on T(R) and arguing the cross terms representing interactions between the wells away, as in [5]. We shall not explicitly write indices on eigenvalues or always indicate dependence on R, in order to avoid complicated notation. Thus we write simply where Q is as in Section II.

The analysis pivots on a gap formula [11]:

PROPOSITION III.1. — Let $\tilde{Q}(x; R) = Q(x)$ for $x_3 < 0$ (resp. $x_3 > 0$) and $\tilde{Q}(x; R) \equiv 0$ for $x_3 > 0$ (resp. $x_3 < 0$). Let $(T_0 + \tilde{Q})\tilde{\psi} = \tilde{E}\tilde{\psi}$. If

$$\int_{\{x_3<0\}} \bar{\tilde{\psi}}\cdot\psi d^3x \neq 0 \qquad \left(\text{resp.} \int_{\{x_3>0\}} \bar{\tilde{\psi}}\cdot\psi d^3x \neq 0\right)$$

then

$$E - \tilde{E} = \frac{-i\displaystyle\int_{\{x_3=0\}} \bar{\tilde{\psi}}\cdot\alpha_3\psi d^2x}{\displaystyle\int_{\{x_3<0\}} \bar{\tilde{\psi}}\cdot\psi d^3x} \tag{3.1-a}$$

$$\left(\text{resp. } E - \tilde{E} = \frac{i\displaystyle\int_{\{x_3=0\}} \bar{\tilde{\psi}}\cdot\alpha_3\psi d^2x}{\displaystyle\int_{\{x_3>0\}} \bar{\tilde{\psi}}\cdot\psi d^3x}\right). \tag{3.1-b}$$

The proof of Proposition III.1 is integration by parts since

$$\begin{aligned} E\int_{\{x_3\lessgtr0\}} \bar{\tilde{\psi}}\cdot\psi d^3x &= \int_{\{x_3\lessgtr0\}} \bar{\tilde{\psi}}\cdot(T_0 + Q)\psi d^3x \\ &= \int_{\{x_3\lessgtr0\}} \overline{(T_0+Q)\tilde{\psi}}\cdot\psi d^3x \mp i\int_{\{x_3=0\}} \bar{\tilde{\psi}}\cdot\alpha_3\psi d^2x \\ &= \tilde{E}\int_{\{x_3\lessgtr0\}} \bar{\tilde{\psi}}\cdot\psi d^3x \mp i\int_{\{x_3=0\}} \bar{\tilde{\psi}}\cdot\alpha_3\psi d^2x. \end{aligned}$$

*Remarks.* — 1. (3.1) also holds for $\tilde{E}$ and $\tilde{\psi}$ defined by $(T_0+Q)\tilde{\psi}=E\tilde{\psi}$.

2. It is clear from the proof that in the region where we set $\tilde{Q}(x; R)\equiv 0$ it could have been chosen largely arbitrary.

Now suppose that $(T_0+Q)\psi=E\psi$, $\|\psi\|=1$ and $E=E(R) \to E(\infty)$ as $R \to \infty$. Assume first that $E(\infty)$ is an eigenvalue (with multiplicity $m$) of $T_0 + V$ but not of $T_0 + W$. Let $\tilde{Q}=\tilde{Q}(x;R)=Q(x)$ for $x_3 > 0$ and $\tilde{Q}\equiv 0$ for $x_3 < 0$. Since $\|\tilde{Q}-V_{-R}\|_{op} \to 0$ as $R \to \infty$, perturbation theory tells us that there are exactly $m$ eigenvalues $\tilde{E}_i$ (with normalized eigenfunctions $\tilde{\psi}_i$, $i = 1 \dots m$) of $T_0+\tilde{Q}$ near $E(\infty)$. Let P denote their total eigenprojection. If P denotes the eigenprojection associated with $E(\infty)$ of $T_0+V_{-R}$, then $\|\tilde{P}-P\| \to 0$ as $R \to \infty$.

PROPOSITION III.2. — For R sufficiently large we can find an eigen index $i = i(R)$ and $\varepsilon > 0$ such that

$$\left|\int_{\{x_3>0\}} \bar{\tilde{\psi}}_i\cdot\psi d^3x\right| \geq \varepsilon > 0 \tag{3.2}$$

*Proof.* — With the J of Section I define $\phi = J\psi/\| J\psi \|$. ($\phi \neq 0$ by arguments of Section I, in fact, $\| J\psi \|$ is bounded away from 0 as $R \to \infty$. In reasonable cases $\| J\psi \| \to 1$ in the absence of a common eigenvalue and $\to 1/\sqrt{2}$ if there is a common eigenvalue from a reflection symmetry as in Section IV.) So $\| (T_0 + V - E(\infty))Z_R\phi \| \to 0$ as $R \to \infty$. Hence $\| P\phi \| \to 1$ by a simple corollary of the spectral theorem (cf. [*15*]) and therefore $\| \tilde{P}\phi \| = \| (\tilde{P} - P + P)\phi \| \to 1$, too. Thus for some $\varepsilon > 0$ and $i = i(R)$ certainly $| (\phi, \tilde{\psi}_i) | \geq \varepsilon$ for sufficiently large R. To establish (3.2), we need only show that $(J\psi, \tilde{\psi}_i)$ differs from $\int_{\{x_3 > 0\}} \overline{\psi} \cdot \tilde{\psi}_i d^3x$ by arbitrarily little as $R \to \infty$. Clearly, it suffices to show that

$$\int_{-R^{\frac{1}{2}} < x_3 < R^{\frac{1}{2}}} \overline{\psi} \cdot \tilde{\psi}_i d^3x$$

goes to zero. This follows from the Schwarz inequality provided

$$\int_{-R^{\frac{1}{2}} < x_3 < R^{\frac{1}{2}}} | \tilde{\psi}_i |^2 d^3x$$

vanishes as $R \to \infty$. The latter fact follows from Lemma III.4 (*i*) below and thus Proposition III.2 is proved.

If $E(\infty)$ is a common eigenvalue of $T_0 + V$, then Proposition III.2 extends with only the change that in addition to $i(R)$ the choice of the half-space $x_3 > 0$ or $x_3 < 0$ depends on R (recall that either $\| J\phi \|$ or $\| (1 - J)\phi \|$ is bigger than $\frac{1}{2}$)).

LEMMA III.3. — Suppose $(T_0 + V)\psi = E\psi$, $E \in (-1, 1)$, and V obeys the assumption of Section I. Then $\psi \in D(e^{\varepsilon |x|})$ for all $\varepsilon$ with $0 < \varepsilon < \sqrt{1 - E^2}$.

*Proof.* — This is a consequence of the argument of Combes and Thomas [*12*]. We will not repeat the details here, but note that the argument is simpler for Dirac operators than for Schrödinger operators, for when one commutes $e^{i\beta x}$ through $T_0$ in

$$e^{-i\beta x}(T_0 + V)e^{i\beta x},$$

one picks up only the constant matrix perturbation $\beta\alpha$.

Let $\tilde{Q}_R(x) = V(x) + W(x + 2R)$ for $x_3 > -R$ and $\tilde{Q}_R(x) \equiv 0$ for $x_3 < -R$ (thus $\tilde{Q}_R = Z_R \tilde{Q} Z_{-R}$ where $\tilde{Q}$ is as in the discussion preceding Proposition III.2). Suppose that $(T_0 + \tilde{Q}_R)\tilde{\psi}_R = \tilde{E}(R)\tilde{\psi}_R$ and $\tilde{E}(R) \to E(\infty)$, where $E(\infty)$ is an eigenvalue of $T_0 + V$.

LEMMA III.4. — *i)* $\| e^{\varepsilon|x|}\tilde{\psi}_R \| \le C_\varepsilon \| \tilde{\psi}_R \|$;

*ii)* $\| e^{\varepsilon|x|}T_0\tilde{\psi}_R \| \le D_\varepsilon \| \tilde{\psi}_R \|$,

*with* $C_\varepsilon$, $D_\varepsilon$ independent of $R (0 < \varepsilon < \sqrt{1 - E(\infty)^2})$.

*Proof.* — *i)* Note that $\tilde{\psi}_R$ obeys

$$- e^{\varepsilon|x|}\tilde{\psi}_R = e^{\varepsilon|x|}(T_0 - E(R))^{-1}\tilde{Q}_R\tilde{\psi}_R.$$

We use (3.3) to estimate $\| e^{\varepsilon|x|}\tilde{\psi}_R \|$ by splitting $\tilde{Q}_R$ as

$$\tilde{Q}_R\chi_{\{|x|<r\}} + \tilde{Q}_R(1 - \chi_{\{|x|>r\}}) \tag{3.4}$$

and inserting (3.4) into (3.3). One easily obtains the estimate

$$\| e^{\varepsilon|x|}\tilde{\psi}_R \| \le c_{\varepsilon,r} \| \tilde{Q}_R\tilde{\psi}_R \| + d_\varepsilon \| \tilde{Q}_R\chi_{\{|x|>r\}} \|_\infty \| e^{\varepsilon|x|}\tilde{\psi}_R \|. \tag{3.5}$$

In the derivation of the second term on the right side of (3.5) one uses that $\| e^{\varepsilon|x|}(T_0 - E(R))^{-1}e^{-\varepsilon|y|} \| \le d_\varepsilon$ is bounded independently of R (R large enough), since $E(R) \to E(\infty)$. Since $\| \tilde{Q}_E\chi_{\{|R|<r\}} \|_\infty$ can be made arbitrarily small (uniformily in R) by choosing $r$ sufficiently large, and $\| \tilde{Q}_R\tilde{\psi}_R \| \le C \| \tilde{\psi}_R \|$ on account of the (R-independent) boundedness of $\tilde{Q}_R(T_0 + \tilde{Q}_R - i)^{-1}$, (*i*) follows.

*ii)* Write $T_0 = (T_0 + \tilde{Q}_R) - \tilde{Q}_R$, use (*i*) and estimate $\| e^{\varepsilon|x|}\tilde{Q}_R\tilde{\psi} \|$ by introducing $\chi_r$ and arguing as in (*i*).

Lemma III.4 also implies that the numerator in (3.1) (where $\tilde{\psi}$ is replaced by a function $\tilde{\psi}_{i(R)}$ as discussed in Proposition III.2) vanishes exponentially as $R \to \infty$. To see this let $\phi(x)$ be a $C_0^\infty$ function with support in $-1 < x_3 < 1$, $\phi(x_3 = 0) = 1$ and let $\phi_R(x) = \phi(x + \mathbf{R})$. Then

$$\left( \int_{\{x_3 = -R\}} | \tilde{\psi}_R |^2 d^2x \right)^{\frac{1}{2}} \le C \| T_0(\phi_R\tilde{\psi}_R) \|, \tag{3.6}$$

where C does not depend on $\tilde{\psi}_R$. This follows from the fact that

$$\tilde{\psi}_R \in D(T_0) = [H^1(\mathbb{R}^3)]^4$$

and the graph norm of $T_0$ is equivalent to the Sobolev norm. As is easy see, Lemma III.4 implies that the right side of (3.6) is bounded by const. $e^{-\varepsilon R} \| \tilde{\psi}_R \|$. Thus the numerator of (3.1) can be estimated by the Schwarz inequality (and translating by $-R$). The integral $\int_{\{x_3 = 0\}} | \psi |^2 d^2x$ can simply be estimated by an R-independent constant, for $\| T_0\psi \|$ is bounded independently of R (a consequence of the boundedness of $Q_R(T_0 + Q_R - i)^{-1}$. As a result of all this we get .

THEOREM III.5. — With the definitions of Proposition III.1, for any $E(R)$ there is a related single-well $\tilde{E}_{i(R)}(R)$ as in III.1 such that

$$| E - \tilde{E}_{i(R)} | < \text{const. } e^{-\varepsilon R}.$$

In the case where W and V are long-range (say, Coulomb) it turns generally out that the eigenvalues $\tilde{E}_i$ have an asymptotic $1/R$ expansion. Then Theorem III.5 tells us that the actual double-well energies have similar expansions. Of course, a change of $i(R)$ can then only occur between single-well energies with identical $1/R$ expansions. The $1/R$ expansion has been dealt with in the context of Schrödinger operators [*5*] [*14*], so we shall concentrate on its foundations only. The details would become at least as unpleasant as those of the Rayleigh-Schrödinger series.

Suppose, for definiteness, that $E(R)$ converges to an eigenvalue of $T_0+V$, with an eigenfunction $\psi_\infty$ such that $(T+V)\psi_\infty = E(\infty)\psi_\infty$. The limiting eigenvalue will ordinarily be degenerate because of the parity symmetry, symmetry under rotation, etc. This is no problem because we will have a well-defined perturbation problem and the usual procedures of degenerate perturbation theory can be resorted to, such as projection to symmetry subspaces.

We have established that the eigenvalues of

$$T_0 + V + W_{2R} = Z_R(T_0 + V_{-R} + W_R)Z_{-R}$$

differ by an exponentially small amount from those of a related operator with $W_{2R}$ modified in a more or less arbitrary way for $x_3 > R$. Now suppose for $x_3 < R$, $W_{2R} = \sum_{k=1}^{n} \frac{\zeta_k}{|\boldsymbol{x}-2\mathbf{R}|^k} + A_n(\boldsymbol{x}, R)$, where $| A_n(\boldsymbol{x}, R) | < \text{const. } R^{-n-1}$ for all $x_3 < R$. Replacement of $W_{2R}$ by $\sum_{k=1}^{n} \frac{\zeta_k}{|\boldsymbol{x}-2\mathbf{R}|^k}$ will thus affect eigenvalues converging to those of $T+V$ by $0(R^{-n-1}) + 0(\exp(-\varepsilon R)) = 0(R^{-n-1})$. Now, with a multiple expansion of $\frac{1}{|\boldsymbol{x}-2\mathbf{R}|}$, $W_{2R}$ can be replaced by

$$\sum_{k=0}^{n} \frac{\eta_k}{R} \left| \frac{\boldsymbol{x}}{R} \right|^k + B_n(\boldsymbol{x}, R),$$

where $| \hat{B}_n(\boldsymbol{x}, R) | \leq \text{const. } R^{-n-1}(1 + |\boldsymbol{x}|^n)$, affecting eigenvalues of $T_0 + V + W_{2R}$ to $0(R^{-n-1})$. The resulting operator is a perturbed single-well problem with a well-defined asymptotic perturbation theory in the parameter $1/R$ to order $R^{-n-1}$: each term in the perturbation series is $\left(\frac{1}{R}\right)^m$ times sums of inner products of $\psi_\infty$ after finitely many applications of the operators $(T_0 + V - z)^{-1}$ and $|\boldsymbol{x}|$, integrated over $z$ away from the spectrum of $T_0+V$. Since $\psi_\infty \in D(e^{\varepsilon x_i}) \Rightarrow \psi_\infty \in D(e^{\varepsilon|\boldsymbol{x}|})$ according to Lemma III.3, $\psi_\infty = e^{-\varepsilon|\boldsymbol{x}|}\phi_\infty$ for some $\phi_\infty \in L^2$, and since $|\boldsymbol{x}|^n$ is bounded by $Ce^{\delta|\boldsymbol{x}|}$ for an arbitrarily small $\delta$, Lemma III.3 implies that all the inner products entering into the perturbation series as coefficients of $R^{-k}$, $k<n+1$, are finite.

## IV. EIGENVALUE GAPS FOR SYMMETRIC POTENTIALS

We conclude with a few remarks about the important special case where V and W represent two symmetric wells, as in relativistic $H_2^+$. The limiting eigenvalue belongs to both $T_0+V$ and $T_0+W$ and the spectral projections converge to those with mixed Dirichlet and Neumann boundary conditions we called X in section III. The 1/R-expansion can still be implemented, as the discussion in section III did not assume that $E_\infty$ belonged only to $\sigma(T_0+V)$. However, the pair or cluster of eigenvalues converging to $E_\infty$ will normally be different for finite R. Now suppose $W = \mathscr{R}V\mathscr{R}$ (for example, $W = V = 1/|\boldsymbol{x}|$). Then

$$(T_0 + V_{-R} + W_R)U\mathscr{R} = U\mathscr{R}(T_0 + V_{-R} + W_R),$$

and thus

$$T_0 + V_{-R} + W_R = (T_0 + V_{-R} + W_R)_+ \oplus (T_0 \oplus V_{-R} + W_R),$$

where the subscripts denote restriction to the symmetry subspaces such that

$$U\mathscr{R}f(\boldsymbol{x}) = \pm f(\boldsymbol{x}).$$

Such functions satisfy the X boundary conditions of section II, and it follows from Theorem II.3 that the eigenvalues of $T_0+V_{-R}+W_R$ always converge in pairs, one + and one −. Also, the phase of a pair of associated normalized eigenvalues $\psi_\pm$ can be chosen so that

$$\int_{\{x_3 \leq 0\}} \overline{\psi}_- \cdot \psi_+ d^3x \to \frac{1}{2}$$

(recall the remarks in the proof of III.2).

But the gap formula (3.1*a*) holds for $E_+ - E_-$ (with $\tilde{Q} = Q$), so

$$E_+ - E_- = \frac{-i\int_{\{x_3=0\}} \overline{\psi}_- \cdot \alpha_3\psi_+ d^2x}{\int_{\{x_3<0\}} \overline{\psi}_- \cdot \psi_+ d^3x} \sim -2i\int_{\{x_3=0\}} \overline{\psi}_- \cdot \alpha_3\psi_+ d^2x,$$

which is exponentially small because of Lemma III.3*c*.

*Note.* — After the preprint of this paper E. B. Davies has found an alternative approach to Theorem II.2 for Schrödinger operators, which also works for Dirac operators [*16*].

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