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The $\psi(0)$ problem for charmonium Hamiltonians

J Killingbeck and S Galicia

Physics Department, University of Hull, Hull HU6 7RX, UK

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Abstract. The problem of calculating $\psi(0)$ for radial Hamiltonians is shown to be reducible to a sequence of energy calculations, which can be performed easily by using a pseudo-angular momentum term in a numerical integration approach. A first-principles approach to s-state hypervirial relations is shown to produce terms not given by the usual commutator approach.

1. Introduction

When matrix-variational methods are used to estimate the eigenvalues of the one-particle Schrödinger equation, it is well known that an error of order η^2 in the energy goes with an error of order η in the wavefunction. This means that the approximate wavefunctions obtained may give fair energy values and yet give poor estimates of expectation values such as $\langle r^N \rangle$. When a *local* quantity (e.g. the value of the wavefunction at some point) is required, it is even less likely that a good value can be obtained from a wavefunction which is obtained by a variational calculation of the energy. One such local quantity which is non-zero for s states is the square of the wavefunction at the origin. This quantity is required in various branches of traditional theory, for example in the theory of hyperfine interaction (Young and Uhlenbeck 1930) and in the theory of excitons (Cabib *et al* 1972). However, it has also played a role in recent non-relativistic models of the charmonium system (the bound quark–antiquark pair), since it is required when estimating the various decay rates of the charmonium system (Kaushal and Müller-Kirsten 1979).

One model Schrödinger equation which has been widely used (e.g. Eichten *et al* 1975, McCartor 1978) to describe charmonium is of the form

$$-\alpha \nabla^2 \psi - \frac{\beta}{r} \psi + \mu r^M \psi = E \psi \quad (1)$$

with $M \geq 1$. The r^M term represents a confining potential which prevents direct break-up of the system, while the coefficient β gives the size of the ‘gluon’ force, which is usually taken to be weak. The coefficient α depends, of course, on the quark mass, and the mass dependence of the eigenfunctions for simple cases has been discussed by Leung and Rosner (1979). The three-parameter problem (1) can be transformed to a one-parameter perturbed hydrogen atom problem if we introduce the change $r \rightarrow Kr$ of the length scale. If we choose the length scale appropriately we find the scaling relationship which indicates how the eigenvalues depend on α , β and μ :

$$E(\frac{1}{2}, 1, \lambda) = K^2 E(\alpha, \beta, \mu) \quad (2)$$

with

$$K = (2\alpha/\beta) \quad \text{and} \quad \lambda = \mu K^{M+2}.$$

If we make the traditional choice and write the radial function as a product $r^{-1}R(r)$, then the relation (2) shows that it is sufficient for us to study the equation

$$-\frac{1}{2}D^2R + VR = ER \quad (3)$$

with

$$V = -r^{-1} + \lambda r^M + \frac{1}{2} \frac{l(l+1)}{r^2} \quad (4)$$

and the normalisation condition

$$\int_0^\infty R^2 dr = 1. \quad (5)$$

The centrifugal term in (4) will, of course, not appear for s states, which are the ones of interest in connection with the $\psi(0)$ problem. The function $R(r)$ will obey the boundary condition $R(0) = 0$ for the regular solutions which we require; this means that the quantity required is actually the slope $DR(0)$, since

$$DR = D(r\psi) = rD\psi + \psi. \quad (6)$$

The problem represented by equations (3) and (4) has been studied for the case $N = 1$ by various authors (Titchmarsh 1952, Killingbeck 1977, Graffi *et al* 1979) and the case $N = 2$ is associated with the theory of the quadratic Zeeman effect (Killingbeck 1979a). In the present work we outline a complete procedure for the numerical treatment of the problem. This procedure yields eigenvalues, expectation values of type $\langle r^N \rangle$, and also $\psi^2(0)$ values which are apparently better than those found by previous methods.

The original contributions contained in this work may be outlined as follows. In § 2 a generalisation of Trivedi's (1980) equation is given, and this leads to a family of inner product formulae analogous to the better known hypervirial formulae. In § 3 a method of deriving hypervirial relations is devised to obtain s-state terms which are omitted by the usual commutator approach: the relations are used in a computation of perturbation series without using wavefunctions. In § 4 a procedure is given which enables $\psi^2(0)$, $\langle r \rangle$, $\langle r^2 \rangle$, etc, to be found using *eigenvalue* calculations only. Section 5 points out a remaining problem which may be amenable to a similar approach.

2. Direct and indirect methods for $\psi(0)$

In their recent work on the $\psi(0)$ problem, Kaushal and Müller-Kirsten (1979) assert that $\psi(0)$ can only be found if the wavefunction is explicitly normalised. They give a lengthy calculation of WKB type for the wavefunction in various regions of space, and the resulting $\psi(0)$ estimate appears to be of low accuracy. As far as we can see, this direct approach is not very efficient, and it is better to do a little mathematical manipulation to convert the $\psi(0)$ problem into another form. Thus, if we take the Schrödinger equation

$$-\frac{1}{2}D^2R + VR = ER, \quad (7)$$

multiply it throughout by a function $F(r)$ and integrate between 0 and ∞ , we quickly obtain the following result (if $FDR = 0$ at ∞ and $RDF = 0$ at 0 and ∞):

$$F(0)DR(0) = \int_0^{\infty} [D^2F + 2F(E - V)]R \, dr. \quad (8)$$

If we take the special case $F = 1$ in (8) we obtain an equation equivalent to that of Trivedi (1980). Trivedi suggested that if an *approximate* normalised R is used in the integral, and if E is replaced by the variational energy associated with R , then a reasonable estimate of $DR(0)$ for the *exact* eigenfunction can be obtained. For example, for the hydrogen atom ground state, use of an energy-optimised Gaussian-type trial function in (8) (with $F = 1$) gives $DR(0) = 1.796$, as opposed to the exact value 2 and the poor value 0.980 obtained by simply substituting $r = 0$ in the approximate function. Equation (8) shows that for the exact R the *same* $DR(0)$ should result for many different choices of F , provided that $F(0)$ is non-zero. It may be that by using various F 's some estimate of the accuracy of the $DR(0)$ value obtained from an approximate R can be obtained. Since we prefer another approach we do not pursue this point here. We also note that if we make the choice $F(r) = 1 + kf(r)$ (with $f(0) = 0$) we must demand that the resulting $DR(0)$ value has *no* k dependence if R is the exact eigenfunction. This leads to the inner product relation

$$\langle D^2f | R \rangle + 2\langle f | (E - V)R \rangle = 0, \quad (9)$$

which is somewhat similar in appearance to the hypervirial relation of § 3, but involves inner products rather than expectation values.

While the approach via equation (8) may lead to useful extensions of Trivedi's (1980) work, we stick more closely to an approach involving expectation values. The basic relation which we need has been given various derivations (usually involving Wronskians) in the literature (Fradkin and Calogero 1966, Fröman 1978a), but it can be obtained simply by multiplying (3) by DR and integrating between 0 and ∞ . The result is (after an integration by parts on the right-hand side)

$$(DR(0))^2 = 2 \int_0^{\infty} R^2(DV) \, dr \quad (10)$$

and it involves the expectation value of the quantity DV , i.e. $\partial V/\partial r$. Using (10) we can reduce the $\psi(0)$ problem to that of finding an expectation value. Fröman (1978b) used (10), but then used a WKB approach to estimate $\langle(DV)\rangle$. In our approach the chain of reasoning is as follows. Using (10) we reduce the problem to the $\langle(DV)\rangle$ problem; we then reduce the *expectation value* problem to a set of *eigenvalue* problems; we use a numerical integration method to solve the eigenvalue problems, and then construct the other desired quantities. For the s states of an unperturbed hydrogen atom, with $V = -r^{-1}$ in (3), the expectation value $\langle r^{-2} \rangle$ equals $2n^{-3}$, n being the principal quantum number of the state concerned. The energy eigenvalue equals $\frac{1}{2}n^{-2}$, so that we have the relationship

$$\psi^2(0) = 2\langle(DV)\rangle = 4 \, dE/dn. \quad (11)$$

Even in the case of perturbed Coulomb potentials, (11) is often used to give an estimate of $\psi(0)$, and is called the Fermi-Segré formula (Fröman and Fröman 1972); we mention it because (like our calculation) it relates $\psi^2(0)$ to entities arising from an energy calculation. However, it has two drawbacks: it involves the estimation of the derivative

of a (hypothetical) smooth function $E(n)$, whereas the actual eigenvalues form a discrete sequence; also, it is not exact if the perturbation is strong. Both these causes of uncertainty render (11) unsuitable for accurate work in theoretical calculations, but (11) allows rough estimates of $\psi^2(0)$ to be obtained from empirically assigned energies.

3. The use of hypervirial relations

The usual way to derive hypervirial relations is to use commutator algebra, starting from the idea that a commutator of form $[H, X]$ has zero expectation value for the exact eigenstates of the Hamiltonian H . The particular family of operators $X_N = r^N D$ then gives equations which relate together the numerical values of the expectation values $\langle r^N \rangle$. However, s states have a non-zero value for $\psi(0)$, and the simple Dirac operator algebra often assumes that operands have zero value or slope at the boundaries of the region of space over which any inner products are formed. To be quite sure that we allow for this, we have adopted a 'first-principles' approach which is very simple indeed; we just work out the integral representing the expectation value of the third derivative of a function $f(r)$:

$$\langle (D^3 f) \rangle = \int_0^\infty R^2 (D^3 f) dr. \quad (12)$$

We repeatedly integrate (12) by parts, and every time $D^2 R$ appears we replace it by $2(V - E)R$, from equation (3). A lengthy but straightforward calculation yields the result

$$8\langle (Df)(E - V) \rangle = 4\langle f(DV) \rangle - \langle (D^3 f) \rangle - 2f(0)(DR(0))^2, \quad (13)$$

which is the usual diagonal hypervirial relation in a simple form, including an s -state boundary term which does not appear in the commutator approach. The boundary terms arising from the integration are actually four in number and involve products of R and DR . However, the only term which survives when we require that $R(0) = 0$ is the one shown in (13), provided, of course, that $f(DR)^2$ vanishes at infinity. The particular choice $f = 1$ leads to equation (10) again, so that our approach unifies the derivation of (10) with that of the usual hypervirial relations, which follow if we set $f = r^N$ in (13). For the problem described by equations (3) and (4) the choice $f = r^{N+1}$ gives the result

$$8(N+1)E\langle r^N \rangle + 4(2N+1)\langle r^{N-1} \rangle + N(N^2-1)\langle r^{N-2} \rangle = 4\lambda(M+2N+2)\langle r^{M+N} \rangle. \quad (14)$$

This result enables us to calculate the various $\langle r^N \rangle$ values for higher N from just a few basic $\langle r^N \rangle$ values for low N . This cuts down considerably the amount of numerical work required; for example, for the case $M = 1$ (i.e. the potential $-r^{-1} + \lambda r$) we only need to calculate E and $\langle r \rangle$ in detail before using (14) to get the values of $\langle r^{-1} \rangle$, $\langle r^3 \rangle$, $\langle r^4 \rangle$, etc. For general integer M the basic quantities required are E and the $\langle r^N \rangle$ up to $\langle r^K \rangle$ where $K = M$. For the pure linear potential, $V = r$, all the $\langle r^N \rangle$ for positive integer N follow if E is known. Equation (14) will always allow *some* expectation values to be found to order η^2 when E is known to order η^2 .

If we postulate that the energy E and the expectation values $\langle r \rangle$, $\langle r^2 \rangle$, etc, are given by power series in λ , then (14) enables us to calculate these series directly, with no wavefunctions being involved in the calculation. The details of this calculation were described by Killingbeck (1978), who calculated the energy coefficients up to E_5 by hand for the case $M = 1$. It is possible to devise a program for the CBM Pet

minicomputer which calculates the perturbation series up to high order, for specified M and for any s state. A second program then applies the algorithm of Wynn (1956) to evaluate Padé approximants to the perturbation series (for some specified λ). Tables 1–3 show some typical results for this calculation. The $[N/N]$ and $[N/N-1]$ approximants are found to straddle the accurate energy, but only for small λ values is the calculation of high accuracy. We suspect that for large M the same effect may occur as for the perturbed oscillator (Graffi and Grecchi 1978), i.e. the $[N/N]$ and $[N/N-1]$ Padé approximant sequences may not converge to the same limit. Richardson and Blankenbecler (1979) have used hypervirial relations in a recursive numerical calculation of E and the $\langle x^N \rangle$ for the *one-dimensional* Hamiltonian $-D^2 + x^4$. From their

Table 1. 1s-state energy perturbation coefficients ($V = r^{-1} + \lambda r^M$).

M	1	2
E_0	-0.5	-0.5
E_1	1.5	3.0
E_2	-1.5	-32.25
E_3	6.75	1362.75
E_4	-49.687 5	-1.032 808 593E05
E_5	480.375	1.147 795 79E07
E_6	-5583	-1.719 187 61E09
E_7	7.455 733 59E04	3.319 536 10E11
E_8	-1.114 319 34E06	-8.035 022 9E13
E_9	1.832 917 15E07	2.388 909 28E16
E_{10}	-3.280 515 88E08	-8.580 782 6E18

Table 2. 2s-state energy perturbation coefficients ($V = -r^{-1} + \lambda r^M$).

M	1	2
E_0	-0.125	-0.125
E_1	6.0	42.0
E_2	-66.0	-14784
E_3	3312	1.992 345 6E07
E_4	-2.716 8E05	-4.5315 056 6E10
E_5	2.884 838 4E07	1.4142 186 7E14
E_6	-3.618 442 75E09	-5.5758 199 8E17
E_7	5.124 051 03E11	2.6668 570 6E21
E_8	-7.983 581 74E13	-1.5129 857 6E25
E_9	1.346 704 14E16	1.0042 786 3E29
E_{10}	-2.433 179 59E18	-7.7264 405 2E32

Table 3. Padé approximants for $V = -r^{-1} + \lambda r^M$.

M	State	λ	$[5/4]$	$[5/5]$
1	1s	0.10	-0.360 899 563	-0.360 900 277
1	2s	0.01	-0.069 671 275	-0.069 671 614
2	1s	0.01	-0.472 392 041	-0.472 393 160
2	2s	0.000 3	-0.113 392 947	-0.113 393 085

data we can extract the radial equation results $E = 2.39364401$, $\langle r \rangle = 0.78667270$, $\langle r^2 \rangle = 0.71560508$, for the $V = r^4$ ground state. Whether their method will work for the Hamiltonian (4), and give $\langle r^N \rangle$ for $N < 0$, remains to be established. For large λ we shall adopt a numerical integration approach.

For non-s states the use of $f = 1$ in (14), with the centrifugal term of (4) added to the 'raw' potential V , gives the result

$$\langle l(l+1)r^{-3} \rangle = \langle (DV) \rangle. \quad (15)$$

Fradkin and Calogero (1966) have already pointed out that (15) is a quantal analogue of the classical balance between the radial force and the centrifugal force. We wish to make a further point: if we find that the minimum in the total potential of equation (4) is at $r = r_0$ (which is the usual Bohr orbit radius), and then suppose that R is concentrated around r_0 , then we obtain (15) as an approximate equality. However, (15) is *exact*; even though it is only a necessary (not a sufficient) condition, it does suggest that the 'Bohr-type' approximation outlined above is probably reasonable. The work of Kaushal and Müller-Kirsten (1979) appears to start from such an approximation, although it involves a change of variable to ensure that even the s-state problem leads to an effective potential which has a strong minimum. In this connection we may also note that for a classical one-dimensional periodic motion with associated potential energy function V , the following result involving *time averages* can be derived:

$$2\langle (Df)(E - V) \rangle_t = \langle f(DV) \rangle_t, \quad (16)$$

where $f(x)$ is an arbitrary smooth function. Equation (16) resembles the quantum-mechanical result (13) for non-s states, but has no (D^3f) term. The (D^3f) term is actually of order \hbar^2 (where \hbar is Planck's constant), as can be seen by noting that it arises from the kinetic energy operator term in (3) when the traditional commutator approach is used to derive (13).

4. Eigenvalue calculations

Equation (10) shows that the calculation of $\psi^2(0)$ is equivalent to an expectation value calculation. As we have explained elsewhere (Killingbeck 1979a), an expectation value such as $\langle r^N \rangle$ can be found numerically from a prescription involving energies:

$$\langle r^N \rangle = \lim_{\epsilon \rightarrow 0} \left(\frac{E(H + \epsilon r^N) - E(H - \epsilon r^N)}{2\epsilon} \right). \quad (17)$$

Provided that we can evaluate the eigenvalues for the perturbed Hamiltonians $H \pm \epsilon r^N$ accurately, equation (17) will allow us to estimate $\langle r^N \rangle$; this approach has been tested for perturbed oscillator problems (Killingbeck 1980) and works well. The calculation has an internal check in any case, since the stability of the predicted $\langle r^N \rangle$ as ϵ varies can be tested. To repeat the calculation for many N values would be tedious, but the comments in § 3 show that only a few $\langle r^N \rangle$ have to be calculated explicitly; the rest follow from the hypervirial relations.

The final step in the calculation, then, is the eigenvalue calculation. Any method which gives accurate results will do, but it turns out (as we shall see below) that the simple method of Killingbeck (1977) has features which make it particularly easy to apply to the $\psi(0)$ problem. If a matrix-variational approach is adopted, equation (17)

yields the same $\langle r^N \rangle$ values as would be found traditionally by directly evaluating $\langle r^N \rangle$ using the approximate eigenvectors. A calculation using numerical integration to find the eigenvalues in (17) usually gives better $\langle r^N \rangle$ values. The method used by Killingbeck (1977), for the problem described by equations (3) and (4), involves the substitution $R(r) = r^{l+1}\phi(r)$. We use this substitution here, but modify the method by introducing a function F , which resembles a logarithmic derivative, and is defined by the equation

$$\phi(r+h) = (1+h^2F(r))\phi(r). \quad (18)$$

h in (18) is the strip width to be used in the numerical integration. Proceeding then to replace D^2 in (18) by its lowest-order finite difference approximation (Killingbeck 1977), we obtain the following equation after a little manipulation:

$$(r+kh)F(r) + \frac{(r-kh)F(r-h)}{1+h^2F(r-h)} = 2r(V(r)-E). \quad (19)$$

In (19), $k = l+1$ and $V(r)$ is the 'raw' potential with *no centrifugal term*. The l value is completely taken care of by the terms on the left of (19). This feature is particularly useful for the $\psi^2(0)$ calculation, since for our charmonium problem we have

$$\epsilon(DV) = \epsilon r^{-2} + \epsilon \lambda M r^{M-1}. \quad (20)$$

The first term on the right of (20) is the derivative of the Coulomb potential, but resembles a centrifugal term for which $\epsilon = \frac{1}{2}l(l+1)$, so that $l \rightarrow 2\epsilon$ as $\epsilon \rightarrow 0$.

To find $\langle(DV)\rangle$ using (17), for an s state, we use the value $k = 2\epsilon + 1$ in (19) (i.e. use a 'pseudo-angular momentum' $l = 2\epsilon$). This takes care of the r^{-2} term in (20). The second term can be added explicitly to V or we can use an 'advanced potential' term, so that the potential becomes

$$V = -r^{-1} + \lambda(r+\epsilon)^M. \quad (21)$$

By using the pseudo-angular momentum and the advanced potential devices together, we can render the calculation particularly simple for a computer, since a program can be written to make the adjustments automatically when ϵ is given as part of the input data. Using two values $\pm\epsilon$ we can estimate $\langle(DV)\rangle$ from the prescription (17).

It should be clear from the above discussion that the method will work for any smooth potential $V(r)$, not just the one of equation (4). The equation (19) has the interesting feature that if we start the integration from $r = kh$ we can specify $F(kh-h)$ arbitrarily; the calculation automatically forces $F(kh+h)$, $F(kh+2h)$, etc, to take definite values. However, these values will depend on the E value which we use on the right of (19). The CBM Pet minicomputer program which we have devised uses three trial E values simultaneously (setting $\phi(kh) = 1$); at large r values it interpolates to find the E value which would have made the wavefunction tend to zero (i.e. which would have given a bound-state function). These ideas have been explained in previous works (Killingbeck 1977, 1979b). The E value obtained using (19) in this way is *not* the required Schrödinger equation eigenvalue, since it is arrived at by using a difference equation involving a finite strip width h . The eigenvalue associated with strip width h is related to the true eigenvalue by a perturbation-type expansion:

$$E(h) = E + Ah^2 + Bh^4 + \dots \quad (22)$$

To get E we do the calculation using several different strip widths, and extrapolate, rather in the manner of Romberg integration. For the potential of equation (4), for

example, we get ground-state eigenvalues accurate to about 1 part in 10^9 by using the values $h = H, 2H, 3H, 4H$ (with $H = 0.025$) and the extrapolation formula

$$E = \frac{1}{35}(56E_1 - 28E_2 + 8E_3 - E_4). \quad (23)$$

For the case of potentials without a Coulombic term (e.g. simple r^M potentials) the method could be improved to suppress the Ah^2 error term in (22), by using the Numerov method or the more simple method of Killingbeck (1979b).

The methods outlined above work just as easily for excited states (of any l value) as they do for the ground state. The orthogonality of different eigenstates, which causes problems in variational approaches, does not play a role. The node number (Z) is the quantity specified and this serves to pick out any required excited state; the numerical integration based on (19) is simply repeated until two trial E values lead to functions with Z and $Z - 1$ nodes, respectively. The required eigenvalue $E(h)$ for that state must then be straddled by the two trial values. These details are handled automatically by the program, and have also been discussed previously (Killingbeck 1979b, 1980). Killingbeck (1980) also indicates briefly how a variational calculation could be set up using the basis states $r^N \psi_0$, where ψ_0 is the ground-state eigenfunction; for potentials of type r^M such a calculation should be quite effective (since it gives exact results for $M = 2$).

5. Some test calculations

Since in the charmonium problem it is usual to take the 'gluon' coefficient to be small, our results are most likely to be useful if we take the 'zero gluon' limit, i.e. use a potential λr^M in (4). With this restriction we can do the calculations for $\lambda = 1$ and get results for any other λ by simple scaling, so that our tabulated results will achieve some degree of universality. By calculating $\langle r^{M-1} \rangle$ we can find $\psi^2(0)$ from (10); by calculating $\langle r^{-1} \rangle$ we can estimate the first-order effect of introducing a weak gluon term. The values of E and $\langle r^M \rangle$ are rigorously related by the virial theorem: $E = \frac{1}{2}(M+2)\langle r^M \rangle$. This allows a check on the independent method of calculating $\langle r^M \rangle$ from equation (17). Although the direct approach of Kaushal and Müller-Kirsten did not work very well, it turns out that a direct approach *can* be made to work fairly well if it is used in conjunction with numerical integration of the Schrödinger equation. For example, while integrating the Schrödinger equation using (19) we can also work out integrals of the type

$$I(N) = \int \phi^2(r) r^N dr \quad (24)$$

by integrating up to the node in $\phi(r)$, using a very good eigenvalue (Killingbeck 1979b). The $I(2)$ value gives the normalisation constant and thus a direct $\psi^2(0)$ estimate; the ratio $I(4)/I(2)$ gives a value for $\langle r^2 \rangle$. The results for the various test potentials of this work show that values of $\langle r \rangle$ and $\langle r^2 \rangle$ obtained by this direct method are accurate to roughly 1 part in 10^5 , which is good enough for many applications. The use of the indirect approach based on equation (17), however, was found to yield more accurate results for quantities such as $\langle r^{-1} \rangle$, $\langle r^{-2} \rangle$ and $\langle (DV) \rangle$. Table 4 shows some results for s states.

Some workers on the charmonium problem have used potentials made up of several different r^N terms; we would like to suggest the potential

$$V = -r^{-1} + 2\lambda r + 2\lambda^2 r^2 \quad (25)$$

Table 4. Results for the lowest three s states ($V = r^M$)†.

$M = 1$	E	1.855 757 09	3.244 607 63	5.386 613 78
	$\langle r \rangle$	1.237 171	2.163 072	3.591 076
	$\langle r^2 \rangle$	1.836 712	5.614 655	15.474 99
	$\langle r^{-1} \rangle$	1.051 866	0.733 486	0.512 970
$M = 2$	E	2.121 320 34	4.949 747 47	7.778 174 59
	$\langle r \rangle$	0.948 850	1.423 275	1.779 094
	$\langle r^2 \rangle$	1.060 660	2.474 874	3.889 087
	$\langle r^{-1} \rangle$	1.341 877	1.118 230	0.995 225
$M = 3$	E	2.276 522 38	6.282 227 60	10.799 758 2
	$\langle r \rangle$	0.842 919	1.143 043	1.363 334
	$\langle r^2 \rangle$	0.827 677	1.617 848	2.322 209
	$\langle r^{-1} \rangle$	1.491 243	1.392 730	1.309 490

† Using $H = 0.025$ for the energies and $\epsilon = 0.02, 0.04$ for the $\langle r^N \rangle$.

as a useful test potential for any proposed method of attacking the problem. For $\lambda > 0$ the insertion of (25) in (3) leads to the *exact* ground-state eigenvalue $-\frac{1}{2} + 3\lambda$, with the eigenfunction $R = r \exp[-r - \lambda r^2]$. Table 5 shows exact results for this potential (with $\lambda = 1$) together with results obtained using the methods proposed in this work. The results illustrate clearly the accuracy of our methods for charmonium-type potentials.

Table 5. Results for $V = -r^{-1} + 2r + 2r^2$.

	E	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 2(DV) \rangle$
Exact	$\frac{5}{2}$	0.605 862 89	0.447 068 56	25.693 806
Integration†	2.500 000 000	0.605 867	0.447 072	24.960 17
ϵ method		0.605 863‡	0.447 069‡	25.693 80§

† Integration up to the node, as explained in text.

‡ Using $\epsilon = 0.04$ and 0.08 .

§ Using $\epsilon = 0.002$ and 0.004 .

6. Conclusion

The methods described in this work can be seen to give accurate values for energies, $\langle r^N \rangle$ values and $\psi^2(0)$ values. The basic principle involved is that of reducing the calculation of any required quantity to the calculation of energy eigenvalues, so that the calculational problem is rendered as simple as possible. Both the approaches of §§ 3 and 4 have the feature that the wavefunction plays a relatively minor role in the proceedings, so that they belong to the same general category as the WKB methods of Fröman (1978a, b). In principle, the 'diagonal problem' (i.e. the calculation of expectation values) has now been handled, but there still remains the 'off-diagonal' problem (e.g. can we find $\langle \psi_0 | r | \psi_1 \rangle$, using only algebra plus eigenvalue calculations, when ψ_0 and ψ_1 are *different* eigenfunctions?). A WKB approach to the problem has been outlined by Fröman and Fröman (1977). We suspect that the problem of adapting the more accurate numerical integration method for the 'off-diagonal' case may be solvable by using off-diagonal hypervirial relations (Hughes 1977, Banerjee 1977) together with

sum rules (Tipping 1976). To allow for boundary term effects, as illustrated by equation (13) of this work, however, it may be necessary to modify the usual double commutator approach to the derivation of off-diagonal hypervirial relations, at least for s states. Preliminary work suggests that the simplest first-principles approach is to work out directly the off-diagonal matrix element of the *fourth* derivative of a smooth function $f(r)$; this leads to s -state results such as

$$\langle R_0 | (DV) | R_1 \rangle = (E_1 - E_0)^2 \langle R_0 | r | R_1 \rangle + \frac{1}{2} DR_0(0) DR_1(0) \quad (26)$$

which have an extra term not obtained by the usual approach. We hope that these comments will stimulate other workers in the field to study the 'off-diagonal' problem.

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