The Jacobi eigenfunctions and the quantum mechanical hypervirial theorems method for bound-state problems

1997 J. Phys. A: Math. Gen. 30 L325

(http://iopscience.iop.org/0305-4470/30/10/005)

J. Phys. A: Math. Gen. **30** (1997) L325–L330. Printed in the UK PII: S0305-4470(97)80498-2

LETTER TO THE EDITOR

The Jacobi eigenfunctions and the quantum mechanical hypervirial theorems method for bound-state problems

T E Liolios and M E Grypeos

Department of Theoretical Physics, University of Thessaloniki, Thessaloniki 54006, Greece

Received 23 December 1996

Abstract. The Jacobi eigenfunctions are suitably adjusted by means of the hypervirial theorems (HVT) scheme in order to obtain, in many cases, a very satisfactory analytic approximation of the s-state eigenfunctions of the radial Gaussian potential. The results obtained show that the HVT scheme is a powerful method for obtaining (analytically) not only approximate eigenvalues but also the corresponding eigenfunctions.

The transformed Jacobi eigenequation can be used to approximately solve the Schrödinger eigenvalue problem for the Gaussian potential $V(r) = -V_0 \exp(-r^2/R^2)$ which has been used as a model in the theory of nucleon–nucleon scattering [1] as well as in numerous other applications in physics. Bessis *et al* [2] applied the Rayleigh–Schrödinger perturbation method to the Gaussian potential, observing that the Jacobi eigenfunctions (that is the solutions of the transformed Jacobi eigenequation) can provide a first approximation to the eigenfunctions of the radial Gaussian potential. Of course one can always find numerical eigenfunctions for that potential but the importance of the analytic ones must not be underestimated. After all, a lot of effort has been made in literature in solving eigenvalue problems analytically since they provide a means of seeing transparently how various quantities vary with respect to the potential parameters.

In the present letter we show that a very handy analytic approximation to the s-state eigenfunctions of the Gaussian potential can be accomplished by imposing a suitable constraint on the Jacobi eigenfunctions through the hypervirial theorems (HVT) scheme [3–10].

The Schrödinger eigenvalue problem for the radial Gaussian potential is

$$\left[\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V_0\,\mathrm{e}^{-r^2/R^2} + E\right]u_{nl} = 0 \qquad (1)$$

$$u_{nl}(0) = 0 \qquad u_{nl}(\infty) = 0.$$

By setting $x = r/R$, equation (1) becomes

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{l(l+1)}{x^2} + s^{-2}\,\mathrm{e}^{-x^2} + \tilde{E}\right]u_{nl} = 0 \qquad (2)$$

$$u_{nl}(0) = 0 \qquad u_{nl}(\infty) = 0$$

where

$$s = \left(\frac{\hbar^2}{2\mu}\frac{1}{V_0 R^2}\right)^{\frac{1}{2}} \qquad \text{and} \qquad \tilde{E} = s^{-2}\frac{E}{V_0}.$$

0305-4470/97/100325+06$19.50

The problem of the determination of the energy eigenvalues in equation (1) has been handled by the (HVT) scheme [7, 10, 11], which yielded satisfactory results especially for the ground and the lower excited states. Moreover, the expression for the mean-square radii $\langle r^2\rangle_{nl}$ have been derived [10] for the Gaussian potential, and can be written as a dimensionless function of s as follows [11]:

$$\left(\frac{\langle r^2\rangle_{nl}}{R^2}\right)_{\mathrm{G}} = a_{nl}s + \frac{1}{16}[12a_{nl}^2 - 4l(l+1) + 3]s^2 + \frac{3a_{nl}}{256}[60a_{nl}^2 - 28l(l+1) + 45]s^3 + \cdots. \tag{3}$$

Equation (2) resembles the transformed Jacobi eigenequation, with the same boundary conditions, which reads as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{l(l+1)}{\sinh^2(x)} + \frac{s^{-2}}{\cosh^2(x)} + \tilde{E}\right]u_{nl} = 0 \tag{4}$$

and can be thought of, in turn, as a Schrödinger equation for the potential

$$V_J(x) = -\left[\frac{s^{-2}}{\cosh^2(x)} - \frac{l(l+1)}{\sinh^2(x)} + \frac{l(l+1)}{x^2}\right]. \tag{5}$$

For the above transformed Jacobi eigenequation the eigenfunctions are [2, 13]

$$u_{nl} = N_{nl}(\sinh x)^{l+1}(\cosh x)^{p+1/2}P_n^{(l+1/2,\,p)}(\cosh(2x)) \tag{6}$$

with

$$N_{nl} = \left[\frac{2^{-p-l-1/2}(-p-a_{nl})\Gamma(n+1)\Gamma(-p-n)}{\Gamma(n+l+3/2)\Gamma(-p-n-l-1/2)}\right]^{\frac{1}{2}} \tag{7}$$

where $a_{nl} = 2n + l + 3/2$ and $p = -\sqrt{s^{-2} + \frac{1}{4}}$.

The corresponding energy eigenvalues $\tilde{E}$ are given simply by

$$\tilde{E} = \tilde{E}_{nl} = -\left[a_{nl} - \sqrt{\frac{1}{s^2} + \frac{1}{4}}\right]^2. \tag{8}$$

The problem of the radial Schrödinger eigenvalue problem of the Poeschl–Teller-type potential [12], ($V_{\mathrm{PT}} = -V_0\cosh^{-2}(r/R)$),

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{l(l+1)}{x^2} + s^{-2}\cosh^{-2}(x) + \tilde{E}_{nl}\right]u_{nl} = 0 \tag{9}$$
$$u_{nl}(0) = 0 \qquad u_{nl}(\infty) = 0$$

has been treated by means of the HVT scheme for any bound state [10]. In fact, apart from the series for the energy eigenvalues, a series for the mean-square radii has been obtained which, as in the case of the Gaussian potential, can be written in the dimensionless form

$$\left(\frac{\langle r^2\rangle_{nl}}{R^2}\right)_{\mathrm{PT}} = a_{nl}s + \frac{1}{12}[12a_{nl}^2 - 4l(l+1) + 3]s^2 + \frac{a_{nl}}{90}[85a_{nl}^2 - 36l(l+1) + 50]s^3 + \cdots. \tag{10}$$

One can easily observe that for the s-states ($l = 0$) equations (4) and (9) are in fact identical and the Jacobi eigenfunction coincides with that of the Poeschl–Teller-type potential. Unfortunately this is not the case for the Gaussian Schrödinger equation (2), which is not exactly solvable even for the ground state.

It has been recently [11] suggested that such cumbersome cases can be handled using a convenient analytic approximation of the wavefunction (composed of an interior and an

exterior part) suitably adjusted. In this work we follow the same general idea by considering the Jacobi eigenfunction and applying the following constraint:

$$\left(\frac{\langle r^2\rangle_{n0}}{R^2}\right)_{\mathrm{G}} \approx \left(\frac{\langle r^2\rangle_{n0}}{R^2}\right)_{\mathrm{Jacobi}} = \left(\frac{\langle r^2\rangle_{n0}}{R^2}\right)_{\mathrm{PT}}. \tag{11}$$

Note that the present approach leads to much more satisfactory results.

Thus one can obtain an s_0 which suitably adjusts the nth s-state Jacobi eigenfunction to approximate the corresponding eigenfunction of the Gaussian potential by solving the equation

$$a_{n0}s_0 + \left[a_{n0}^2 + \frac{1}{4}\right]s_0^2 + \frac{a_{n0}}{90}[85a_{n0}^2 + 50]s_0^3 = g_{n0} \tag{12}$$

where

$$g_{n0} = a_{n0}s + \frac{1}{16}[12a_{n0}^2 + 3]s^2 + \frac{3a_{n0}}{256}[60a_{n0}^2 + 45]s^3. \tag{13}$$

(Note that s is of course calculated with respect to the Gaussian potential parameters.)

Alternatively one could use the formulae of the analytic solution of cubic equations:

$$s_0 = S + T - \tfrac{1}{3}b_1 \tag{14}$$

$$S = (W + \sqrt{Q^3 + W^2})^{\frac{1}{3}} \qquad T = (W - \sqrt{Q^3 + W^2})^{\frac{1}{3}} \tag{15}$$

$$Q = \frac{3b_2 - b_1^2}{9} \qquad W = \frac{9b_1b_2 - 27b_3 - 2b_1^3}{54} \tag{16}$$

$$b_1 = \frac{45(4a_{n0}^2 + 1)}{2a_{n0}(85a_{n0}^2 + 50)} \qquad b_2 = \frac{90}{(85a_{n0}^2 + 50)} \qquad b_3 = -\frac{90g_{n0}}{a_{n0}(85a_{n0}^2 + 50)} \tag{17}$$

which can be readily fed into a computer for a fast and accurate calculation of s_0.

Finally the nth s-state normalized eigenfunction which is proposed for the Gaussian potential (in equation (2)) is

$$u_{n0}(x) = N_{n0}(\sinh x)(\cosh x)^{p_0+1/2}P_n^{(1/2,\,p_0)}(\cosh(2x)) \tag{18}$$

with

$$N_{n0} = \left[\frac{2^{-p_0-1/2}(-p_0 - a_{n0})\Gamma(n+1)\Gamma(-p_0-n)}{\Gamma(n+3/2)\Gamma(-p_0-n-1/2)}\right]^{\frac{1}{2}} \tag{19}$$

where $a_{n0} = 2n + 3/2$ and $p_0 = -\sqrt{s_0^{-2} + \frac{1}{4}}$.

Obviously, in addition to the Gaussian potential, other potentials can be handled in an analogous way.

Visualization of the results can be achieved by plotting the eigenfunctions obtained through the present method against those obtained by numerical integration (see figures 1–3). To be more specific we consider, as an application, a problem of physical interest, namely that of the binding energy of a Λ–particle in hypernuclei, in which the self-consistent Λ–nuclei potential is approximated by a Gaussian one (with the rigid core model expression [14] for R: $R = r_0A^{\frac{1}{3}}$, A being the mass number of the core nucleus). This is a reasonable approximation for relatively light hypernuclei. The values of the potential parameters may be determined by a least-squares fit to known experimental values [14], $V_0 = 34.16$ MeV, $r_0 = 1.199$ fm.

We further note that a measure of the quality of the achieved approximation is the value of the integral

$$I_{n0} = \int_0^\infty |u_{n0}^{\mathrm{num}}(r) - u_{n0}(r)|^2\,\mathrm{d}r \tag{20}$$

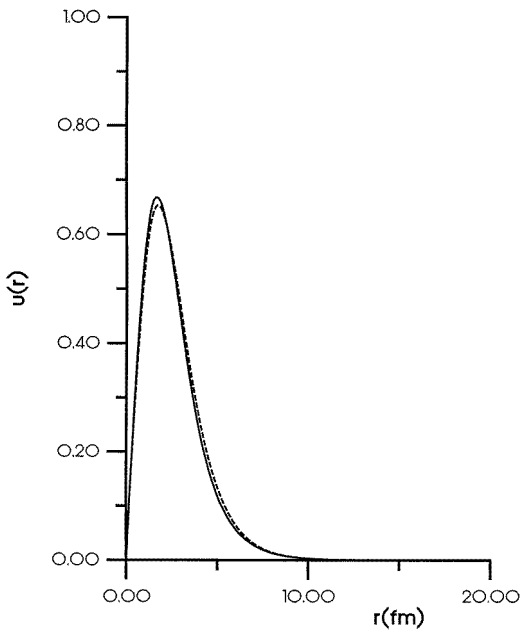

Figure 1. The plot of the adjusted s-state Jacobi eigenfunction (broken curve), with $n = 0$, $A = 11$, against that of the corresponding eigenfunction (full curve) obtained through numerical integration of the Schrödinger equation.

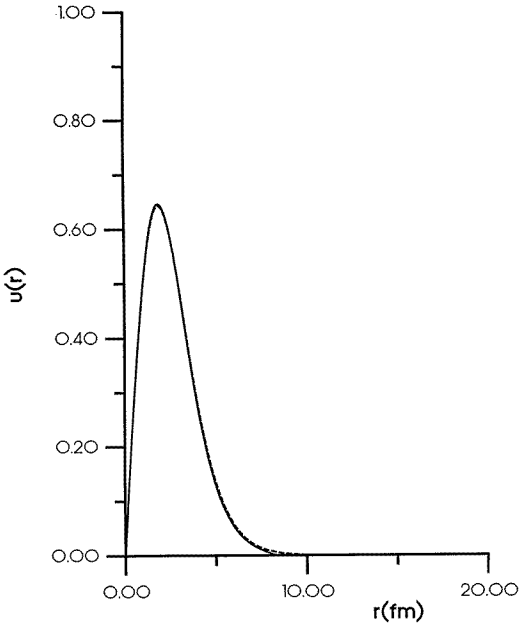

Figure 2. The plot of the adjusted s-state Jacobi eigenfunction (broken curve), with $n = 0$, $A = 40$, against that of the corresponding eigenfunction (full curve) obtained through numerical integration of the Schrödinger equation.

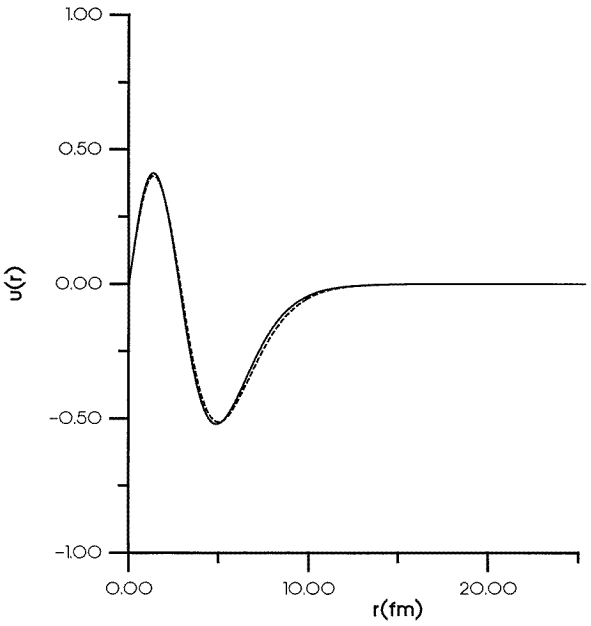

Figure 3. The plot of the adjusted s-state Jacobi eigenfunction (broken curve), with $n = 1$, $A = 120$, against that of the corresponding eigenfunction (full curve) obtained through numerical integration of the Schrödinger equation.

where $u_{n0}^{\text{num}}(r)$ is the corresponding, numerically obtained, normalized eigenfunction. For various nuclei one obtains:

n	A	s	I_{n0}
0	11	0.460	0.0030
0	40	0.358	0.0001
1	120	0.295	0.0032

It is seen that the value of I_{n0} decreases rapidly with A so that the heavier the nuclei the better the approximation, as is also clear from the figures.

In conclusion, the important results of this paper (and to some extent those of [11]) is that the (HVT) scheme, which is 'a perturbation theory without a wavefunction', becomes capable of providing approximate analytic eigenfunctions for certain states in a simple and efficient way.

References

[1] Buck B 1977 *Nucl. Phys.* A **275** 246
[2] Bessis N, Bessis G and Joulakian B 1982 *J. Phys. A: Math. Gen.* **15** 3679
[3] Hirschfelder J O 1960 *J. Chem. Phys.* **33** 1462
[4] Marc G and McMilllan W G 1985 *Adv. Chem. Phys.* **58** 209
Fernandez F M and Castro E A 1987 *Hypervirial Theorems (Lecture Notes in Chemistry 43)* (Berlin: Springer)
McRae S M and Vrscay E R 1992 *J. Math. Phys.* **33** 3004
[5] Swenson R J and Danforth S H 1972 *J. Chem. Phys.* **57** 1734
[6] Killingbeck J 1978 *Phys. Lett.* **65A** 87

Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** L1925
Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** 245
[7] Grant M and Lai C S 1979 *Phys. Rev.* A **20** 718
Lai C S 1981 *Phys. Rev.* A **23** 455
Lai C S 1982 *Phys. Rev.* A **26** 2245
Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* **15** 1495
Lai C S 1983 *J. Phys. A: Math. Gen.* **16** L181
[8] Mateo F G, Zúñiga J, Requena A and Hidalgo A 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 2771
[9] Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 5291
Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 4535
Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 3053
Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 3041
Witwit M R M 1992 *Phys. Rev.* C **48** 198
[10] Liolios T E and Grypeos M E 1995 *Advances in Nuclear Physics (Proc. 5th Hellenic Symp. Nuclear Physics (Patras, Greece))* ed C Syros and C Ronchi (European Commission) EUR 16302 EN, p 104
[11] Grypeos M E and Liolios T E 1996 submitted
[12] Lalazissis G A, Grypeos M E and Massen S E 1988 *Phys. Rev.* C **37** 2098
Lalazissis G A 1989 *PhD Thesis* Aristotle University of Thessaloniki
[13] Lalazissis G A 1993 *Phys. Rev.* C **48** 198
[14] Lalazissis G A 1994 *Phys. Rev.* C **49** 1412
Lalazissis G A 1994 *Preprint* Aristotle University of Thessaloniki