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1987 J. Phys. A: Math. Gen. 20 2773

(http://iopscience.iop.org/0305-4470/20/10/021)

J. Phys. A: Math. Gen. **20** (1987) 2773-2780. Printed in the UK

External field Dirac equation with separable potential

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Received 2 June 1986

Abstract. The general form of the rotation, space reflection, time reversal and charge conjugation invariant separable potential for the Dirac equation is investigated. A concrete potential is constructed which reproduces the $1s_{1/2}$ and $2p_{1/2}$ eigenvalues of the cut-off Coulomb potential.

1. Introduction

The separable potentials have served as very useful tools in facilitating the solution of various dynamical problems in non-relativistic quantum mechanics. It might be useful to consider their application for studying certain questions in relativistic quantum mechanics as well, e.g. in the so-called external field problems their use can lead to important calculational simplifications. Sucher (1985) used a separable potential for investigation of the continuum dissolution problem. A closely related problem, namely the pair creation in a time-dependent electromagnetic field, was studied using separable potentials (Hraskó *et al* 1986).

The two-centre Dirac problem, concerning a Dirac particle moving in the field of two potentials, is another example where the use of separable potentials leads to considerable simplifications in the solution of the dynamical equations. In fact, for local potentials this problem involves solution of partial differential equations without separation of variables. The potentials obtained in the present work will be used for a two-centre study in a following paper (Tóth *et al* 1987).

In this paper we want to construct a simple separable interaction which reproduces one of the most interesting qualitative features of a static Coulomb field in the Dirac equation: with increasing potential strength the energy of the $1s_{1/2}$ ground state becomes smaller than $-mc^2$, i.e. it disappears in the lower continuum. This fact plays an important role in the instability of the QED vacuum in strong electromagnetic fields (e.g. Rafelski *et al* 1978).

In § 3 we construct the general separable potential which is invariant under rotation, space reflection, time reversal and charge conjugation. In § 4 using the partial wave expansion we derive the energy eigenvalue equation and the normalised wavefunctions. In § 5 we investigate the behaviour of these eigenfunctions at the origin and at infinity. For a concrete construction we turn to the cut-off Coulomb potential, whose eigenvalue problem was solved by Pieper and Greiner (1969). Using their binding energies and wavefunctions we construct a separable potential which reproduces the $1s_{1/2}$ and $2p_{1/2}$ energy eigenvalues for $80 \leqslant Z \leqslant 170$.

0305-4470/87/102773+08$02.50

2. Notation

We use units in which $\hbar = c = 1$. The Dirac equation in coordinate representation is

$$i\frac{\partial\psi(t,\boldsymbol{r})}{\partial t} = (H_0 + V)\psi(t,\boldsymbol{r}) = (\alpha\boldsymbol{p} + \beta m + V(t,\boldsymbol{r}))\psi(t,\boldsymbol{r}) \tag{1}$$

where

$$p_i = -i\frac{\partial}{\partial x_i} \qquad \alpha_i = \begin{pmatrix} & \sigma_i \\ \sigma_i & \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathbb{1} & \\ & -\mathbb{1} \end{pmatrix}$$

the σ_i are the Pauli matrices and $\mathbb{1}$ is the 2×2 unit matrix.

We will use the common eigenvectors of the following commuting operators: the square of the momentum, the square and third component of the total angular momentum, space reflection and β.

By definition

$$\begin{aligned}
&\hat{\boldsymbol{p}}^2|pjlmQ\rangle = p^2|pjlmQ\rangle && p \geqslant 0\\
&\hat{\boldsymbol{J}}^2|pjlmQ\rangle = j(j+1)|pjlmQ\rangle && j = \tfrac{1}{2}, \tfrac{3}{2}, \ldots\\
&\hat{J}_3|pjlmQ\rangle = m|pjlmQ\rangle && m = -j, -j+1, \ldots, j\\
&\hat{P}|pjlmQ\rangle = (-1)^l|pjlmQ\rangle && l = j \pm \tfrac{1}{2}\\
&\beta|pjlmQ\rangle = Q|pjlmQ\rangle && Q = \pm 1.
\end{aligned} \tag{2}$$

(In the non-relativistic theory β is absent and the *pjlm* quantum numbers define these common eigenvectors unambiguously. In the relativistic case there are two linearly independent vectors with these quantum numbers. We can distinguish these two vectors by another quantum number which can be, for example, the sign of the energy or it can be the eigenvalue of the β operator.)

In momentum representation

$$\langle \boldsymbol{p}', \alpha|pjlmQ\rangle = \frac{1}{p^2}\delta(p-p')\begin{pmatrix} \delta_{Q1}[Y_l(\hat{\boldsymbol{p}}')\chi_{1/2}]_{jm} \\ \delta_{Q-1}[Y_{l'}(\hat{\boldsymbol{p}}')\chi_{1/2}]_{jm} \end{pmatrix}_\alpha \tag{3}$$

where α is the spinor index ($\alpha = 1, 2, 3, 4$), $\hat{\boldsymbol{p}} = \boldsymbol{p}/|p_-|$ and $l' = 2j - l$.

Using the completeness and orthonormality relations for the $|\boldsymbol{p}, \alpha\rangle$ we can derive analogous relations for the $|pjlmQ\rangle$:

$$\begin{aligned}
&\langle pjlmQ|p'j'l'm'Q'\rangle = \frac{1}{p^2}\delta(p-p')\delta_{jj'}\,\delta_{ll'}\delta_{mm'}\delta_{QQ'}\\
&\sum_{jlmQ}\int_0^\infty \mathrm{d}p\, p^2|pjlmQ\rangle\langle pjlmQ| = \hat{1}.
\end{aligned} \tag{4}$$

3. Symmetries

The general form of a separable potential is

$$\hat{V}_{\mathrm{sep}} = \sum_{k,l=1}^{N} |k\rangle\lambda_{kl}\langle l| \tag{5}$$

where λ_{kl} are real constants and the $|k\rangle$ are arbitrary vectors normalised to unity. This freedom can be reduced by requiring that the general properties of V_{sep} and V, the exact potential, be the same. One of the basic properties of a potential is its symmetry: this symmetry assures the conservation of different quantum numbers during physical processes. V_{sep} will conserve these quantum numbers, too, if it is diagonal in them. The cut-off Coulomb potential is invariant under rotation, space reflection and time reversal, so the most general possible separable potential is

$$\hat{V}_{\text{sep}} = \sum_{j=1/2}^{j_{\max}} \sum_{l=j\pm 1/2} \sum_{m=-j}^{j} \sum_{i,i'=1}^{N} \sum_{Q,Q'=\pm 1} |ijlmQ\rangle \lambda_{ii'jlQQ'} \langle i'jlmQ'| \tag{6}$$

where

$$|ijlmQ\rangle = \int_0^\infty \mathrm{d}p\, p g_{ijlQ}(p) |pjlmQ\rangle.$$

This vector is normalised to unity if the $g_{ijlQ}(p)$ form factors satisfy

$$\int_0^\infty \mathrm{d}p |g_{ijlQ}(p)|^2 = 1. \tag{7}$$

In momentum representation

$$\langle \boldsymbol{p}, \alpha | ijlmQ\rangle = \begin{pmatrix} \dfrac{g_{ijlQ}(p)}{p} \delta_{Q1} [Y_l(\hat{\boldsymbol{p}}) \chi_{1/2}]_{jm} \\ \dfrac{g_{ijlQ}(p)}{p} \delta_{Q-1} [Y_{l'}(\hat{\boldsymbol{p}}) \chi_{1/2}]_{jm} \end{pmatrix}_\alpha . \tag{8}$$

By a unitary transformation this potential can be diagonalised in the i and a quantum numbers, too:

$$\hat{V}_{\text{sep}} = \sum_{j=1/2}^{j_{\max}} \sum_{l=j\pm 1/2} \sum_{m=-j}^{j} \sum_{i=1}^{N} \sum_{Q=\pm 1} |ijlmQ\rangle \lambda_{ijlQ} \langle ijlmQ|. \tag{9}$$

Time reversal invariance imposes another constraint on the form factors: V_{sep} commutes with $\hat{T}$ only if

$$g^*_{ijlQ}(p) g_{ijlQ}(p') = g_{ijlQ}(p) g^*_{ijlQ}(p'). \tag{10}$$

This condition is fulfilled if the phase of g_{ijlQ} does not depend on p. This phase factor does not appear in the potential, so it can be chosen to be unity. This is why all the form factors are real functions of their argument.

In QED there is another exact symmetry: charge conjugation. For the Dirac equation with an external field it is no longer a symmetry. Nevertheless it has an effect on the form of the external field: V (and so V_{sep} too) must commute with $\hat{C}$, the charge conjugation operator. This requirement is satisfied if the potential strength and the form factors with the same i, j but different l and a are equal.

We conclude this section by the general form of the possible separable potential:

$$\begin{aligned} &\hat{V}_{\text{sep}} = \sum_{j=1/2}^{j_{\max}} \sum_{p=j\pm 1/2} \sum_{m=-j}^{j} \sum_{i=1}^{N} \sum_{q=\pm 1} |ijlmQ\rangle \lambda_{ijlQ} \langle ijlmQ| \\ &\lambda_{ijlQ} \equiv \lambda_{ijl'-Q'} \qquad g_{ijlQ}(p) \equiv g_{ijl'-Q'}(p). \end{aligned} \tag{11}$$

4. Solution of the eigenvalue problem

The Hamiltonian is invariant under rotation and space reflection, so we can use the partial wave expansion. The wavefunction in a given partial wave is

$$\langle \boldsymbol{p}, \alpha|\psi\rangle = \begin{pmatrix} \dfrac{g(p)}{p}[Y_l\chi]_{jm} \\ \dfrac{h(p)}{p}[Y_{l'}\chi]_{jm} \end{pmatrix}_\alpha . \tag{12}$$

From now on we omit the $1/p$ denominator and the angle-dependent fractions and denote this wavefunction by

$$\langle p|\psi\rangle = \begin{pmatrix} g(p) \\ h(p) \end{pmatrix}. \tag{13}$$

We restrict ourselves to a given partial wave and also omit these *jlm* indices.

The separable potential is diagonal as the original V:

$$\langle p_1|\hat{V}_{\text{sep}}|p_2\rangle = \sum_{i=1}^{N} \begin{pmatrix} \lambda_{i1} g_{i1}(p_1) g_{i1}(p_2) & 0 \\ 0 & \lambda_{i-1} g_{i-1}(p_1) g_{i-1}(p_2) \end{pmatrix}. \tag{14}$$

The energy eigenvalue equation is

$$\left(H_0 + \sum_{iQ} |iQ\rangle\lambda_{iQ}\langle iQ|\right)|\psi_B\rangle = E_B|\psi_B\rangle. \tag{15}$$

If $E_B \in [-m, +m]$ then the operator $E - H_0$ has a unique inverse, the free Green operator G_0. Using this operator we obtain

$$|\psi_B\rangle = \sum_{iQ} \lambda_{iQ} \hat{G}_0(E_B)|iQ\rangle\langle iQ|\psi_B\rangle. \tag{16}$$

Multiplying by the $|i'Q'\rangle$ we obtain an algebraic equation for the $\langle iQ|\psi_B\rangle$ which can be solved unambiguously only if its determinant is zero:

$$\det(\delta_{ii'}\delta_{QQ'} - \lambda_{iQ}\langle i'Q'|\hat{G}_0(E_B)|iQ\rangle) = 0. \tag{17}$$

This—generally transcendent—equation determines the energy eigenvalues. The normalised eigenfunction is

$$\begin{aligned} |\psi_B\rangle &= N\sum_{iQ} \hat{G}_0(E_B)|iQ\rangle \\ N &= \left(\sum_{i,i'}\sum_{Q,Q'} \langle iQ|\hat{G}_0^2(E_B)|i'Q'\rangle\right)^{-1/2}. \end{aligned} \tag{18}$$

In momentum representation

$$\begin{aligned} \langle p_1|\hat{G}_0(E)|p_2\rangle &= \frac{\delta(p_1 - p_2)}{E^2 - m^2 - p_1^2}\begin{pmatrix} E+m & -p_1 \\ -p_1 & E-m \end{pmatrix} \\ \langle p|\psi_B\rangle &= \frac{N}{E^2 - m^2 - p^2}\begin{pmatrix} E+m & -p \\ -p & E-m \end{pmatrix}\begin{pmatrix} \sum_i g_{i1}(p) \\ \sum_i g_{i-1}(p) \end{pmatrix}. \end{aligned} \tag{19}$$

5. Constraints imposed by the exact wavefunction

We require that the wavefunction obtained with the separable potential behave as the exact one at the origin and at infinity.

The exact eigenfunction is given in coordinate representation. The transformation between the two representations is

$$g(p)=\left(\frac{2}{\pi}\right)^{1/2} p\int_0^\infty \mathrm{d}r\, r j_l(pr)u(r)$$
$$h(p)=\left(\frac{2}{\pi}\right)^{1/2} p\int_0^\infty \mathrm{d}r\, r j_{l'}(pr)v(r) \tag{20}$$

if

$$\langle p|\psi\rangle=\begin{pmatrix} g(p)\\ h(p)\end{pmatrix} \qquad \text{and} \qquad \langle r|\psi\rangle=\begin{pmatrix} u(r)\\ v(r)\end{pmatrix}.$$

The exact wavefunction for $r\to 0$ behaves as

$$\langle r|\psi_B\rangle=\begin{pmatrix} u(r)\\ v(r)\end{pmatrix}\sim\begin{pmatrix} r^{l+1}\\ r^{l'+1}\end{pmatrix}. \tag{21}$$

Via the above transformation this behaviour limits the possible behaviour of the form factors at infinity:

$$\langle p|\psi_B\rangle=\begin{pmatrix} g(p)\\ h(p)\end{pmatrix}\sim\begin{pmatrix} p^{-a}\\ p^{-b}\end{pmatrix} \qquad \begin{matrix} a\geqslant l+2\\ b\geqslant l'+2\end{matrix} \qquad \text{for } p\to\infty. \tag{22}$$

The exact eigenfunction decreases exponentially at the infinity. The transformation for this case gives

$$\langle p|\psi_B\rangle=\begin{pmatrix} g(p)\\ h(p)\end{pmatrix}\sim\begin{pmatrix} p^{l+1}\\ p^{l'+1}\end{pmatrix} \qquad \text{for } p\to 0. \tag{23}$$

6. Numerical results

In this section we construct a separable potential which reproduces the $1s_{1/2}$ and $2p_{1/2}$ eigenvalues of the cut-off Coulomb potential

$$V=\begin{cases} \dfrac{Ze^2}{R_0}\left(-\dfrac{3}{2}+\dfrac{1}{2}\left(\dfrac{r}{R_0}\right)^2\right) & r\leqslant R_0\\ -\dfrac{Ze^2}{r} & r\geqslant R_0\end{cases} \tag{24}$$

$$R_0=1.2\text{ fm }A^{1/3} \qquad A=0.007\,33Z^2+1.30Z+63.6.$$

The jl quantum numbers are therefore $\frac{1}{2}, 0$ and $\frac{1}{2}, 1$, respectively. The exact potential is diagonal and all the diagonal elements are non-zero. This means that we must take both the $a=1$ and the $a=-1$ values of a. We choose the simplest case where $i=1$.

A possible choice of the normalised form factors which satisfy the constraints investigated in the preceding section is

$$g_{+1}(p)=\left(\frac{32}{\pi}\right)^{1/2}\mu_1^{5/2}\frac{p}{(p^2+\mu_1^2)^2}$$
$$g_{-1}(p)=\left(\frac{32}{\pi}\right)^{1/2}\mu_2^{3/2}\frac{p^2}{(p^2+\mu_2^2)^2}. \tag{25}$$

The μ_1 and μ_2 parameters will be determined later.

With these form factors both the G_0 matrix elements and the coordinate representation wavefunction can be calculated analytically. The energy eigenvalue equations are

$$\text{for } 1s_{1/2} \qquad \det\begin{vmatrix} G^s_{0_{+1,+1}}-1/\lambda_{+1} & G^s_{0_{+1,-1}} \\ G^s_{0_{-1,+1}} & G^s_{0_{-1,-1}}-1/\lambda_{-1}\end{vmatrix}=0$$
$$\text{for } 2p_{1/2} \qquad \det\begin{vmatrix} G^p_{0_{+1,+1}}-1/\lambda_{-1} & G^p_{0_{+1,-1}} \\ G^p_{0_{+1,-1}} & G^p_{0_{-1,-1}}-1/\lambda_{+1}\end{vmatrix}=0. \tag{26}$$

The G_0 matrix elements in the two partial waves—due to charge conjugation—are not independent of each other:

$$G^p_{0_{+1,+1}}(E)=-G^s_{0_{-1,-1}}(-E)$$
$$G^p_{0_{-1,-1}}(E)=-G^s_{0_{+1,+1}}(-E) \tag{27}$$
$$G^p_{0_{-1,+1}}(E)=G^p_{0_{+1,-1}}(E)=G^s_{0_{+1,-1}}(E)=G^s_{0_{-1,+1}}(E).$$

The μ_1 and μ_2 parameters can be varied freely because for each μ_1 and μ_2 such λ_{+1} and λ_{-1} exist that the energy eigenvalues are equal to the exact ones. We can choose them for example by requiring that

$$\| |\psi_{\text{exact}}\rangle - |\psi_{\text{sep}}\rangle \|$$

be minimal as a function of μ_1 and μ_2. However, this norm is a very flat function of the parameters, so instead of a definite value we get intervals for μ_1 and μ_2 from which we can choose freely.

It would be desirable to give $\mu_1(Z)$, $\mu_2(Z)$, $\lambda_{+1}(Z)$, $\lambda_{-1}(Z)$ functions which give the correct value for every Z. Unfortunately, the $2p_{1/2}$ energies for $Z \leq 40$ are in the

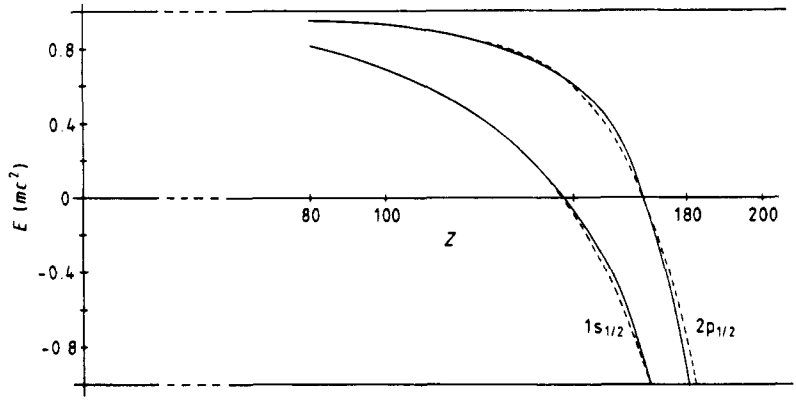

Figure 1. Comparison of the exact (full curve) and separable potential (broken curve) $1s_{1/2}$ and $2p_{1/2}$ energy eigenvalues for $80 \leq Z \leq 180$.

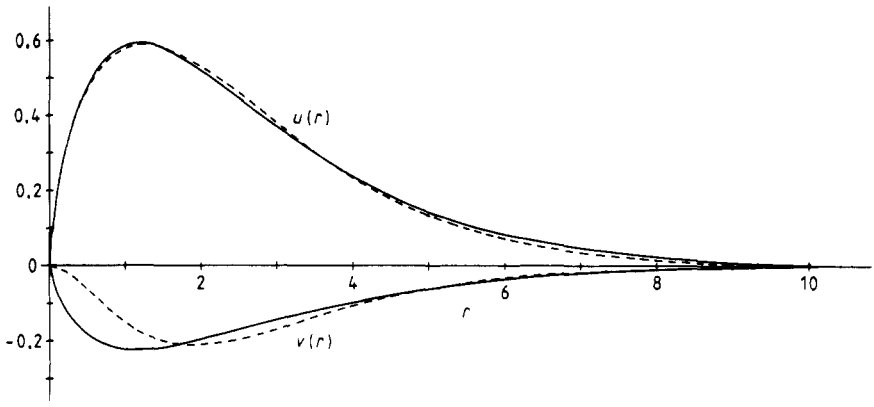

Figure 2. Comparison of the exact (full curve) and separable potential (broken curve) $1s_{1/2}$ wavefunctions for $Z=90$. $u(r)$ is the upper, $v(r)$ is the lower component. (r is measured in Compton wavelength units).

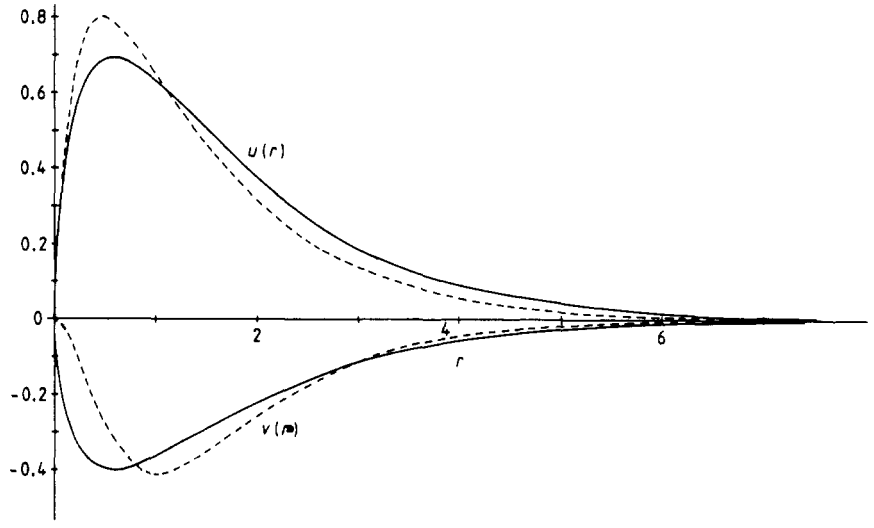

Figure 3. As figure 2 for $Z=120$.

$0.99 \leqslant E_B \leqslant 1.0$ interval and to give back these values the above functions must have a relative error of 10^{-3} which cannot be achieved by simple functions. However, in the $80 \leqslant Z \leqslant 170$ region greater relative error is allowed and we succeed with the functions

$$\begin{aligned}
&\mu_1(Z) = 5.28\times 10^{-4}Z^2 - 0.0625Z + 2.70\\
&\mu_2(Z) = 3.33\times 10^{-4}Z^2 - 0.040Z + 3.60\\
&\lambda_{+1}(Z) = 0.64 + 0.064Z + 7.76\times 10^{-4}Z^2 - 9.12(\mathrm{e}^{0.01Z} - 1)\\
&\lambda_{-1}(Z) = -2.80 + 0.013Z - 2.18\times 10^{-4}Z^2 - 8.17\times 10^{-9}\,\mathrm{e}^{0.113Z}.
\end{aligned} \tag{28}$$

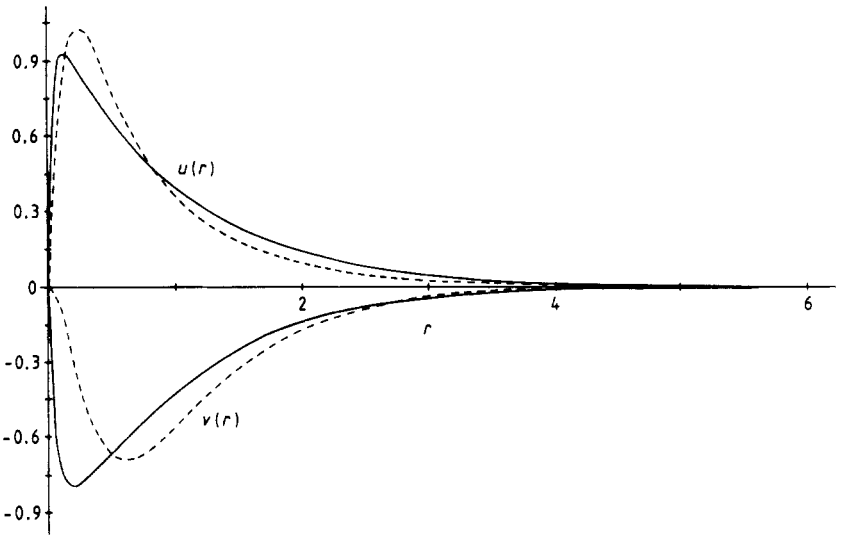

Figure 4. As figure 2 for $Z = 150$.

The presence of the exponential factors is due to the fact that for large Z the exact binding energies—which do not involve the electron's rest mass—increase very quickly which require the rapid increase in λ_{+1} and λ_{-1}.

Using these Z dependencies we can calculate the energy eigenvalues and the wavefunctions. The energies are compared to the exact ones in figure 1 and the $1s_{1/2}$ wavefunction for three different values of Z in figures 2-4.

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