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1998 J. Phys. A: Math. Gen. 31 397

(http://iopscience.iop.org/0305-4470/31/1/033)

J. Phys. A: Math. Gen. **31** (1998) 397–408. Printed in the UK PII: S0305-4470(98)84768-9

Variational energy spectra of relativistic Hamiltonians

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Received 4 June 1997

Abstract. In ordinary and relativistic quantum mechanics the energy spectra of most of the Hamiltonians cannot be obtained exactly. Approximate methods have to be used among which the variational one is particuarly popular. The purpose of this paper is to show that when the 4×4 matrices $\boldsymbol{\alpha}, \beta$ appearing in a Dirac equation with interaction, are replaced by a direct product of 2×2 matrices associated with ordinary and what we call sign spins, then a standard complete set of non-relativistic wavefunctions can be used to carry out the variational calculations. To illustrate the power of our method we analyse first the variational energies of ordinary and Dirac relativistic oscillator Hamiltonians, and then indicate the procedure for the general one-particle case. The extensions to higher spins, or to a larger number of particles, are briefly mentioned in the conclusion.

1. Introduction

The three-dimensional single-particle stationary Schrödinger equation has had innumerable applications [1]. Except for special potentials such as the oscillator or Coulomb ones, its energy spectra cannot be obtained exactly. Thus, in general, approximation methods are used, among which the variational one is particularly popular. Frequently the basis of states on which the variational procedure is applied, is an explicit orthonormal one with some variational parameters, for example the harmonic oscillator states whose frequency ω is varied to get the best approach to the actual bound state levels of the problem.

The observations of the previous paragraph have been extensively used and applied in ordinary quantum mechanics [1], but when we are in the relativistic range the literature is not as vast [2]. In this paper we shall analyse a variational procedure, based on a complete set of harmonic oscillator states but coupled to spin $\frac{1}{2}$, applied to a Dirac Hamiltonian with arbitrary interaction of the form

$$H' = c\boldsymbol{\alpha} \cdot \boldsymbol{p}' + mc^2\beta + V(r') \tag{1.1}$$

where

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{1.2}$$

with $\boldsymbol{\sigma}$ being the vector of Pauli spin matrices, and all the observables carry a prime to indicate that they are in standard c.g.s. units. We shall later introduce $H, \boldsymbol{p}, \boldsymbol{r}$ without primes for units that are more convenient to our analysis. The potential $V(r')$ usually depends only on the magnitude of the position vector $\boldsymbol{r}'$ if it comes from the fourth component of the

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0305-4470/98/010397+12$19.50

Dirac equation [1], or is of the form $V(r')\beta$ if its origin is related to a mass that is position dependent.

Before deriving the matrix formulation of H' in an appropriate basis it is convenient to consider some special cases of H' in which the method can be discussed numerically, to see about its convergence and validity as compared with exact results, and thus we shall first apply our analysis to relativistic harmonic oscillators, in the first case when in (1.1) we have

$$V(r') = \tfrac{1}{2}m\Omega^2 r'^2 \tag{1.3}$$

with Ω being the frequency, while in the second we shall discuss what we have called the Dirac oscillator given by (1.1) when $V(r') = 0$ but in which we make the replacement

$$\boldsymbol{p}' \to \boldsymbol{p}' - \mathrm{i}m\Omega \boldsymbol{r}'\beta. \tag{1.4}$$

In the following sections we shall show that our variational procedure is very good at giving us the energy spectra of the two problems mentioned above.

2. Variational energy spectra of the ordinary relativistic harmonic oscillator

As mentioned above, the present problem corresponds to $V(r')$ given by (1.3) and we shall start by subtracting the rest energy mc^2 from the Hamiltonian and making it dimensionless through the definition

$$H = (\hbar\Omega)^{-1}(H' - mc^2). \tag{2.1}$$

Furthermore, we shall employ as the set of variational functions one that includes harmonic oscillator states of frequency ω. As it would be bothersome to have this frequency in the wavefunction when we calculate matrix elements, we prefer to introduce it in the Hamiltonian as was done in [4], by making in H of (2.1) the change of variables

$$\boldsymbol{p}' = (m\omega\hbar)^{1/2}\boldsymbol{p} \qquad \boldsymbol{r}' = \left(\frac{\hbar}{m\omega}\right)^{1/2}\boldsymbol{r} \tag{2.2}$$

so as to obtain

$$H = a\epsilon\boldsymbol{\alpha}\cdot\boldsymbol{p} + \frac{1}{2\epsilon^2}r^2\mathcal{I} + a^2(\beta - \mathcal{I}) \tag{2.3}$$

where

$$a = \sqrt{\frac{mc^2}{\hbar\Omega}} \qquad \epsilon = \sqrt{\frac{\omega}{\Omega}} \tag{2.4}$$

and $\mathcal{I}$ is a 4×4 unit matrix.

With the help of ϵ we have incorporated the oscillator frequency in the Hamiltonian and thus in our variational function we need only to use [4] oscillator states of frequency 1.

Our next point is to note that the 4×4 matrices $\boldsymbol{\alpha}, \beta, \mathcal{I}$ in (2.3) can be converted into direct products of 2×2 ones by introducing the definitions [5]

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad s_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad s_2 = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \qquad s_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.5}$$

$$\check{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad t_1 = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad t_2 = \frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} \qquad t_3 = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2.6}$$

The matrices $s_i, i = 1, 2, 3$, are those of the ordinary spin $\frac{1}{2}$, while $t_i, i = 1, 2, 3$ which we distinguish by a square instead of a round bracket, have the same definition as the s_i

but play a very different role and we called them *sign spin* since they are associated with the sign of the energy [5]. The set of matrices (2.5), (2.6) are identical to those appearing in supermultiplet theory as introduced by Wigner [6] but in which the $t_i, i = 1, 2, 3$ were interpreted as the components of isotopic spin.

From definitions (1.2), (2.5), (2.6) we clearly see that $\boldsymbol{\alpha}, \beta, \mathcal{I}$ can be expressed as the direct products

$$\boldsymbol{\alpha} = 4\boldsymbol{s} \otimes t_1 \qquad \beta = 2\check{I} \otimes t_3 \qquad \mathcal{I} = \hat{I} \otimes \check{I}. \tag{2.7}$$

Replacing (2.7) in (2.3) we finally obtain

$$H = 4a\epsilon(\boldsymbol{s} \cdot \boldsymbol{p}) \otimes t_1 + \frac{1}{2\epsilon^2} r^2(\hat{I} \otimes \check{I}) + a^2[2(\hat{I} \otimes t_3) - (\hat{I} \otimes \check{I})]. \tag{2.8}$$

For the variational analysis of the Hamiltonian (2.8) we start, as in the non-relativistic problem [4], with the orbital harmonic oscillators of frequency 1 expressed as

$$|Nl\mu\rangle = R_{Nl}(r)Y_{l\mu}(\theta, \varphi) \tag{2.9}$$

with $Y_{l\mu}$ being spherical harmonics and R_{Nl} being the radial functions of equation (1.8) of [4], but now characterized by the total number of quanta

$$N = 2n + l \tag{2.10}$$

where $n = 0, 1, 2, \ldots$ is the radial quantum number.

In the relativistic case we are dealing with here we must replace (2.9) by a ket that includes the ordinary spin $\frac{1}{2}$ state which we denote by $\chi_\sigma, \sigma = \pm\frac{1}{2}$, so that we get the ket

$$|N(l, \tfrac{1}{2})jm\rangle \equiv \sum_{\mu\sigma} \langle l\mu, \tfrac{1}{2}\sigma | jm\rangle |Nl\mu\rangle \chi_\sigma \tag{2.11}$$

where $\langle|\rangle$ is a Clebsch–Gordan coefficient and j, m the total angular momentum and its projection. The latter are eigenvalues for integrals of motion of the problem as

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{s} \tag{2.12}$$

(with the components of $\boldsymbol{s}$ given by (2.5) and $L = \boldsymbol{r} \times \boldsymbol{p}$) obviously commutes with the Hamiltonian (2.8).

We are not yet through with our basic variational states as we still have to include the part related with the sign spin $\frac{1}{2}$, which could be denoted by the ket $|\frac{1}{2}\tau\rangle$ with the eigenvalue τ of t_3 being $\tau = \pm\frac{1}{2}$. Thus the states with respect to which we have to determine the matrix elements of H can be denoted by the kets

$$|N(l, \tfrac{1}{2})j; \tau\rangle \equiv |N(l, \tfrac{1}{2})jm\rangle \otimes |\tfrac{1}{2}\tau\rangle \tag{2.13}$$

in which we suppressed the m because the matrix elements of the Hamiltonian do not depend on it [7], and also the index $\frac{1}{2}$ as it is fixed.

From (2.8) and (2.13) we see that the variational matrix elements of the Hamiltonian are given by

$$\begin{aligned}
&\langle N'(l', \tfrac{1}{2})j; \tau'|H|N(l, \tfrac{1}{2})j; \tau\rangle \\
&\quad = 4a\epsilon\left\{\langle N'(l', \tfrac{1}{2})j|\boldsymbol{s} \cdot \boldsymbol{p}|N(l, \tfrac{1}{2})j\rangle\langle\tfrac{1}{2}\tau'|t_1|\tfrac{1}{2}\tau\rangle\right\} \\
&\qquad + \frac{\delta_{ll'}\delta_{\tau\tau'}}{2\epsilon^2}\left\{\langle N'l\|r^2\|Nl\rangle\right\} + a^2\left\{(2\tau - 1)\delta_{\tau'\tau}\delta_{N'N}\delta_{l'l}\right\} \\
&\quad = 4a\epsilon\left\{(-1)^{l'+\frac{1}{2}-j} W(ll'\tfrac{1}{2}\tfrac{1}{2}; 1j)[2(2l' + 1)]^{1/2}\langle N'l'\|p\|Nl\rangle\sqrt{\tfrac{3}{4}}\langle\tfrac{1}{2}\tau'|t_1|\tfrac{1}{2}\tau\rangle\right\}
\end{aligned}$$

$$+\frac{\delta_{ll'}\delta_{\tau\tau'}}{2\epsilon^2}\Bigg\{-\tfrac{1}{2}\Big[(N-l)(N+l+1)\Big]^{1/2}\delta_{N'N-2}$$
$$+(N+\tfrac{3}{2})\delta_{N'N}-\tfrac{1}{2}\Big[(N-l+2)(N+l+3)\Big]^{1/2}\delta_{N'N+2}\Bigg\}$$
$$+a^2\Big\{(2\tau-1)\delta_{\tau'\tau}\delta_{N'N}\delta_{l'l}\Big\} \tag{2.14}$$

where the first curly bracket on the right-hand side comes from formula (6.21) of Rose's book [8], while the second curly bracket is obtained from (3.11) in [1], if we write $r^2=(p^2+r^2)-p^2$.

The reduced matrix element $\langle N'l'\|p\|Nl\rangle$ can be immediately determined by writing

$$\boldsymbol{p}=(\mathrm{i}/\sqrt{2})(\boldsymbol{\eta}-\boldsymbol{\xi}) \tag{2.15}$$

where $\boldsymbol{\eta},\boldsymbol{\xi}$ are creation and annihilation operators, whose reduced matrix elements can be obtained from equation (10.35) of [1]. Substituting in (2.14) the value mentioned of $\langle N'l'\|p\|Nl\rangle$ as well as the Racah coefficients $W(ll'\frac{1}{2}\frac{1}{2};1j)$ and the matrix element $\langle\frac{1}{2}\tau'|t_1|\frac{1}{2}t\rangle$ given respectively in [8, pp 227, 83] we finally obtain:

$$\langle N'(l',\tfrac{1}{2})j,\tau'|H|N(l,\tfrac{1}{2})j,\tau\rangle$$
$$=\frac{\mathrm{i}a\epsilon}{\sqrt{2}}\Bigg\{-\Bigg[\frac{(j+l+\frac{5}{2})(j+l+\frac{1}{2})(l-j+\frac{3}{2})(j-l+\frac{1}{2})}{(2l+1)(2l+3)}\Bigg]^{1/2}$$
$$\times\Big[(N+l+3)^{1/2}\delta_{N'N+1}+(N-l)^{1/2}\delta_{N'N-1}\Big]\delta_{l'l+1}$$
$$+\Bigg[\frac{(j+l+\frac{3}{2})(l-j-\frac{1}{2})(j+l-\frac{1}{2})(j-l-\frac{3}{2})}{(2l+1)2l-1)}\Bigg]^{1/2}$$
$$\times[(N-l+2)^{1/2}\delta_{N'N+1}+(N+l+1)^{1/2}\delta_{N'N-1}]\delta_{l'l-1}\Bigg\}$$
$$\times\{[(\tfrac{1}{2}-\tau)(\tfrac{3}{2}+\tau)]^{1/2}\delta_{\tau'\tau+1}+[(\tfrac{1}{2}+\tau)(\tfrac{3}{2}-\tau)]^{1/2}\delta_{\tau'\tau-1}\}$$
$$+\frac{\delta_{l'l}\delta_{\tau'\tau}}{2\epsilon^2}\{-\tfrac{1}{2}[(N-l)(N+l+1)]^{1/2}\delta_{N'N-2}+(N+\tfrac{3}{2})\delta_{N'N}$$
$$-\tfrac{1}{2}[(N-l+2)(N+l+3)]^{1/2}\delta_{N'N+2}\}$$
$$+a^2\{(2\tau-1)\delta_{\tau'\tau}\delta_{N'N}\delta_{l'l}\}. \tag{2.16}$$

The question now is to write the matrix itself for a definite j up to a maximum number of quanta $\mathfrak{N}$, i.e. write N,N' restricted to the interval $0\leqslant N,N'\leqslant\mathfrak{N}$, and then diagonalize it for a fixed a getting the energies E as a function of ϵ and looking for values of the latter that give a minimum, at least for those related to positive values of the energy.

The simplest case of (2.16) corresponds to $j=\frac{1}{2}$, which implies $l=0$ or 1, for which N is either even or odd. Thus, in this case the kets (2.13) can be written in the short hand notation

$$|N^{\tau}\rangle \tag{2.17}$$

where $\tau=\pm\frac{1}{2}$ will be denoted by $\pm$.

Our matrix elements can then be written as

$$\langle N'^{\tau'}|H|N^{\tau}\rangle \tag{2.18}$$

and we see from (2.16) that the kinetic energy connects the kets $|N^{\pm}\rangle$ with the bra's $\langle(N\pm1)^{\mp}|$, while the potential energy relates $|N^{\pm}\rangle$ with the bra's $\langle(N\pm2)^{\pm}|$, $\langle(N^{\pm}|$. If

we then start with the state denoted by 0^+ in the ket, we can take the values of columns and rows in the matrix of elements (2.18) in the following order

$$0^+, 1^-, 2^+, 3^-, \ldots 14^+, 15^- \ldots \tag{2.19}$$

while if we start with 0^- we get an independent matrix whose ordering is

$$0^-, 1^+, 2^-, 3^+, \ldots 14^-, 15^+ \ldots . \tag{2.20}$$

In (2.19) the states of positive or negative energy (given by the $+$ or $-$ sign above the numbers) are associated respectively with an even or odd number of quanta N and parity $(-1)^N$, while in (2.20) the relation is reversed.

We shall discuss in detail the case when the ket $|N^{\pm}\rangle$ are given in the order (2.19), as the results for the order (2.20) will be similar.

In the numerical calculation we have to specify first the value of a, defined by (2.4), that we shall use. We will consider the two cases

$$a = 10 \qquad \text{and} \qquad a = 1. \tag{2.21}$$

In the first case we have $\bar{h}\Omega = (mc^2/100)$ and this implies that the oscillator interaction is much weaker than the rest energy, so we would expect for positive energies, curves for the energy E as function of ϵ very similar to those of the non-relativistic problem [1] with a minimum close to $\epsilon = 1$, i.e. $\omega = \Omega$. On the other hand, for this value of $a = 10$ we also get the negative energy curves that start with energy E being close to $+\infty$ if $\epsilon \to 0$, and then give a set of almost parallel lines at negative energies when $\epsilon \simeq 1$ and finally collapse to $E \to -\infty$ if $\epsilon \to \infty$. These negative energies are monotonically decreasing so they would not correspond to bound states of negative energy but rather represent, in a discrete fashion, the continuous negative energy spectrum of this problem.

All of the above comments are illustrated in figure 1 in which $a = 10$. In part (a) we have the positive energies with the characteristics we mentioned above, where at $\epsilon \simeq 1$, and the energies are very close to

$$(2n + \tfrac{3}{2}) \qquad n = 0, 1, 2, \ldots \tag{2.22}$$

while in figure 1(b) we give the curves for negative energies again with the characteristics we mentioned above. In figure 1(c), we change the scale to draw together the positive and negative parts of the energies as a function of ϵ, and show the gap of $2a^2 \simeq 200$ between them at the minima when $\epsilon \simeq 1$, as we would expect in a relativistic problem, as it corresponds to $2mc^2$ in units of $\bar{h}\Omega$.

We turn now our attention to the case when $a = 1$, which implies $\bar{h}\Omega = mc^2$, so that we are in a fully relativistic situation. Again we draw the energy curves as a function of ϵ in figure 2. To see the situation clearly this figure is divided into three parts. First, in figure 2(a) we give the positive energies as a function of ϵ where we find that the curves take the value $+\infty$ both when $\epsilon = 0$ and $\epsilon = \infty$. This implies that we have minima and thus bound states continue to exist but now they appear for the lowest energy at $\epsilon \simeq 2.2$, i.e. $\omega = \simeq 4.84\Omega$, and their values are given in table 1, where, for comparison, we also give the values when $a = 10$.

Then in figure 2(b) we give the negative energy values which start at $+\infty$ if $\epsilon = 0$ and then decrease monotonically with ϵ until they reach the value $-\infty$ when $\epsilon \to \infty$. There are thus no negative bound states and what we are seeing is then the discrete representation of the continuous negative spectrum. Finally in figure 2(c), we choose the scale so that both positive and negative energy curves can be drawn together but here, while not crossing [9] they appear almost together up to values close to $\epsilon = 2$, and then they start to separate as seen on the right-hand side of figure 2(c).

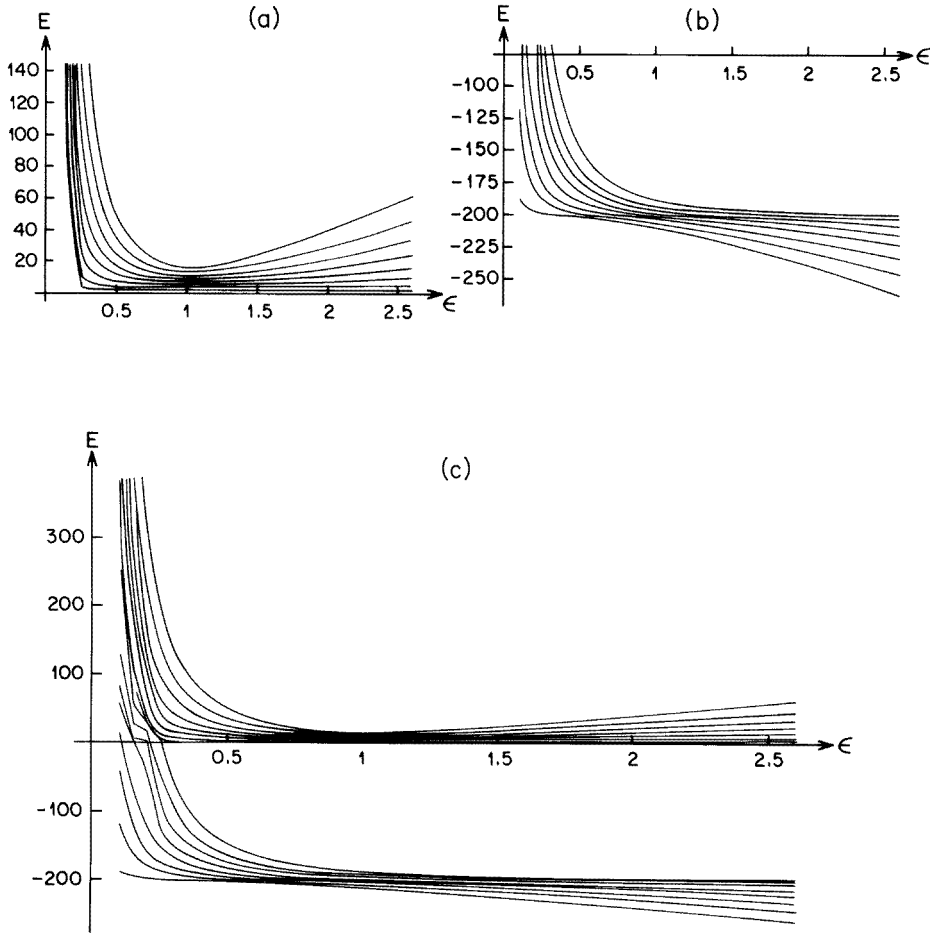

Figure 1. We draw the variational energy curves for the ordinary relativistic oscillator with E as a function $\epsilon \equiv (\omega/\Omega)^{1/2}$ when $a = 10$, and where we take all the states in (2.19) from $|0^+\rangle$ to $|15^-\rangle$. We have thus a 16×16 matrix that will give rise to 16 curves, of which eight start at $E = +\infty$ when $\epsilon = 0$ and end at $E = +\infty$ when $\epsilon = \infty$. Thus they have a minimum as seen in (*a*), and it occurs close to $\epsilon = 1$, as for $a = 10, \overline{h}\Omega = (mc^2/100)$ and we are in the non-relativistic limit where $E = (2n + \frac{3}{2}), n = 0, 1, \ldots 7$ as seen in table 1. The other eight curves start at $E = +\infty$ when $\epsilon = 0$ but then decrease monotonically to $E = -\infty$ when $\epsilon = \infty$ as seen in (*b*). Thus they have no bound states and in fact at $\epsilon \simeq 1$ they are given by almost parallel lines that represent, in a discrete fashion, the continuous negative energy spectrum of the problem. In (*c*), we change the scale to draw together the positive and negative energy curves of E as function of ϵ and show the gap of $2a^2 = 200$ that separates them at $\epsilon \simeq 1$, which we could expect in a relativistic problem, as it corresponds to $2mc^2$ in units of $\overline{h}\Omega$.

Incidentally at $\epsilon = 2.2$, the separation between the positive minimum energy and the first negative one is approximately 2. As, in this particular case, we are taking $a \equiv (mc^2/\overline{h}\Omega) = 1$, this means that again the gap $2mc^2$ in units of $\overline{h}\Omega$ is maintained.

Thus, we see that a variational analysis using the kets (2.13) as trial wavefunctions, gives valid results for $a = 10$ that we can compare with the non-relativistic limit at least for the positive energies. For $a = 1$ we just have to trust the calculations of table 1 for the energies of bound states as already $\overline{h}\Omega$ is equal to mc^2 and thus non-relativistic results are not applicable.

Table 1. Variational energies of relativistic harmonic oscillator at the values of a and ϵ indicated, where the latter gives the minimum of the positive energies. On the left-hand side, we indicate the values of n corresponding to formula (2.22) of the text.

n	E for $a = 10, \epsilon = 1$	E for $a = 1, \epsilon = 2.2$
0	1.499	1.438
1	3.481	2.680
2	5.444	3.838
3	7.401	4.959
4	9.341	6.129
5	11.268	7.360
6	13.184	8.670
7	15.124	10.162

To gain more confidence in our procedures we shall also apply them to the Dirac oscillator of (1.4) as the energy spectra of this relativistic problem can be calculated exactly, and so we can compare it with the variational analysis for any value of the parameter $a = (mc^2/\hbar\Omega)^{1/2}$.

3. Variational energy spectra for the Dirac oscillator

From equation (1.1) and (1.4) we see that in c.g.s. units the Hamiltonian of the Dirac oscillator [3] can be written as

$$H' = c[\boldsymbol{\alpha} \cdot (\boldsymbol{p}' - \mathrm{i}m\Omega \boldsymbol{r}'\beta)] + mc^2\beta \tag{3.1}$$

and we can analyse it variationally by following the same steps that we used in the previous section.

We first replace H' by H through definition (2.1), and then also substitute the $\boldsymbol{r}', \boldsymbol{p}'$ by the $\boldsymbol{r}, \boldsymbol{p}$ as defined in equation (2.2). Finally the $\boldsymbol{\alpha}, \beta$ are replaced by the direct products of 2×2 matrices as in equation (2.7). Thus we arrive at the Hamiltonian

$$\begin{aligned} H &= 4a\{\epsilon[(\boldsymbol{s} \cdot \boldsymbol{p}) \otimes t_1] - \epsilon^{-1}[(\boldsymbol{s} \cdot \boldsymbol{r}) \otimes t_2]\} \\ &+ a^2[2(\hat{I} \otimes t_3) - (\hat{I} \otimes \check{I})] \end{aligned} \tag{3.2}$$

where a and ϵ have the same definition as in (2.4) and we use the fact that

$$\boldsymbol{\alpha}\beta = 4[(\boldsymbol{s} \otimes t_1)(\hat{I} \otimes t_3] = 4\boldsymbol{s} \otimes t_1 t_3 = -4\mathrm{i}\boldsymbol{s} \otimes t_2. \tag{3.3}$$

We now take as variational functions the same ones that we used before, i.e. those given by equation (2.13), so that again with the help of formula (6.21) of [8] we have that

$$\begin{aligned} \langle N'(l', \tfrac{1}{2})j; \tau'|H|N(l, \tfrac{1}{2})j; \tau\rangle &= 4a\{\epsilon\langle N'(l', \tfrac{1}{2})j|\boldsymbol{s} \cdot \boldsymbol{p}|N(l, \tfrac{1}{2})j\rangle\langle \tfrac{1}{2}\tau'|t_1|\tfrac{1}{2}\tau\rangle \\ &- \epsilon^{-1}\langle N'(l', \tfrac{1}{2})j|\boldsymbol{s} \cdot \boldsymbol{r}|N(l, \tfrac{1}{2})j\rangle\langle \tfrac{1}{2}\tau'|t_2|\tfrac{1}{2}\tau\rangle\} \\ &+ a^2(2\tau - 1)\delta_{N'N}\delta_{l'l}\delta_{\tau'\tau} \\ &= 4a\left\{(-1)^{l'+\frac{1}{2}-j}W(ll'\tfrac{1}{2}\tfrac{1}{2}; 1j)[2(2l'+1)]^{1/2}\sqrt{\tfrac{3}{4}}\right\} \\ &\times\left\{\epsilon\langle N'l'\|p\|Nl\rangle\langle \tfrac{1}{2}\tau'|t_1|\tfrac{1}{2}\tau\rangle - \epsilon^{-1}\langle N'l'\|r\|Nl\rangle\langle \tfrac{1}{2}\tau'|t_2|\tfrac{1}{2}\tau\rangle\right\} \\ &+ a^2(2\tau - 1)\delta_{N'N}\delta_{l'l}\delta_{\tau'\tau}. \end{aligned} \tag{3.4}$$

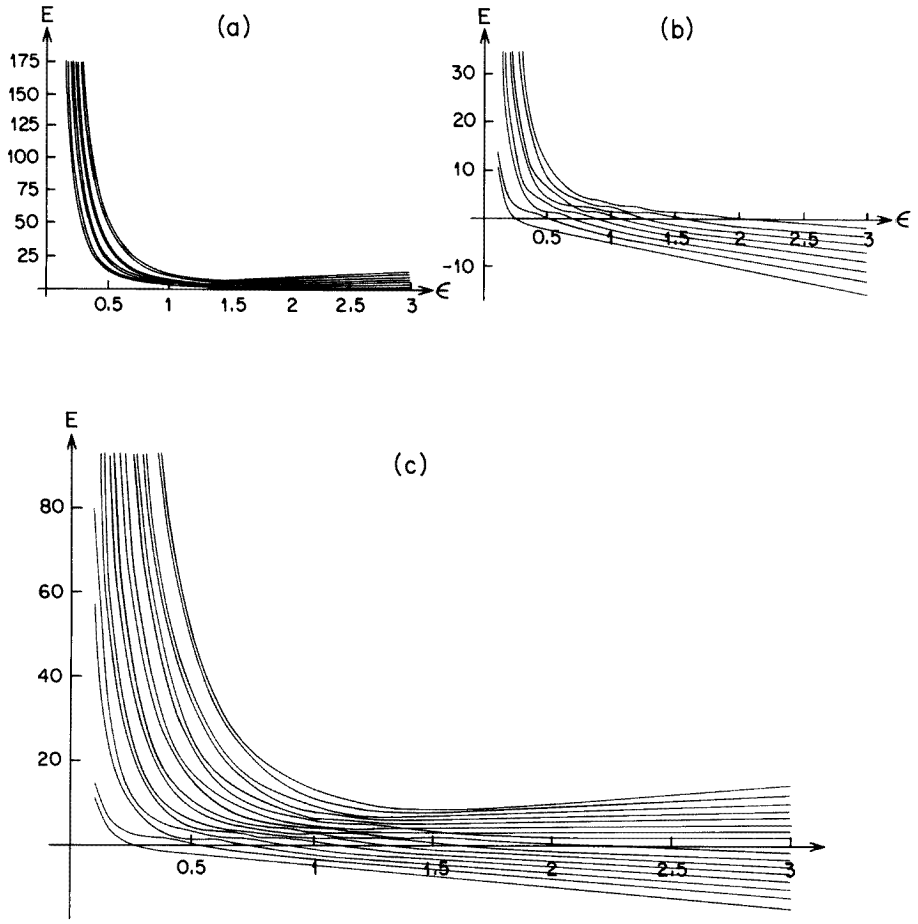

Figure 2. We draw the variational energy curves for the ordinary relativistic oscillator with E as a function of ϵ when $a = 1$ and where, as before, we take all states (2.10) from $|0^+\rangle$ to $|15^-\rangle$. We have thus 16 curves of which again eight start at $E = +\infty$ when $\epsilon = 0$ and end $E = +\infty$ when $\epsilon = \infty$. Thus they have a minimum, as seen in (a), but as $a = 1$, which means $\hbar\Omega = mc^2$, we are in the relativistic region and the minimum does not occur at $\epsilon = 1$ but at $\epsilon \simeq 2.2$, while the energy spectrum is compressed as seen in table 1. The other eight curves start at $E = +\infty$ when $\epsilon = 0$ but then decrease monotonically to $E = -\infty$ when $\epsilon = \infty$, as seen in (b). Thus they have no bound states and at $\epsilon \simeq 2.2$ they give almost parallel lines that represent, in a discrete fashion, the continuous negative energy spectrum of the problem. In (c) we change the scale to show both curves together which overlap at small ϵ but do not cross, and later get separated into positive and negative energies with eight curves in each part as seen at the end of (c). At $\epsilon = 2.2$ the separation between the minimum positive energy and highest negative one is approximately 2, so again a gap of $2mc^2$ in units of $\hbar\Omega$ is maintained.

The reduced matrix element $\langle N'l' \| p \| Nl \rangle$ was already discussed in the previous section and that of $\langle N'l' \| r \| Nl \rangle$ can be obtained in a similar fashion as

$$\boldsymbol{r} = (1/\sqrt{2})(\boldsymbol{\eta} + \boldsymbol{\xi}). \tag{3.5}$$

By using the explicit form of the Racah coefficient $W(ll'\frac{1}{2}\frac{1}{2}; 1j)$ and of the matrix of $t_i, i = 1, 2, 3$, we could obtain for the matrix element (3.4) of H an expression similar to (2.16). We are going to do numerical calculations only for the simplest case which, as in

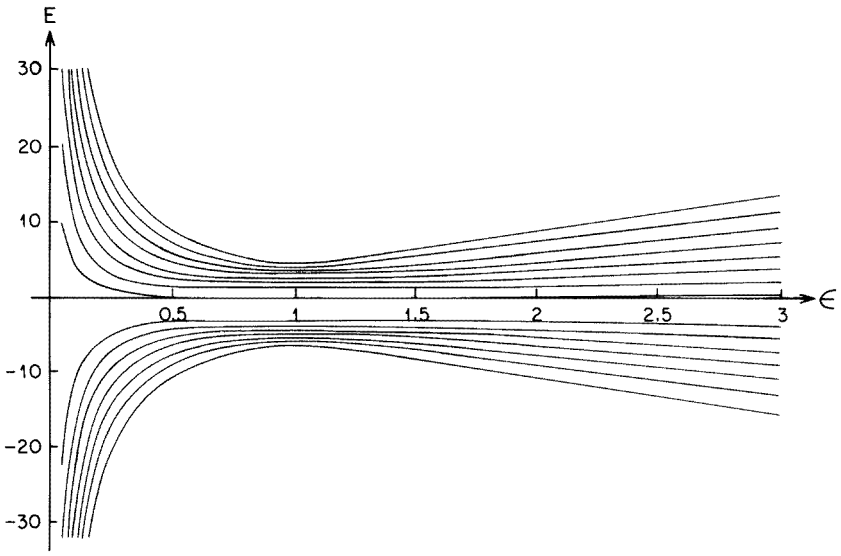

Figure 3. We draw the variational energy curves of the Dirac oscillator with E as a function of ϵ when $a = 1$ and we take all states (2.19) from $|0^+\rangle$ to $|15^-\rangle$. We have thus 16 curves, but here they break up elegantly into two parts, eight in positive and eight in negative energies and the minima or maxima occur both at $\epsilon = 1$ and coincide with the exact values for the reasons discussed in the text. Note that at $\epsilon = 1$ the upper and lower values of E correspond respectively to N even or odd as indicated in equations (3.7) and (3.8).

the previous case, turns out to be $j = \frac{1}{2}$. In that case l, l' can only take the value 0 or 1. When $l = l'$ the only contribution is from the last term in (3.4), i.e. $a^2(2\tau - 1)\delta_{N'N}\delta_{l'l}\delta_{\tau'\tau}$. Thus, we just need to give explicitly the matrix elements (3.4) when $l = 0$ and $l' = 1$ or vice versa, with the latter being the Hermitian conjugate of the former. Thus, from the discussion given above the only matrix element of interest when $j = \frac{1}{2}$ is given by

$$\begin{aligned}
&\langle N'(l', \tfrac{1}{2})\tfrac{1}{2}, \tau'|H|N(l, \tfrac{1}{2})\tfrac{1}{2}, \tau\rangle \\
&\quad = \frac{-ia\epsilon}{\sqrt{2}}[\sqrt{N+3}\delta_{N'N+1} + \sqrt{N}\delta_{N'N-1}]\{[(\tfrac{1}{2} - \tau)(\tfrac{3}{2} + \tau)]^{1/2}\delta_{\tau'\tau+1} \\
&\quad\quad + [(\tfrac{1}{2} + \tau)(\tfrac{3}{2} - \tau)]^{1/2}\delta_{\tau'\tau-1}\} \\
&\quad\quad + \frac{ia}{\epsilon\sqrt{2}}[\sqrt{N+3}\delta_{N'N+1} - \sqrt{N}\delta_{N'N-1}]\{-[(\tfrac{1}{2} - \tau)(\tfrac{3}{2} + \tau)]^{1/2}\delta_{\tau'\tau+1} \\
&\quad\quad + [(\tfrac{1}{2} + \tau)(\tfrac{3}{2} - \tau)]^{1/2}\delta_{\tau'\tau-1}\}. \qquad (3.6)
\end{aligned}$$

Using (3.6) as well as the diagonal part mentioned above we have written down a 16×16 matrix based on the chain (2.19) starting with $|0^+\rangle$ and ending with $|15^-\rangle$. This matrix has a and ϵ as parameters, and we select first $a = 1$, so only ϵ remains. We then diagonalize the matrix for different values of ϵ and obtain the curves of the energy E as function of ϵ as shown in figure 3.

It turns out that curves have two branches, the positive ones starting at $E = +\infty$ when $\epsilon = 0$, and going back to $+\infty$ when $\epsilon \to \infty$. The negative ones do the reverse, i.e. take the values $E = -\infty$ when $\epsilon = 0$ or ∞. Thus the positive curves have a minimum that turns out to occur at $\epsilon = 1$, while at the same value the negative ones have a maximum. Had we taken instead of E negative, its absolute value $|E|$, as suggested by Quesne [10]

using arguments of Dirac's hole theory, then $|E|$ as function of ϵ would behave in a similar way as the positive E, i.e. it would have minima at $\epsilon = 1$.

The minima would then give the variational energy of the bound states of the problem, which are the only ones present in the exact solution that has a discrete spectrum [3].

In figure 3 we took $a = 1, j = \frac{1}{2}$ and also see that in (2.19) the even or odd N correspond to positive or negative energy as they have the superscript $+$ and $-$.

In fact our variational approximation is so good that for $\epsilon = 1$ it already gives the actual energy eigenvalues [3, 10] as equation (3.2) with $\epsilon = 1, a = 1, j = \frac{1}{2}$ gives, as a function of N, for positive E_+ and negative E_- energies, the *exact* values [3, 10]

$$E_+ = -1 + (1 + 2N)^{\frac{1}{2}} \qquad \text{if } N \text{ is even} \tag{3.7}$$

$$E_- = -1 - (3 + 2N)^{\frac{1}{2}} \qquad \text{if } N \text{ is odd.} \tag{3.8}$$

Thus, we have to compare these values with those of figure 3 when $\epsilon = 1$ and by using a ruler one can see that they exactly agree. This excellent convergence is related with the fact that the state $|N(l, \frac{1}{2})jm\rangle$ of (2.11) turns out to be an eigenstate of the Dirac oscillator problem [3, 10], but this in no way demerits our variational calculation as it is done for any ϵ and we just happen to apply it to a problem whose energy spectra has an exact solution to which it corresponds at the minima, i.e. when $\epsilon = 1$.

We note incidentally that our variational calculation also gives a spurious state that we do not draw, which corresponds to the negative energy $E_- = -2$, at $\epsilon = 1$, which from (3.8) would be associated to the ket with $N = -1$ that does not exist, a fact also noted by Quesne [10].

Again we note from (3.7) and (3.8) that for $\epsilon = 1$ the separation between the energy levels corresponding to $N = 0$ and $N = 1$ is $1 + \sqrt{5} > 2$ and it implies (as we already observed in the ordinary relativistic oscillator), that there is a gap of $2mc^2$ or larger in units of $\hbar\Omega$ between the positive and negative energy states. We also recall that our analysis was restricted to $a = 1$, but for arbitrary a, the results are very similar and provide no new relevant information.

In the present example our variational analysis gives us exactly what we expect, and thus we can use it with confidence in getting the spectra of other relativistic Hamiltonians, as we proceed to outline in the next section.

4. Variational energy spectra for an arbitrary relativistic Hamiltonian

We now wish to outline the procedure to be followed in a variational analysis, when applied to Hamiltonian (1.1) with $V(r')$ being some arbitrary functions of r' and, in some cases, even containing the matrix β. We first subtract from (1.1) the rest energy mc^2 and then divide $H' - mc^2$ by some constant number of the dimension of energy appropriate to the potential. For example, if we deal with the Coulomb potential $(-e^2/r')$ it is convenient to divide by the Bohr energy $E_B = (mc^4/2\hbar^2)$ as was done in [11].

Once we carry out the operation indicted in the previous paragraph, it gives us a dimensionless Hamiltonian

$$H = b^{-1}(H' - mc^2) \tag{4.1}$$

where b is the number mentioned above. We also carry in H the replacement of $\boldsymbol{r}', \boldsymbol{p}'$ by the dimensionless variables $\boldsymbol{r}, \boldsymbol{p}$ defined in (2.2). We thus obtain an equation for H that depends besides $\boldsymbol{r}, \boldsymbol{p}, \boldsymbol{\alpha}, \beta$ on the parameter

$$\epsilon \equiv (\hbar\omega/b)^{\frac{1}{2}}. \tag{4.2}$$

In equation (4.1) we replace then $\boldsymbol{\alpha}, \beta$ by their expressions as direct products of 2×2 matrices of ordinary and sign spin as indicated in (2.7). From this point on the analysis for determining the variational matrix elements follows the same steps as in section 2. We use as variational states the same kets as those defined in (2.13), (2.11), (2.9), and obtain the matrix elements.

$$\langle N'(l', \tfrac{1}{2})j, \tau' | H | N(l, \tfrac{1}{2})j, \tau \rangle \tag{4.3}$$

in which for the kinetic and rest energy matrix elements we have the same expression that appears in the first and last parts of (2.16). The middle of (2.16) corresponds to a matrix element of potential energy proportional to r^2, so it has to be replaced by

$$\begin{aligned}\langle N'l' \| V(r) \| Nl \rangle \delta_{l'l} \delta_{\tau'\tau} &= \left[\int_0^\infty R_{N'l}(r) V(r) R_{Nl}(r) r^2 \, \mathrm{d}r \right] \delta_{l'l} \delta_{\tau'\tau} \\ &= \sum_p \left[B\left(\frac{N-l}{2} l, \frac{N'-l}{2} l, p \right) I_p \right] \delta_{l'l} \delta_{\tau'\tau}\end{aligned} \tag{4.4}$$

where $R_{Nl}(r)$ are the radial functions of the three-dimensional oscillator of frequency 1 given in (1.8), (1.9) of [4], where we have to replace n by $[(N-l)/2]$ as indicated in (2.10).

On the right-hand side of (4.4) we have the coefficients B given by the algebraic expression (2.6) of [4], where again we use relation (2.10), and these coefficients have been tabulated numerically in [12].

The I_p is the Talmi integral defined by [12]

$$I_p = \frac{2}{\Gamma(p + \frac{3}{2})} \int_0^\infty r^{2p+2} V(r) \mathrm{e}^{-r^2} \, \mathrm{d}r \tag{4.5}$$

and in many cases it is very easy to evaluate. For example, we have for

$$V(r) = r^\lambda \qquad I_p = [\Gamma(p + \tfrac{1}{2}\lambda + \tfrac{3}{2}) / \Gamma(p + \tfrac{3}{2})] \tag{4.6}$$

$$V(r) = \mathrm{e}^{-u^2 r^2} \qquad I_p = (1 + u^2)^{-p - \frac{3}{2}} \tag{4.7}$$

as seen in [4, p 4].

Thus we are in a position to obtain explicit expressions for $\langle N'l' \| V(r) \| Nl \rangle$ so that the matrix elements (4.3) are completely defined as functions of ϵ.

Again, as in section 2, we have to take a set of states $|N(l, \frac{1}{2})j; \tau\rangle$ with fixed j connected by the Hamiltonian and we consider these states from $N = 0$ to a maximum value $N = \mathfrak{N}$. We then diagonalize the resulting matrix for series of values of ϵ to get the energy $E(\epsilon)$, and trace curves such as those appearing in figures 1–3. We can then determine the ϵ for the minima of the lowest curve, and with this value of ϵ get variational energy spectra for the potential in question.

Thus, we have outlined a general procedure for getting the variational energy spectra of an arbitrary relativistic Hamiltonian.

5. Conclusion

What is the most important point of the procedure we have outlined in this article? The answer [5] is the writing of $\boldsymbol{\alpha}, \beta$ as direct products of (2×2) matrices associated with ordinary and sign spin. This allows us to use as variational functions those of (2.13) that are identical to those employed in nuclear physics when isotopic spin is present instead of

the cumbersome procedure of Dirac functions that have two components associated with positive and negative energies.

Once the previous paragraph is understood, it opens many possible generalizations of the procedure that we have developed in this paper. For example, instead of the radial part of harmonic oscillator states we could use any other complete set of orthonormal functions, among which the Sturmian–Coulomb radial functions given in equation (41.17) of [4], seem particularly appropriate for the variational discussions of the relativistic Coulomb problem, as their exponential part goes as $e^{-\lambda r}$, instead of $e^{-\Lambda r^2}$ for the harmonic oscillator states.

One can also extend our analysis to relativistic Hamiltonians of arbitrary spin, using the technique outlined in [5, 11] for determining the corresponding wave equations. The variational procedure will be very similar but with the complication that we will need the reduce matrix elements of the generators of a U(4) group, with respect to states belonging to irreps of the chain $U(4) \supset \hat{U}(2) \otimes \check{U}(2)$. Finally we may also use the concept of sign spin to analyse, by a very different method, the important problem of relativistic many-electron atoms.

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