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Comparison of perturbative and variational procedures in a relativistic problem

M. Moshinsky*, L. Benet, G. Loyola and A. Salinas
Instituto de Física, Universidad Nacional Autónoma de México
Apartado postal 20-364, 01000 México, D.F., México

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Abstract. For bound states two of the most popular approximative procedures are the perturbative and variational ones. These procedures have been extensively used and compared in ordinary quantum mechanics. The situation is more delicate in the relativistic case where we need not only to develop the methods appropriately, but also to separate in them the contribution of positive energy states, as those from the negative ones are not allowed by Dirac's procedure, which assumes them occupied by particles satisfying an exclusion principle. To illustrate the problems that appear we discuss in this paper the particle-antiparticle system with a Dirac oscillator interaction in a one dimensional space for each particle. We then develop the appropriate perturbative and variational procedures, compare their results, and discuss their range of validity as function of the value of the frequency ω of the Dirac oscillator.

Resumen. Para estados ligados, dos de los más populares procedimientos de aproximación son los de perturbaciones y variaciones. Estos procedimientos han sido extensamente usados y comparados en la mecánica cuántica ordinaria. La situación es más delicada en el caso relativista, donde no sólo necesitamos desarrollar los métodos en forma apropiada, sino también separar en ellos la contribución de los estados de energía positiva, ya que los de energía negativa no están permitidos por la consideración de Dirac, que supone que están ocupadas por partículas que satisfacen un principio de exclusión. Para ilustrar los problemas que aparecen, discutimos en este artículo el sistema de partícula-antipartícula, con una interacción del tipo de oscilador de Dirac, y en un espacio unidimensional para cada partícula. Desarrollamos entonces los procedimientos perturbativos y variacionales apropiados, comparamos sus resultados, y discutimos su rango de validez como función del valor de la frecuencia del oscilador de Dirac.

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1. Introduction

When dealing with problems in quantum mechanics that do not admit an exact solution, there are many approximative procedures. For bound states two of the most popular are the perturbative and variational ones [1]. In the range of validity of both their results should coincide. When outside these ranges, the comparison is more difficult even in ordinary quantum mechanics, and this may be compounded in relativistic problems, where besides we have to deal with the interpretation of negative energy states.

The purpose of this note is to apply both procedures to the two-body system of a particle-antiparticle in one space dimension, with a Dirac oscillator interaction [2,3,4].

*Member of El Colegio Nacional.

This example will illustrate the difficulties one finds in comparing the perturbative and variational methods in a relativistic problem. We shall start though, in the next section, with a simple problem in ordinary quantum mechanics, to first discuss the range of validity of our two approximate procedures.

2. A NON-RELATIVISTIC EXAMPLE

In the usual perturbative analysis discussed in Schiff's book [1], one starts with the Hamiltonian H of the form

$$H = H_0 + \lambda H', \tag{2.1}$$

where the eigenvalues ϵ_n and eigenfunctions $|n\rangle$ of H_0 are well known, and λ is a parameter in terms of which the eigenvalues E_n and eigenfunctions $|n]$ of H can be developed.

To be able to evaluate the validity of this analysis, we shall consider an example in which $E_n, |n]$ of H can be determined exactly, of the form

$$H_0 = \bar{p}^2 + \bar{x}^2, \qquad H' = -\bar{x}^2. \tag{2.2a, b}$$

Clearly then, with the help of the canonical transformation

$$\bar{x}' = (1-\lambda)^{1/4}\bar{x}, \qquad \bar{p}' = (1-\lambda)^{-1/4}\bar{p}, \tag{2.3a, b}$$

when $0 \leq \lambda < 1$, we get

$$H = (1-\lambda)^{1/2}(\bar{p}'^2 + \bar{x}'^2), \tag{2.4}$$

so that

$$E_n = (1-\lambda)^{1/2}(2n+1), \quad n = 0, 1, 2, \ldots \tag{2.5}$$

and $|n]$ are the one dimensional harmonic oscillator states of n-quanta, but functions of $\bar{x}'$ of (2.3a).

If $1 < \lambda < \infty$ then the canonical transformation we must use is of the form

$$\bar{x}'' = (\lambda-1)^{1/4}\bar{x}, \qquad \bar{p}'' = (\lambda-1)^{-1/4}\bar{p} \tag{2.6a, b}$$

and the Hamiltonian becomes

$$H = (\lambda-1)^{1/2}(\bar{p}''^2 - \bar{x}''^2), \tag{2.7}$$

so that it corresponds to a repulsive harmonic oscillator with a continuous spectrum of eigenvalues and eigenstates given by confluent hypergeometric functions [5].

For the value $\lambda = 1$ we have the free particle Hamiltonian, *i.e.*,

$$H = \bar{p}^2. \tag{2.8}$$

The perturbative procedure [1] only makes sense for $\lambda \ll 1$ if we are going to start from the oscillator eigenfunctions $|n\rangle$ of the H_0 of unit frequency in (2.2*a*). In that case, the value of E_n is given by [1]

$$E_n = \epsilon_n + \lambda\langle n|H'|n\rangle + \lambda^2 {\sum_m}' \left\{(\epsilon_n - \epsilon_m)^{-1}\left|\langle m|H'|n\rangle\right|^2\right\} + \cdots, \tag{2.9}$$

where the prime in the summation indicates that the term $m = n$ is excluded.

Using the creation and annihilation operators

$$\bar{\eta} = \tfrac{1}{\sqrt{2}}(\bar{x} - i\bar{p}), \qquad \bar{\xi} = \tfrac{1}{\sqrt{2}}(\bar{x} + i\bar{p}), \tag{2.10}$$

we obtain that

$$H' = -\bar{x}^2 = -\tfrac{1}{2}\bar{\eta}^2 - \tfrac{1}{2}\bar{\xi}^2 - \left(\bar{\eta}\bar{\xi} + \tfrac{1}{2}\right), \tag{2.11}$$

and as the eigenstates of the oscillator are

$$|\bar{n}\rangle = \frac{\bar{\eta}^n}{(n!)^{1/2}}|0\rangle \tag{2.12}$$

with the ground state $|0\rangle$ being

$$|0\rangle = \pi^{-1/4}\exp(-\bar{x}^2/2), \tag{2.13}$$

we see immediately that

$$\begin{aligned}\langle m|H'|n\rangle = &-\tfrac{1}{2}[(n+2)(n+1)]^{1/2}\delta_{m,n+2} \\ &- \tfrac{1}{2}[n(n-1)]^{1/2}\delta_{m,n-2} - [n + (1/2)]\delta_{mn}.\end{aligned} \tag{2.14}$$

Up to second order in perturbation theory we obtain that E_n of (2.9) becomes

$$E_n = [1 - \tfrac{1}{2}\lambda - \tfrac{1}{8}\lambda^2 + \cdots](2n+1), \tag{2.15}$$

which is the same result we get from (2.5) if we use the binomial theorem for $(1-\lambda)^{\frac{1}{2}}$.

Turning now our attention to the variational procedure, we note that the matrix elements for the full Hamiltonian have the form

$$\langle m|H|n\rangle = (2n+1)\delta_{m,n} + \lambda\langle m|H'|n\rangle, \tag{2.16}$$

TABLE I. Comparison of the first six eigenvalues, $n = 0$ to 5 for the variational procedure, the perturbative procedure up to 1st order, and the exact results ($\lambda = 0.1$). We also indicate the maximum number of quanta N to which we carry our variational analysis.

N/n	0	1	2	3	4	5
5	0.948683299	2.846049902	4.743436941	6.640830695	8.557879760	10.46311940
10	0.948683298	2.846049894	4.743416490	6.640783087	8.538149683	10.43551682
15	0.948683298	2.846049894	4.743416490	6.640783086	8.538149682	10.43551629
20	0.948683298	2.846049894	4.743416490	6.640783086	8.538149682	10.43551628
Perturbative procedure	0.94875	2.84625	4.73375	6.64125	8.53875	10.43625
Exact results	0.948683298	2.846049894	4.743416490	6.640783086	8.538149682	10.43551628

TABLE II. Comparison of the first six eigenvalues $n = 0$ to 5 for the variational procedure, the perturbative procedure up to 1st order, and the exact results ($\lambda = 0.9$). We also indicate the maximum number of quanta N to which we carry our variational analysis.

N/n	0	1	2	3	4	5
5	0.335478537	1.042210965	2.139964779	3.206398351	5.774556683	7.301390684
10	0.316770496	0.961970351	1.631117754	2.474312727	3.328924711	4.757516993
15	0.316274187	0.949225271	1.589460148	2.242025733	2.989678713	3.753465154
20	0.316228850	0.948739202	1.581549189	2.218666121	2.8625855210	3.562213901
Perturbative procedure	0.44875	1.34625	2.24375	3.14125	4.03875	4.93625
Exact results	0.316227766	0.948683298	1.581138830	2.213594362	2.846049894	3.478505426

where the last term is given by (2.14). In principle, for any value of λ, one could calculate the eigenvalues E_n by diagonalizing the finite symmetrical matrix

$$\left\| \langle m|H|n\rangle \right\|, \tag{2.17}$$

for values m, n that go from 0 to a maximum that we could call N.

Our exact analysis shows though that we can expect sensible results only for λ in the interval $0 \leq \lambda < 1$, as after 1 the spectrum becomes continuous. As an example we discuss the case $\lambda = 0.1$ in Table I. Even if λ approaches 1, we expect the situation to be unstable *i.e.* the lowest eigenvalues are not the same if we take $N, 2N, 3N, \ldots$ as the maximum values of n, as shown for $\lambda = 0.9$ and $N = 5, 10, 15, 20$, in Table II, although for $N = 20$ the eigenvalues already start to approach the exact result.

Thus, we see from this elementary example, that the variational procedure involving a parameter, may not be valid for all values of it. This situation will also appear in the relativistic example to be discussed below.

3. THE PARTICLE-ANTIPARTICLE SYSTEM IN ONE DIMENSION WITH A DIRAC OSCILLATOR INTERACTION

The single particle one dimensional Dirac oscillator equation is suggested in a similar way as in the three dimesnional case, *i.e.* by the replacement [2]

$$\alpha p \to \alpha(p - i\omega x\beta), \tag{3.1}$$

in the Dirac free particle equation giving rise to [2,3]

$$i\frac{\partial\psi}{\partial t} = \left[\alpha(p - i\omega x\beta) + \beta\right]\psi, \tag{3.2}$$

where ω is the frequency of the oscillator, all in units

$$\hbar = c = m = 1 \tag{3.3}$$

where m is the mass of the particle. Note furthermore that in one dimension x, p are scalar variables and α, β are two dimensional matrices given by

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.4a,b}$$

As shown in references [4] the equation for the antiparticle has also the form (3.2) if we exchange ω by $-\omega$.

When dealing with a non-interacting system of particle-antiparticle, in which they are characterized, respectively, by the indices 1 and 2, the Hamiltonian can be written as

$$\begin{aligned} H &= \alpha_1 p_1 + \alpha_2 p_2 + \beta_1 + \beta_2 \\ &= \tfrac{1}{\sqrt{2}}\left[(\alpha_1 + \alpha_2)P\right] + \left\{\tfrac{1}{\sqrt{2}}(\alpha_1 - \alpha_2)p + \beta_1 + \beta_2\right\}, \end{aligned} \tag{3.5}$$

where

$$P = \tfrac{1}{\sqrt{2}}(p_1 + p_2), \qquad p = \tfrac{1}{\sqrt{2}}(p_1 - p_2), \tag{3.6}$$

and α_s, β_s, $s = 1, 2$ are the direct products

$$\alpha_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \alpha_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{3.7a,b}$$

$$\beta_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \beta_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.7c,d}$$

In the center of mass frame, $P = 0$ and thus we are left only with the curly bracket Hamiltonian in (3.5).

We showed, through a Poincaré invariant analysis [4], that if we now wish to introduce a Dirac oscillator interaction between particle and antiparticle, all we have to do in (2.5) (when $P = 0$) is to make the replacements

$$\alpha_1 p \rightarrow \alpha_1(p - i\omega x B), \tag{3.8a}$$

$$\alpha_2 p \rightarrow \alpha_2(p + i\omega x B), \tag{3.8b}$$

where

$$x = \tfrac{1}{\sqrt{2}}(x_1 - x_2), \qquad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.9a, b}$$

The new operator we form in this way has as an eigenvalue the total energy of the particle-antiparticle system interacting through a Dirac oscillator. As this energy is in the frame of reference where the center of mass is at rest, we can identify it with the mass of the composite particle and denote it by $\mathcal{M}$ which is then given by the operator

$$\mathcal{M} = \tfrac{1}{\sqrt{2}}\{(\alpha_1 - \alpha_2)p - i\omega(\alpha_1 + \alpha_2)xB\} + \beta_1 + \beta_2, \tag{3.10}$$

where

$$\alpha_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \alpha_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{3.11a, b}$$

$$\beta_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad \beta_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{3.11c, d}$$

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{3.11e}$$

and the wave function can be written as [3]

$$\psi = \begin{pmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{pmatrix}. \tag{3.12}$$

Denoting by μ the eigenvalue of the operator $\mathcal{M}$ of (3.10), and making use of (3.11) we obtain the equation

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & (p+i\omega x) & -(p-i\omega x) & 0 \\ (p-i\omega x) & 0 & 0 & -(p+i\omega x) \\ -(p+i\omega x) & 0 & 0 & (p-i\omega x) \\ 0 & -(p-i\omega x) & (p+i\omega x) & 0 \end{pmatrix}\begin{pmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{pmatrix}$$

$$= \begin{pmatrix} (\mu-2) & \psi_{11} \\ \mu & \psi_{21} \\ \mu & \psi_{12} \\ (\mu+2) & \psi_{22} \end{pmatrix} \tag{3.13}$$

where $p = -i\partial/\partial x$.

Introducing now creation and annihilation operators by the definitions

$$\eta = \tfrac{1}{\sqrt{2}}(\omega^{1/2}x - i\omega^{-1/2}p), \qquad \xi = \tfrac{1}{\sqrt{2}}(\omega^{1/2}x + i\omega^{-1/2}p), \tag{3.14a, b}$$

we get the equations

$$i\omega^{1/2}\begin{pmatrix} \eta & \xi \\ \xi & \eta \end{pmatrix}\begin{pmatrix} \psi_{21} \\ \psi_{12} \end{pmatrix} = \begin{pmatrix} (\mu-2) & \psi_{11} \\ (\mu+2) & \psi_{22} \end{pmatrix}, \tag{3.15a}$$

$$-i\omega^{1/2}\begin{pmatrix} \xi & \eta \\ \eta & \xi \end{pmatrix}\begin{pmatrix} \psi_{11} \\ \psi_{22} \end{pmatrix} = \mu\begin{pmatrix} \psi_{21} \\ \psi_{12} \end{pmatrix}. \tag{3.15b}$$

Defining now a vector ϕ of components

$$\phi = \begin{pmatrix} \phi_{11} \\ \phi_{22} \\ \phi_{21} \\ \phi_{12} \end{pmatrix} \tag{3.16a}$$

where

$$\phi_{11} = \psi_{11}, \quad \phi_{22} = \psi_{22}, \quad \phi_{21} = i\psi_{21}, \quad \phi_{12} = i\psi_{12}, \tag{3.16b}$$

we see that equations (3.15) can be written in the matrix form

$$\begin{pmatrix} 2 & 0 & \omega^{1/2}\eta & \omega^{1/2}\xi \\ 0 & -2 & \omega^{1/2}\xi & \omega^{1/2}\eta \\ \omega^{1/2}\xi & \omega^{1/2}\eta & 0 & 0 \\ \omega^{1/2}\eta & \omega^{1/2}\xi & 0 & 0 \end{pmatrix}\begin{pmatrix} \phi_{11} \\ \phi_{22} \\ \phi_{21} \\ \phi_{12} \end{pmatrix} = \mu\begin{pmatrix} \phi_{11} \\ \phi_{22} \\ \phi_{21} \\ \phi_{12} \end{pmatrix}. \tag{3.17}$$

We shall use the expression (3.15) when dealing with the perturbative method in the next section and the expression (3.17) when we consider the variational method in Sect. 6.

4. THE PERTURBATIVE PROCEDURE

Multiplying Eq. (3.15a) by μ and substituting in it Eq. (3.15b) we get

$$\omega \begin{pmatrix} \eta\xi + \xi\eta & \eta^2 + \xi^2 \\ \eta^2 + \xi^2 & \eta\xi + \xi\eta \end{pmatrix} \begin{pmatrix} \psi_{11} \\ \psi_{22} \end{pmatrix} = \begin{pmatrix} \mu^2 - 2\mu & 0 \\ 0 & \mu^2 + 2\mu \end{pmatrix} \begin{pmatrix} \psi_{11} \\ \psi_{22} \end{pmatrix}. \tag{4.1}$$

It is convenient to substitute ψ_{11}, ψ_{22} by φ_+, φ_- through the relation

$$\begin{pmatrix} \psi_{11} \\ \psi_{22} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix}, \tag{4.2}$$

so that equation (4.1) becomes

$$\omega \begin{pmatrix} -(\eta - \xi)^2 & 0 \\ 0 & (\eta + \xi)^2 \end{pmatrix} \begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix} = \begin{pmatrix} \mu^2 & -2\mu \\ -2\mu & \mu^2 \end{pmatrix} \begin{pmatrix} \varphi_+ \\ \varphi_- \end{pmatrix}. \tag{4.3}$$

Writing the two equations in φ_+, φ_- explicitly and eliminating φ_- between them we obtain for φ_+, which from now on we denote simply by φ, the equation

$$\left\{\mu^4 - \left[4 + 2\omega(2\eta\xi + 1)\right]\mu^2 - \omega^2(\eta + \xi)^2(\eta - \xi)^2\right\}\varphi = 0. \tag{4.4}$$

Unfortunately, because of the term with ω^2, this problem is not exactly soluble. We note though that the operator (4.4) contains the ω as a parameter, where this frequency is given in units of the rest mass $m = 1$ of the particle. If $\omega \ll 1$ we can begin by neglecting the term ω^2 and get

$$\mu^2\left\{\mu^2 - [4 + 2\omega(2\eta\xi + 1)]\right\}\varphi = 0. \tag{4.5}$$

Clearly then the eigenfunction is $u_n(x)$ of the one dimensional harmonic oscillator and the eigenvalue, which we shall denote by μ_0, becomes

$$\mu_0^2 = 4 + 2\omega(2n + 1). \tag{4.6}$$

Our interest though is in Eq. (4.4) which we can solve by a perturbation procedure. We first define

$$W = \mu^2, \tag{4.7a}$$

$$H_0 = 4 + 2\omega(2\eta\xi + 1), \tag{4.7b}$$

$$H' = -\omega^2(\eta + \xi)^2(\eta - \xi)^2, \tag{4.7c}$$

so Eq. (4.4) becomes

$$(W^2 - WH_0 + H')\varphi = 0. \tag{4.8}$$

We then, as for example in Schiff's book [1], replace H' by $\lambda H'$ where λ is a parameter and write

$$W = W_0 + \lambda W_1 + \lambda^2 W_2 + \cdots, \tag{4.9a}$$

$$\varphi = \varphi_0 + \lambda\varphi_1 + \lambda^2\varphi_2 + \cdots, \tag{4.9b}$$

where $W_0^2 = \mu_0^2$ of (4.6) and $\varphi_0 = u_n(x)$.

From (4.9a) we obtain

$$W^2 = W_0^2 + \lambda(2W_0W_1) + \lambda^2(2W_0W_2 + W_1^2) + \cdots, \tag{4.9c}$$

so that using (4.9) we see that, to first order in λ, (4.8) takes the form

$$[W_0(W_0 - H_0)\varphi_0] + \lambda[(2W_0W_1 - W_1H_0 + H')\varphi_0 + W_0(W_0 - H_0)\varphi_1] + \cdots, \tag{4.10}$$

where each of the square brackets must vanish [1]. For the first one this is automatic as from (4.5) we have

$$H_0\varphi_0 = W_0\varphi_0. \tag{4.11}$$

From the second square bracket, when we take its scalar product [1] with $\phi_0 = u_n(x)$, we obtain

$$W_1 = -W_0^{-1}(\varphi_0, H'\varphi_0), \tag{4.12}$$

where we made use of the hermitian character of H_0 and of Eq. (4.11).

Thus to first order perturbation theory, when we take, as usual [1], $\lambda = 1$, we have that

$$\mu^2 = \mu_0^2 - \mu_0^{-2}(\varphi_0, H'\varphi_0) + \cdots \tag{4.13}$$

where μ_0 is given by (4.6), $\varphi_0 = u_n(x)$ and H' by (4.7c).

The only terms in H' of (4.7c) that contribute to the scalar product in (4.13) are those that do not change the number of quanta n so H' can be replaced by

$$H' \to \omega^2[2(\eta\xi)^2 + 2(\eta\xi) - 1]. \tag{4.14}$$

The square of the mass μ^2, as function of the number of quanta n, is then given to first order perturbation theory by

$$\mu^2(n, \omega) = 4 + 2\omega(2n + 1) - (\omega^2/4)(2n^2 + 2n - 1) + \cdots, \tag{4.15}$$

where we are keeping only those terms up to order ω^2 so μ_0^{-2} is replaced by just (1/4).

We want finally to develop a feeling for the behaviour of the exact equations (4.3) when $\omega \gg 1$. For that we define σ as

$$\sigma \equiv \omega^{-1/2}\mu, \tag{4.16}$$

and dividing (4.3) by ω we get in the limit when $\omega \to \infty$ that

$$-(\eta - \xi)^2\varphi_+ = \sigma^2\varphi_+, \quad (\eta + \xi)^2\varphi_- = \sigma^2\varphi_-. \tag{4.17a,b}$$

Introducing the coordinate $\check{x}$ and momentum $\check{p}$ by the definition

$$\check{x} = \tfrac{1}{\sqrt{2}}(\eta + \xi), \quad \check{p} = \tfrac{i}{\sqrt{2}}(\eta - \xi), \tag{4.18a,b}$$

the Eqs. (4.17) become

$$2\check{p}^2\varphi_+ = -2\frac{d^2\varphi_+}{d\check{x}^2} = \sigma^2\varphi_+, \qquad 2\check{x}^2\varphi_- = \sigma^2\varphi_-, \tag{4.19a,b}$$

which admit the solutions

$$\varphi_+ = \exp\left[i(\sigma/\sqrt{2})\check{x}\right], \quad \varphi_- = \delta(2\check{x}^2 - \sigma^2), \tag{4.20a,b}$$

for any real value of σ in the interval $-\infty < \sigma < \infty$. Thus it seems that for $\omega \to \infty$ the spectrum tends to be continuous, and no approximative procedure for bound states is likely to work. We shall return to this point in the next section.

5. THE VARIATIONAL PROCEDURE

In the variational method we start from Eq. (3.17) and write ϕ_{st}; $s, t = 1, 2$, as an expansion in terms of one dimensional oscillator functions of the form

$$\phi_{st}(x) = \sum_{n=0}^{\infty} a_{st}(n)u_n(x). \tag{5.1}$$

Substituting (5.1) in (3.17), multiplying both sides by $u_m^*(x)$, integrating with respect to x, and making use of the relations

$$\int_{-\infty}^{\infty} u_m^*(x)[\eta u_n(x)]\,dx = (n+1)^{1/2}\delta_{mn+1}, \tag{5.2a}$$

$$\int_{-\infty}^{\infty} u_m^*(x)[\xi u_n(x)]\,dx = n^{1/2}\delta_{mn-1}, \tag{5.2b}$$

we finally obtain the equations

$$\sum_n \{2a_{11}(n)\delta_{mn} + 0 + [\omega(n+1)]^{1/2}\delta_{m,n+1}a_{21}(n) + (\omega n)^{1/2}\delta_{m,n-1}a_{12}(n)\} = \mu a_{11}(m)$$

$$\sum_n \{0 - 2a_{22}(n)\delta_{mn} + (\omega n)^{1/2}\delta_{m,n-1}a_{21}(n) + [\omega(n+1)]^{1/2}\delta_{m,n+1}a_{12}(n)\} = \mu a_{22}(m)$$

$$\sum_n \{(\omega n)^{1/2}\delta_{m,n-1}a_{11}(n) + [\omega(n+1)]^{1/2}\delta_{m,n+1}a_{22}(n) + 0 + 0\} = \mu a_{21}(m)$$

$$\sum_n \{[\omega(n+1)]^{1/2}\delta_{m,n+1}a_{11}(n) + (\omega n)^{1/2}\delta_{m,n-1}a_{22}(n) + 0 + 0\} = \mu a_{12}(m), \tag{5.3}$$

where we kept the zeros of (3.17) as coefficients of the missing $a_{st}(n)$ in (5.3).

The matrix corresponding to the operator on the left hand side of (3.17) is then given in terms of 4×4 blocks and for a given n there are only values for $m = n+1$, n, $n-1$ so a typical set of three blocks can be written as

n

$m = n+1$

		$[\omega(n+1)]^{1/2}$	
			$[\omega(n+1)]^{1/2}$
	$[\omega(n+1)]^{1/2}$		
$[\omega(n+1)]^{1/2}$			

$m = n$

2			
	-2		

$m = n-1$

			$(\omega n)^{1/2}$
		$(\omega n)^{1/2}$	
$(\omega n)^{1/2}$			
	$(\omega n)^{1/2}$		

where empty blocks indicate zeros.

Clearly then if we go from $n = 0$ to a maximum value $n = N$ we get a symmetric real matrix of $[4(N+1)] \times [4(N+1)]$ dimensions. For $N = 5, 10, 15$ and 20 it is then respectively of dimensions $24 \times 24, 48 \times 48, 64 \times 64$ and 96×96.

We have diagonalized these matrices for different values of ω. For $w \ll 1$, as for example $\omega = 0.01$, we get values very close to $\mu = 2, 0, -2$, as seen in Table III for $N = 5$. We are

TABLE III. Mass spectra μ for $\omega = 0.01$ obtained by a variational procedure ($N = 5$) for the particle-antiparticle system. Results should be read from left to right and going down. The masses are symmetric with respect to 0, and all of them are in the vicinity of $2, 0, -2$, with only the six in the vicinity of 2 having a physical significance.

-2.044100613491596	-2.034561986347728	-2.024816301028781
-2.024779717114118	-2.014925558988651	-2.005000007732200
$-3.9617169669586387E-02$	$-1.9165017880114182E-02$	$-1.8958617641650164E-02$
$-1.7852055500015840E-02$	$-4.9734734312391416E-03$	$-2.5557899401092870E-03$
$2.5557899401091552E-03$	$4.9734734312382248E-03$	$1.7852055500015299E-02$
$1.8958617641650164E-02$	$1.9165017880115719E-02$	$3.9617169669586567E-02$
2.005000007732201	2.014925558988650	2.024779717114118
2.024816301028780	2.034561986347725	2.044100613491599

TABLE IV. Comparison of the variational and perturbative procedures (up to lst order) for the first six eigenvalues $n = 0$ to 5 of μ^2 with $\omega = 0.01$. Only the variational values in the vicinity of 4 were considered.

N/n	0	1	2	3	4	5
5	4.020025031	4.059925008	4.099732903	4.099881053	4.139442476	4.178347318
10	4.020025031	4.059926385	4.099731549	4.139442942	4.179062886	4.199730664
15	4.020025031	4.059926385	4.099731549	4.139442942	4.179062886	4.218593615
20	4.020025031	4.059926385	4.099731549	4.139442942	4.179062886	4.218593615
Perturbative procedure	4.020025	4.059925	4.099725	4.139425	4.179025	4.218525

TABLE V. Mass spectra μ for $\omega = 1.0$ obtained by a variational procedure ($N = 5$) for the particle-antiparticle system. The results should be read from left to right and then going down. They are symmetric with respect to 0, but no longer in the vicinity $2, 0, -2$, so they have strong admixtures of negative energy states.

-4.250017149585462	-4.050302684986235	-3.748635260236295
-3.668101518788701	-3.072512756171069	-2.501987776734324
-1.808797996416922	-1.179135806690647	-0.9489438276047327
-0.7648302660395511	-0.3565397907700288	-0.2240492387188997
0.2240492387189008	0.3565397907700284	0.7648302660395526
0.9489438276047337	1.17913580669064 9	1.808797996416919
2.501987776734322	3.072512756171067	3.668101518788697
3.748635260236298	4.050302684986240	4.250017149585466

only interested in those close to 2 that correspond to positive energy values for both particle and antiparticle and, when we square them, they are close to the values obtained by the perturbative procedure of the previous section, as shown in Table IV.

When ω is of the order or larger than 1, then the variational procedure becomes unstable, *i.e.* the results for $N = 5, 10, 15, 20$ can not be compared. This may be due to the appearance of a continuous spectrum as showed at the end of the previous section. There is also an important relativistic effect. The eigenvalues of μ are no longer close to $-2, 0, 2$ as happened for $\omega \ll 1$, as shown in Table V for $\omega = 1$, so that we no longer know if they come from positive energies for both particle and antiparticle, or from the level of energy 0 which, for a free particle and antiparticle, could occur when the negative energies of one combine with positive ones of the other as was discussed in Ref. [8]. As Dirac theory predicts that all negative energy states are filled, the levels coming from this 0 energy state will not have any physical significance. Thus we arrive at the conclusion that the variational method makes only sense when $\omega \ll 1$ and this is an important restriction when we wish to apply it to some three dimensional problems.

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