

Dimensionality and Energy Levels of Quantum Mechanical Systems

Harry A. MAVROMATIS
Physics Department
King Fahd University of
Petroleum and Minerals
Dhahran 31261 SAUDI ARABIA

Received 04.12.1996

Abstract

The N -dimensional Schrödinger equation involving a general, central potential $V_N(r)$, is decomposed into a 3-dimensional component plus a term that may be treated as a dimension-dependent perturbation. This allows discussion of the general N -dimensional system from a 3-dimensional perspective.

Introduction

Recently several papers have focused on the role the dimensionality “ N ” of the space plays in determining the energy levels of quantum mechanical systems. One assumes in such discussions that the system under consideration is subject to a “central” potential $V_N(r)$, where $r = \sqrt{r_1^2 + r_2^2 + \cdots + r_N^2}$. Thus Hagen [1] discusses how the dimensionality affects the energies of the generalized hydrogen atom and rewrites the N -dimensional Coulomb potential as a two-dimensional Coulomb term plus a harmonic oscillator perturbation in the other dimensions. A related discussion for hydrogen appears in the paper of Ho [2] where the author compares the energies of a two-dimensional, possibly multivalued-wavefunction Coulomb system, with those of the standard three-dimensional Coulomb problem. The exact solution for the N -dimensional Coulomb system is well known [3]. Similarly well-researched is the N -dimensional harmonic oscillator, whose exact solutions can be obtained immediately if one uses “ N -dimensional” Cartesian coordinates. The N -dimensional oscillator is also exactly solvable in spherical co-ordinates [4].

In the present work we show how the N -dimensional Hamiltonian for an arbitrary system subject to any general potential $V_N(r)$ can be decomposed in a simple peda-

gical way into a three-dimensional component, plus a perturbation. This allows one to make general statements about the energies of an arbitrary N -dimensional, relative to the corresponding 3-dimensional system. For a few special cases, using lowest-order perturbation theory one can additionally explicitly evaluate the energy differences that arise because of the difference of dimension. This provides an interesting illustration of first-order perturbation theory, where comparison with the exact eigenvalues indicates under what conditions this approximation gives accurate results.

Decomposition Procedure

The N -dimensional radial Hamiltonian of a system subject to a potential $V_N(r)$ is [5, 6, 7]:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2(\ell + N/2 - 3/2)(\ell + N/2 - 3/2 + 1)}{2mr^2} + V_N(r) \right] u_{n\ell}^{(N)}(r) = E_N u_{n\ell}^{(N)}(r), \quad (1)$$

where $u_{n\ell}^{(N)}(r)$ is the N -dimensional radial eigenfunction,

$$\int_0^\infty \left\{ u_{n\ell}^{(N)}(r) \right\}^2 dr = 1,$$

and ℓ is assumed to be integer such that the total wavefunction is single-valued.

One can re-write eq. (1) as follows:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell + 1)}{2mr^2} + V_N(r) + \frac{\hbar^2(\ell + N/2 - 3/2)(\ell + N/2 - 3/2 + 1)}{2mr^2} - \frac{\hbar^2 \ell(\ell + 1)}{2mr^2} \right] u_{n\ell}^{(N)}(r) = E_N u_{n\ell}^{(N)}(r),$$

i.e. after a little algebra one obtains:

$$[H_0 + H_1] u_{n\ell}^{(N)}(r) = E_N u_{n\ell}^{(N)}(r)$$

where

$$H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell + 1)}{2mr^2} + V_N(r), \quad (2)$$

$$H_1 = \frac{\hbar^2(N/2 - 3/2)(2\ell + N/2 - 1/2)}{2mr^2}. \quad (3)$$

Thus to first order in perturbation theory:

$$E_N \sim E_3 + \Delta E, \quad (4)$$

where E_3 are the 3-dimensional energy levels corresponding to the Hamiltonian H_0 , and to first-order in perturbation theory:

$$\Delta E = \int_0^\infty \{u_{n\ell}^{(3)}(r)\}^2 H_1 dr = \frac{\hbar^2(N-3)(4\ell+N-1)}{8m} \int_0^\infty \frac{\{u_{n\ell}^{(3)}(r)\}^2}{r^2} dr. \quad (5)$$

One immediately notes that by construction $\Delta E = 0$ if $N = 3$, and since $\{u_{n\ell}^{(3)}(r)\}^2/r^2$ is positive definite, ΔE is positive if $N > 3$, and negative if $N < 3$ (i.e. $N = 2$). Hence for a given system, relative to the $N = 3$ space the system's energy levels are always shifted upwards as N increases and downwards for $N = 2$. Increasing the dimensionality of the space can thus be viewed as introducing an additional N -dependent centrifugal potential.

The case $N = 1$ deserves special care because, whereas for $N \neq 1$, $u_{n\ell}^{(N)}(0) = 0$, and r is only defined for $r \geq 0$, for the case $N = 1$, $u_{n0}^{(1)}(r)$ extends from $-\infty \leq r \leq \infty$. Thus, the normalization condition for the one-dimensional case is

$$\int_{-\infty}^{\infty} \{u_{n0}^{(1)}(r)\}^2 dr = 1.$$

Additionally, and more importantly [15], $u_{n0}^{(1)}(0)$ is not necessarily zero. This does not however mean we must completely eliminate $N = 1$ from the discussion which follows. If one works with central potentials $V(r)$, necessarily the solutions $u_{n0}^{(1)}(r)$ are either of even or of odd parity. The even parity $N = 1$ solutions need not be zero at the origin, hence must be eliminated from our discussion. For the odd-parity $N = 1$ solutions however, $u_{n0}^{(1)}(0)$ is necessarily zero. Thus, with the proviso that the $N = 1$ states considered are of odd parity, one can also discuss what happens to these states using the above expression. For these states $\Delta E = 0$ according to Eq. (5). This is because, aside from a $\sqrt{2}$ difference in normalization constant, these correspond to the $\ell = 0$, $N = 3$ states (and energies).

Two N -dimensional cases where Eq. (5) can be evaluated analytically are the familiar (a) harmonic oscillator, and the related [8-11] (b) Coulomb potential. These are discussed in the following two sections. For these same systems the exact N -dimensional eigenvalues are also known. They can be obtained directly from the 3-dimensional solutions by the straightforward substitution $\ell \rightarrow \ell + (N-3)/2$ [4, 7]. Thus, for these two potentials, several interesting comparisons between perturbation theory and the exact solutions can be made. In this paper we also discuss the problem of (c) a particle in an N -dimensional vs a 3-dimensional infinite box, after the discussion of cases (a), and (b).

(a) N -dimensional Harmonic Oscillator: $V_N(r) = \frac{1}{2}mw^2r^2 = \frac{\hbar^2r^2}{2mb^4}$; ($b = \sqrt{\hbar/mw}$).

Here [4] the exact N -dimensional energies are:

$$E_N = (2n + \ell + N/2)\hbar w, \quad n = 0, 1, 2, \dots \quad \ell = 0, 1, 2, \dots, \quad (6)$$

while the 3-dimensional eigenfunctions are:

$$u_{n\ell}^{(3)}(r) = \left[\frac{2n!}{\Gamma(n + \ell + 3/2)^3 b} \right]^{1/2} \left(\frac{r}{b} \right)^{\ell+1} \exp(-r^2/2b^2) L_n^{\ell+1/2}(r^2/b^2). \quad (7)$$

Thus, substituting in Eq. (5)

$$\begin{aligned} \Delta E &= \frac{2n! \hbar^2 (N-3)(4\ell + N - 1)}{\Gamma(n + \ell + 3/2)^3 8m} \int_0^\infty \left(\frac{r}{b} \right)^{2\ell+2} \exp(-r^2/b^2) \frac{\{L_n^{\ell+1/2}(r^2/b^2)\}^2}{r^2} \frac{dr}{b} \\ &= \frac{2n! \hbar \omega (N-3)(4\ell + N - 1)}{\Gamma(n + \ell + 3/2)^3} \frac{1}{2} \int_0^\infty (u)^{\ell-1/2} \exp(-u) \{L_n^{\ell+1/2}(u)\}^2 du. \end{aligned}$$

Using the formula [12, 13]:

$$\int_0^\infty (u)^{a-1} \exp(-u) \{L_n^a(u)\}^2 du = \frac{\Gamma(n+a+1)^3}{an!}, \quad (8)$$

one directly obtains the result:

$$\begin{aligned} \Delta E &= \hbar \omega \frac{(N-3)}{2} \left[1 + \frac{N-3}{4\ell+2} \right] \\ &= \frac{\hbar \omega (N-3)}{2} + \frac{\hbar \omega (N-3)^2}{2(4\ell+2)} \\ &\rightarrow \frac{\hbar \omega (N-3)}{2} \quad \text{for large } \ell. \end{aligned} \quad (9)$$

This correction, in agreement with the previous general arguments, is $> 0 (< 0)$ for $N > 3 (< 3)$. It also reduces to the exact energy difference for large ℓ where, using Eq. (6) one has

$$\begin{aligned} E_N &= E_3 + \Delta E_{\text{exact}} \\ (2n + \ell + N/2)\hbar \omega &= (2n + \ell + 3/2)\hbar \omega + \frac{(N-3)}{2}\hbar \omega. \end{aligned} \quad (10)$$

The result that the first-order expression is approximately equal to the exact energy difference, i.e. $\Delta E \rightarrow \Delta E_{\text{exact}}$ for large ℓ is not unexpected since for large angular momentum one knows that the particle is on the average far away from the origin, hence is not very much affected by the perturbation H_1 which is proportional to $1/r^2$. In this case H_1 will be a small perturbation as compared to H_0 and first-order calculations should, and do turn out to be very accurate. On the other hand there are cases (small ℓ , large $N-3$) where the first-order result is seen not to be very accurate. From Eq. (9) we see that for $N=1$, $\ell=0$, $\Delta E=0$, consistent with the remarks in the decomposition section that for $N=1$, $\ell=0$, ΔE should always be zero for the odd-parity states.

(b) N -dimensional Coulomb Potential: $V_N(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$.

Here the exact N -dimensional energies are

$$\begin{aligned} E_N &= -\frac{\alpha^2 mc^2}{2(p+\ell+1+(N-3)/2)^2}, \\ \alpha &= \frac{e^2}{4\pi\epsilon_0 \hbar c}, \quad p=0,1,\dots \quad \ell=0,1,\dots \quad n=p+\ell+(N-3)/2+1, \end{aligned} \quad (11)$$

while the exact 3-dimensional eigenfunctions (with $\kappa = m\alpha/(n\hbar)$) are:

$$u_{n\ell}^{(3)}(r) = \left[\frac{2\kappa(n-\ell-1)!}{2n[(n+\ell)!]^3} \right]^{1/2} (2\kappa r)^{\ell+1} \exp(-\kappa r) L_{n-\ell-1}^{2\ell+1}(2\kappa r). \quad (12)$$

Thus, substituting in Eq. (5):

$$\begin{aligned} \Delta E &= \frac{\hbar^2(N-3)(4\ell+N-1)(n-\ell-1)!}{8m \cdot 2n[(n+\ell)!]^3} \int_0^\infty (2\kappa r)^{2\ell+2} \exp(-2\kappa r) \frac{\{L_{n-\ell-1}^{2\ell+1}(2\kappa r)\}^2}{r^2} 2\kappa dr \\ &= \frac{mc^2\alpha^2(N-3)(4\ell+N-1)(n-\ell-1)!}{2 \cdot 2n[(n+\ell)!]^3} \int_0^\infty (u)^{2\ell} \exp(-u) \{L_{n-\ell-1}^{2\ell+1}(u)\}^2 du. \end{aligned}$$

Using Eq. (8) one obtains finally:

$$\begin{aligned} \Delta E &= \frac{mc^2\alpha^2}{2(p+\ell+1)^2} \frac{N-3}{p+\ell+1} \left[1 + \frac{N-3}{4\ell+2} \right] \\ &\rightarrow \frac{mc^2\alpha^2}{2(p+\ell+1)^2} \frac{N-3}{p+\ell+1} \quad \text{for large } \ell. \end{aligned} \quad (13)$$

This result, is also in agreement with the previous general arguments, i.e. $\Delta E > 0 (< 0)$ for $N > 3 (< 3)$. For large ℓ , and for the same reasons as in case (a), it also reduces to the leading term in the exact energy difference where, using Eq. (11) one has

$$\begin{aligned} E_N &= E_3 + \Delta E_{\text{exact}} \\ -\frac{\alpha^2 mc^2}{2(p+\ell+1+(N-3)/2)^2} &= -\frac{\alpha^2 mc^2}{2(p+\ell+1)^2} + \frac{mc^2\alpha^2}{2(p+\ell+1)^2} \frac{N-3}{p+\ell+1} + \dots \end{aligned} \quad (14)$$

From Eq. (13) we see that for $N=1$, $\ell=0$, $\Delta E=0$, again consistent with the remarks in the decomposition section that for $N=1$, $\ell=0$, ΔE should always be zero for the odd-parity states.

(c) N -dimensional Particle in a Box:

$$V_N(r) = \begin{cases} 0, & 0 < r < a, \\ \infty, & a < r < \infty. \end{cases} \quad (15)$$

For this case the exact N -dimensional eigenfunctions are:

$$u_{n\ell}^{(N)}(r) = \begin{cases} A_{n\ell}^{(N)} r^{j_{\ell+N/2-3/2}(k_{n\ell}r)}, & 0 < r < a, \\ 0, & a < r < \infty \end{cases} \quad (16)$$

where $E_N = \hbar^2 k_{n\ell}^2 / 2m$, and $A_{n\ell}^{(N)}$ is a normalization constant given by:

$$1 = \left(A_{n\ell}^{(N)} \right)^2 \int_0^a j_{\ell+N/2-3/2}^2(k_{n\ell}r) r^2 dr.$$

As for the allowed $k_{n\ell}$ s, these are given by the requirement:

$$j_{\ell+N/2-3/2}(k_{n\ell}a) = 0, \quad (\text{or } J_{\ell+N/2-1}(k_{n\ell}a) = 0.) \quad (17)$$

For the three-dimensional case the energies can be decomposed in the usual way into the solutions for $\ell = 0$, i.e. the roots of $j_0(k_{n0}a)$, namely $E_3^{(n0)} = \hbar^2 k_{n0}^2 / 2m$, $n = 1, 2, \dots$ the solutions for $\ell = 1$, i.e. the roots of $j_1(k_{n1}a)$, namely $E_3^{(n1)} = \hbar^2 k_{n1}^2 / 2m$, and generally $E_3^{(n\ell)} = \hbar^2 k_{n\ell}^2 / 2m$, where $j_\ell(k_{n\ell}a) = 0$. It is interesting to compare these to the energies for dimension $N = 5$. The solutions in this case for $\ell = 0$ correspond to the solutions for the roots of $j_1(k_{n0}a)$, i.e. are identical to the 3-dimensional solutions for the case $\ell = 1$. Similarly for $N = 5$ and $\ell = 1$, one has all the 3-dimensional solutions for $\ell = 2$. However, all the 3-dimensional $\ell = 0$ solutions (which begin at a lower energy) are missing for the $N = 5$ case. Similarly if $N = 7$ all the $\ell = 0$, and $\ell = 1$, $N = 3$ levels are missing but the 3-dimensional $\ell = 2$ levels correspond exactly to the $N = 7$, $\ell = 0$ levels, etc. A similar analysis may be carried out for $N = 2, 4, 6$, etc.

For this system, substituting Eq. (16) in Eq. (5) yields:

$$\begin{aligned} \Delta E &= \frac{\hbar^2(N-3)(4\ell+N-1)}{8m} \left(A_{n\ell}^{(3)} \right)^2 \int_0^a j_\ell^2(k_{n\ell}r) dr \\ &= E_3(n, \ell) \frac{(N-3)(4\ell+N-1)}{4} \frac{\int_0^b j_\ell^2(u) du}{\int_0^b j_\ell^2(u) u^2 du} \end{aligned} \quad (18)$$

where $b = k_{n\ell}a$.

Eq. (18) must be evaluated numerically. This may be done for example using Mathematica [14]. Three sets of numerical results are listed in Table 1 (where it is assumed $\hbar = m = a = 1$).

From examples (a) and (b) above, one expects (and obtains) good agreement between ΔE_{exact} and ΔE , for large ℓ ($\ell = 10$), and bad agreement for small ℓ ($\ell = 0$). The lowest n state is considered throughout in this numerical calculation, for all three cases. The result ΔE is seen to always be greater than ΔE_{exact} , as expected from variational considerations, and as ℓ increases $\Delta E / E_3$ is seen to rapidly decrease in value.

Table 1. Numerical Evaluation of ΔE for N -dimensional particle in a box

ℓ	N	$k_{1\ell}$	$k_{1\ell+1}$	$E_5(1, \ell)$	$E_3(1, \ell)$	ΔE_{exact}	ΔE Eq. (18)	$\Delta E/E_3$
0	5	π	4.49	10.08	4.93	5.15	8.87	1.80
5	5	9.35	10.50	55.13	43.71	11.42	11.89	0.272
10	5	15.03	16.14	130.25	112.95	17.30	17.54	0.155

Conclusions

The N -dimensional problem for a general potential $V_N(r)$ has been studied from a 3-dimensional perspective, by decomposing the Hamiltonian into a 3-dimensional component and a $1/r^2$ -dependent perturbation. For $N > 3$ this behaves as an additional centrifugal potential, and for $N = 2$ as a centripetal potential. The perturbation is accurately treated using first-order perturbation theory in the case of states with large angular momenta. For two cases: the N -dimensional oscillator and the N -dimensional Coulomb potential, exact first-order analytic calculations are compared to the exact dimension-induced energy correction. For the particle in the N -dimensional infinite box it is pointed out that the energy levels are identical for $N = 3, 5, 7 \dots (N = 2, 4, 6 \dots)$ but as N increases, lower ℓ levels are progressively eliminated. Additionally for this case, numerical calculations are performed that yield results consistent with those obtained for the cases which were treated analytically.

KFUPM support is acknowledged.

References

- [1] C. R. Hagen, "Dimensionality as a perturbation parameter in the generalized hydrogen atom", Am. J. Phys. **(63)**, 1039-1040 (1995).
- [2] Vu, B. Ho, "On the quantization of angular momentum", J. Phys. A. **(27)**, 6237-6241 (1994).
- [3] M. M. Nieto, "Hydrogen atom and relativistic pi-mesic atom in N -space dimensions", Am. J. Phys. **(47)**, 1067-1072 (1979).
- [4] H.A. Mavromatis, Exercises in Quantum Mechanics, p. 120, Kluwer Academic Publishers (1992).
- [5] A. Chatterjee, "Large- N expansions in Quantum Mechanics", Phys. Rep. **(186)**, 249-370 (1990).
- [6] C. Mller, Spherical Harmonics, Lecture Notes in Mathematics **(17)**, Springer, Berlin (1966).
- [7] I.L. Cooper, "An Integrated Approach to Ladder and Shift Operators for the Morse Oscillator, Radial Coulomb and Radial Oscillator Potential", J. Phys. A **(26)**, 1601-1623 (1993).

MAVROMATIS

- [8] D.S. Bateman, C. Boyd, and B. Dutta-Roy, "The mapping of the Coulomb problem into the oscillator", *Am. J. Phys.* **(60)**, 833-836 (1992).
- [9] P. Pradhan, "Comment on 'The mapping of the Coulomb problem into the oscillator', by David S. Bateman, Clinton Boyd and Binayak Dutta-Roy [*Am. J. Phys.* 60 (9), 833-836 (1992)]", *Am. J. Phys.* **(63)**, 664 (1995).
- [10] H.A. Mavromatis, "Mapping of the Coulomb problem into the oscillator: a comment on the papers by Bateman et.al. [*Am. J. Phys.* 60 (9), 833-836 (1992)], and Pradhan [*Am. J. Phys.* 63 (7), 664 (1995)]", *Am. J. Phys.* 64, 1074 (1996).
- [11] V.A. Kostelecký, M.M. Nieto, and D.R. Truax, "Supersymmetry and the relationship between the Coulomb and oscillator problems in arbitrary dimensions", *Phys. Rev. D.* **(32)**, 2627-2633 (1985).
- [12] H.A. Mavromatis, "An Interesting New Result Involving Associated Laguerre Polynomials", *Intern. J. Comp. Math.* **(36)**, 257-261 (1990).
- [13] J.L. Power and B. Crasemann, "Quantum Mechanics", p. 235, Addison-Wesley Publishers (1965).
- [14] S. Wolfram, *Mathematica*, Addison-Wesley Publishers (1988).
- [15] H.A. Mavromatis, *Exercises in Quantum Mechanics*, p. 111, Kluwer Academic Publishers (1992).