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Exactly solvable noncentral potentials in two and three dimensions

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We show that the list of analytically solvable potentials in nonrelativistic quantum mechanics can be considerably enlarged. In particular, we show that those noncentral potentials for which the Schrödinger equation is separable are analytically solvable provided the separated problem for each of the coordinates belongs to the class of exactly solvable one dimensional problems. As an illustration, we discuss in detail two examples, one in two and the other in three dimensions. A list of analytically solvable noncentral potentials in spherical polar coordinates is also given. Extension of these ideas to other standard orthogonal coordinate systems as well as to higher dimensions is straightforward.

I. INTRODUCTION

The analytically solvable potentials in nonrelativistic quantum mechanics have pedagogical value. The explicit expressions for the eigenvalues, the eigenfunctions, and the scattering matrix in such examples give insight in the physical concepts of quantum mechanics. Besides, some of these may have physical applications; some could be used as the unperturbed part of a more realistic Hamiltonian. Most of the analytically solvable examples that are found in the text books,[1] however, are either one dimensional, or are central potentials which are essentially one dimensional on the half line. The noncentral potential that is sometimes discussed in the text books[2] is the anisotropic harmonic oscillator. The purpose of this paper is to present other examples of analytically solvable noncentral potentials in two and three spatial dimensions. This is accomplished by considering those noncentral potentials (in spherical polar coordinates) for which the Schrödinger equation is separable in each of the coordinates and reduces to three uncoupled one dimensional equations that can be exactly solved. The method is applicable to other orthogonal coordinate frames,[3] and may be extended to higher dimensions. In this paper, two examples, one in two, and the other in three dimensions, are treated in some detail. A list of solvable noncentral potentials in spherical polar coordinates in three dimensions is also given.

It is worth pointing out that these potentials may not only be of academic interest. For example, it has been known for a long time[4] that the exact solution of a potential in two dimensions can be directly mapped to an exact solution of a corresponding three-body problem in one dimension. In fact, the particular example in two dimensions discussed in some detail in Sec. II has some novel application in solvable many body problems also. Hopefully, a few applications of the noncentral potentials in three dimensions to some physical problems may be forthcoming.

The plan of the paper is as follows: In Sec. II, a two dimensional noncentral potential is discussed in detail, together with its application in a novel many body problem. Next, in Sec. III, a new analytically solvable three dimensional example is presented. In the last section, other examples in both two and three dimensions are listed. It is worth pointing out that all these may also be solved alge-

braically by using the concept of shape invariant potentials within the formalism of supersymmetric quantum mechanics.[5]

II. SOLVABLE NONCENTRAL POTENTIALS IN TWO DIMENSIONS

Consider a potential $V(r,\phi)$ in polar coordinates of the form

$$V(r,\phi)=\tilde{U}(r)+\frac{U(\phi)}{r^2}. \tag{2.1}$$

Such a form is classically integrable,[6] and has two constants of motion. The Schrödinger equation for the eigenvalue problem is ($\hbar=1$, $2M=1$)

$$\left(-\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right)\Psi_{nl}=\left(E_{nl}-\tilde{U}(r)-\frac{U(\phi)}{r^2}\right)\Psi_{nl}. \tag{2.2}$$

On writing the eigenfunction $\Psi_{nl}(r,\phi)$ as

$$\Psi(r,\phi)=\frac{1}{\sqrt{r}}u(r)K(\phi), \tag{2.3}$$

the radial equation may be written as

$$\left(-\frac{d^2}{dr^2}+\tilde{U}(r)+\frac{(m^2-1/4)}{r^2}\right)u(r)=Eu(r). \tag{2.4}$$

In the above, m^2 is the eigenvalue of the angular equation

$$\left(-\frac{d^2}{d\phi^2}+U(\phi)\right)K(\phi)=m^2K(\phi). \tag{2.5}$$

The two constants of motion in the quantum problem are the eigenvalues E and m^2. An interesting example of the angular potential is given by

$$U(\phi)=G/\sin^2(p\phi). \tag{2.6}$$

This potential is actually a special case of the more general Pöschl–Teller potential that is treated in detail in Flügge's text[2] on quantum mechanics. We shall nevertheless solve this simpler problem here to clarify the quantisation procedure. Note that in general, from physical considerations, the potential should be single-valued and periodic,

$$U(\phi)=U(\phi+2\pi). \tag{2.7}$$

This puts the restriction that the parameter p occurring in Eq. (2.6) be an integral multiple of 1/2. We will infact take p to be an integer so that the eigenfunctions are necessarily periodic [see Eq. (2.15)]. Moreover, since the potential $U(\phi)$ is singular, the wave function must vanish at $\phi=0$ and $\phi=\pi/p$ for a repulsive potential, and it is sufficient to solve the equation in the range $0\leqslant\phi\leqslant\pi/p$. Thus the range of ϕ is broken into disjointed sectors, with the boundary condition on the wave function

$$K(\phi=0)=K(p\phi=\pi)=0. \tag{2.8}$$

Within this range, the wave function should be smooth with no discontinuity in its derivative. At this point, it is instructive to examine the behavior of $K(\phi)$ as $\phi\to0$, noting that $U(\phi)$ given by Eq. (2.6) dominates the Schrödinger equation in this situation. Equation (2.5) then reduces to

$$\left(-\frac{d^2}{d\phi^2}+\frac{G}{p^2\phi^2}\right)K(\phi)=0.$$

The solution of this equation is $K(\phi)=\phi^\alpha$, where direct substitution shows that α has to satisfy $\alpha^2-\alpha-G/p^2=0$. Only the positive root is allowed in view of the boundary condition (2.8), giving

$$\alpha=\frac{1}{2}+\frac{1}{2}\left(1+\frac{4G}{p^2}\right)^{1/2}. \tag{2.9}$$

Keeping in mind Eq. (2.8), it is natural to assume, for the entire range $0\leqslant\phi\leqslant\pi/p$, the form

$$K(\phi)=(\sin p\phi)^\alpha R(\phi), \tag{2.10}$$

where α is given by Eq. (2.9), and $R(\phi)$ is a smooth function which is nonzero and finite at $\phi=0$. It is further convenient to make the substitution

$$t=\tfrac{1}{2}[1-\cos(p\phi)] \tag{2.11}$$

in Eq. (2.5) when $U(\phi)$ is given by Eq. (2.6). Some straightforward algebra then yields that $R(t)$ satisfies the equation

$$t(1-t)R''(t)+\left[\frac{1}{2}+\alpha-2t\left(\frac{1}{2}+\alpha\right)\right]R'(t)-\left[\alpha^2-\frac{m^2}{p^2}\right]R(t)=0. \tag{2.12}$$

In the above, a prime denotes differentiation with respect to the variable t. This is precisely the form obeyed by a hypergeometric function[7] in the variable t. Thus the wave function $K(\phi)$ is given by

$$K(\phi)=(\sin p\phi)^\alpha F\left[\alpha+\frac{m}{p},\alpha-\frac{m}{p},\alpha+\frac{1}{2},\frac{1}{2}(1-\cos p\phi)\right]. \tag{2.13}$$

The hypergeometric function as given in Eq. (2.13) is in general not an acceptable wave function, since it diverges at $p\phi=\pi$. For it to be well behaved, the series has to terminate to a finite polynomial, leading to the condition that the argument $(\alpha-m/p)$ is a negative integer or zero, i.e.,

$$m=p(\alpha+n_1),\quad n_1=0,1,2,\cdots. \tag{2.14}$$

Note again that m in general is not an integer, but the above condition on m yields the discrete quantum number n_1 corresponding to azimuthal quantization. Further simplification results by noting that the Gegenbauer polynomial[8] $C^\alpha_{n_1}(\cos p\phi)$ is proportional to $F[n_1+2\alpha,-n_1,\alpha+\frac{1}{2},\frac{1}{2}(1-\cos p\phi)]$. The function $C^\alpha_{n_1}(\cos p\phi)$, defined in the range $0\leqslant p\phi\leqslant\pi$, is a polynomial of degree n_1. Thus the acceptable (unnormalized) angular wave function labeled by the quantum number n_1 is given by

$$K_{n_1}(\phi)=(\sin p\phi)^\alpha C^\alpha_{n_1}(\cos p\phi). \tag{2.15}$$

The corresponding eigenvalue m^2 of Eq. (2.5) is defined by the discrete spectrum

$$m^2=p^2(\alpha+n_1)^2,\quad n_1=0,1,2,\cdots. \tag{2.16}$$

This solution was given by Calogero[4] while solving the three body problem in one dimension with a pairwise inverse square potential. This will be discussed presently.

The reality of the parameter α, as defined in Eq. (2.9), implies that $4G/p^2\geqslant-1$. In the radial Eq. (2.4), $m^2\geqslant\frac{1}{4}$, and analytical solutions may be obtained if the potential $\tilde{U}(r)$ is

taken to be simple harmonic or of Coulomb type. For example, for $\tilde{U}(r)=\frac{1}{4}\omega^2 r^2$, the eigenfunctions of Eq. (2.4) are[1]

$$u_{n,n_1}(r)=r^{m+1/2}e^{-\omega r^2/4}L_n^m(\tfrac{1}{2}\omega r^2), \tag{2.17}$$

with $n=0,1,2,\ldots$ and m is defined by Eq. (2.14) for $n_1=0,1,2,\cdots$. The corresponding eigenvalues are given by[1]

$$E_{n,n_1}=(2n+m+1)\omega. \tag{2.18}$$

One may now ask if there is any problem of physical interest with a noncentral potential of the type discussed above. As mentioned already, Calogero[4] considered a model three body quantum problem in one spatial dimension with the Hamiltonian

$$H=\sum_{i=1}^{3}-\frac{\partial^2}{\partial x_i^2}+\frac{\omega^2}{12}\sum_{i<j}(x_i-x_j)^2+\frac{1}{2}g\sum_{i<j}(x_i-x_j)^{-2}. \tag{2.19}$$

The three particles, after the center-of-mass motion is factored out, have two independent degrees of freedom, which may be mapped on to the (r,ϕ) coordinates of a particle in a noncentral potential. To be more specific, define the Jacobi coordinates

$$X=\tfrac{1}{3}(x_1+x_2+x_3),\qquad x=\frac{(x_1-x_2)}{\sqrt{2}},\quad y=\frac{(x_1+x_2-2x_3)}{\sqrt{6}}. \tag{2.20}$$

The potentials in Eq. (2.19) depend only on the relative coordinates x, y, and therefore the wave function in the center-of-mass variable X is a plane wave that can be separated out. A mapping of the problem to the motion of a particle on a plane in the field of a noncentral potential may be done by defining

$$x=r\sin\phi,\quad y=r\cos\phi,\qquad r^2=\tfrac{1}{3}[(x_1-x_2)^2+(x_2-x_3)^2+(x_3-x_1)^2], \tag{2.21}$$

with the range of the variables $0\leq r\leq\infty$, $0\leq\phi\leq 2\pi$. A little algebra shows that

$$(x_1-x_2)=\sqrt{2}\,r\sin\phi,\qquad (x_2-x_3)=\sqrt{2}\,r\sin(\phi+2\pi/3),\qquad (x_3-x_1)=\sqrt{2}\,r\sin(\phi+4\pi/3). \tag{2.22}$$

Furthermore, by using the trigonometric identity

$$\sum_{m=1}^{3}\operatorname{cosec}^2[\phi+2(m-1)\pi/3]=9\operatorname{cosec}^2(3\phi), \tag{2.23}$$

it is straightforward to verify that the problem reduces to the noncentral potential (2.1) for a particle on a plane, with

$$\tilde{U}(r)=\frac{1}{4}\omega r^2,\quad U(\phi)=\frac{9}{2}\frac{g}{(\sin 3\phi)^2}. \tag{2.24}$$

In the range $0\leq\phi\leq(\pi/3)$, the solution is then given by Eq. (2.16) with $p=3$, and the wave function vanishing at the edges $\phi=0$ and $\pi/3$. Within this range, Eq. (2.22) shows that the spatial ordering of the particles is given by $x_1\geq x_2\geq x_3$. Because of the singular nature of the potential $U(\phi)/r^2$, the particles cannot cross, and the ordering is fixed. In another sector, e.g., $\pi/3\leq\phi\leq 2\pi/3$, Eq. (2.22) shows that $x_1\geq x_3\geq x_2$; it is as if the coordinates x_2 and x_3 have been interchanged. The wave function $K_{n_1}(\phi)$ may be then extended to this region from the original range by imposing the appropriate symmetry requirement due to the exchange of particles 2 and 3. The interested reader may look up these details in Calogero's paper.[4]

This somewhat academic example becomes more significant when it is realized[9] that the N-body problem ($N>3$) with the Hamiltonian given by Eq. (2.19) is exactly solvable (though by a different method). Sutherland,[10] in a variation of the theme, solved the problem by considering an inverse square pair potential between particles on a circle, with the interaction summed over all possible windings

$$V(r)=g\sum_{n=-\infty}^{\infty}(r+nL)^{-2}=\frac{g\pi^2}{L^2}\left[\sin\left(\frac{\pi r}{L}\right)\right]^{-2}. \tag{2.25}$$

Here, r is the distance between the two particles on a ring of circumference L, so that $\sin(\pi r/L)=\sin(\phi/2)$, where ϕ is the angle subtended at the center of the circle by the pair. Sutherland showed that the N-body Hamiltonian

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+\frac{g\pi^2}{L^2}\sum_{i<j}\left[\sin\left(\frac{\phi_{ij}}{2}\right)\right]^{-2} \tag{2.26}$$

is exactly solvable with periodic boundary condition. Here, the coordinates x_i are measured along the ring, and $\phi_{ij}=2\pi(x_i-x_j)/L$. The Hamiltonian (2.26) is an example with a pairwise potential that gives rise to nontrivial correlations in the ground state. For a periodic boundary condition, direct substitution shows that the ground state wave function is

$$\Psi=\prod_{i<j}\left|\sin\frac{\pi(x_i-x_j)}{L}\right|^{\alpha}, \tag{2.27}$$

with α given by Eq. (2.9), where $(4G/p^2)$ is replaced by $2g$. The corresponding eigenvalue is given by

$$E_N=\frac{1}{3}\alpha^2\pi^2\frac{N(N^2-1)}{L^2}, \tag{2.28}$$

where N denotes the number of particles.

Although the many body problem with the inverse pair potential is an example of a fully integrable system, there appears to be a deep connection between the expression of $|\Psi|^2$ obtained from Eq. (2.27), and the quantum spectral distribution of systems that are chaotic.[10,11] A discussion of this fascinating connection is beyond the scope of this paper. The many-body models of the Calogero–Sutherland type have been popular in recent times in statistical mechanics[12] and in the physics of spin chains.[13]

III. SOLUBLE NONCENTRAL POTENTIALS IN THREE DIMENSIONS

In spherical polar coordinates, a noncentral potential of the form

$$V(r,\theta,\phi)=\tilde{U}(r)+\frac{V(\theta)}{r^2}+\frac{U(\phi)}{r^2\sin^2\theta}, \tag{3.1}$$

is classically integrable,[6] with three constants of motion. The Schrödinger equation is also separable in the coordinates, and with suitable choices for the potentials $\tilde{U}(r)$, $V(\theta)$ and

$U(\phi)$, the uncoupled equations can be exactly solved. The Schrödinger equation for the wave function $\Psi(r,\theta,\phi)$ is given by

$$\left[-\left(\frac{\partial^2\Psi}{\partial^2 r}+\frac{2}{r}\frac{\partial\Psi}{\partial r}\right)-\frac{1}{r^2}\left(\frac{\partial^2\Psi}{\partial\theta^2}+\cot\theta\frac{\partial\Psi}{\partial\theta}\right)-\frac{1}{r^2\sin^2\theta}\frac{d^2\Psi}{\partial\phi^2}\right]=(E-V)\Psi. \tag{3.2}$$

It is convenient to write $\Psi(r,\theta,\phi)$ as

$$\Psi(r,\theta,\phi)=\frac{u(r)}{r}\frac{H(\theta)}{(\sin\theta)^{1/2}}K(\phi). \tag{3.3}$$

Substituting Eq. (3.3) in Eq. (3.2), we obtain

$$\left[-\frac{1}{u}\frac{d^2u}{dr^2}+\tilde{U}(r)-\frac{1}{4r^2}\right]+\frac{1}{r^2}\left[-\frac{1}{H}\frac{d^2H}{d\theta^2}+V(\theta)-\frac{1}{4}\operatorname{cosec}^2\theta\right]+\frac{1}{r^2\sin^2\theta}\left[-\frac{1}{K}\frac{d^2K}{d\phi^2}+U(\phi)\right]=E. \tag{3.4}$$

Again, let $K(\phi)$ obey the same equation as Eq. (2.5),

$$-\frac{d^2K}{d\phi^2}+U(\phi)K(\phi)=m^2K(\phi). \tag{3.5}$$

Substituting this in Eq. (3.4), the ϕ dependence in it is eliminated, resulting in the equation,

$$-\frac{1}{u}\frac{d^2u}{dr^2}+\left[\tilde{U}(r)-\frac{1}{4r^2}\right]+\frac{1}{r^2}\left[-\frac{1}{H}\frac{d^2H}{d\theta^2}+V(\theta)+\left(m^2-\frac{1}{4}\right)\operatorname{cosec}^2\theta\right]=E. \tag{3.6}$$

Next, let $H(\theta)$ obey the equation

$$-\frac{d^2H}{d\theta^2}+\left[V(\theta)+\left(m^2-\frac{1}{4}\right)\operatorname{cosec}^2\theta\right]H(\theta)=l^2H(\theta), \tag{3.7}$$

where l need not be an integer. A further substitution of this equation in Eq. (3.6) then completes the separation of the variables, giving the radial equation,

$$-\frac{d^2u}{dr^2}+\left[\tilde{U}(r)+\frac{(l^2-1/4)}{r^2}\right]u(r)=Eu(r). \tag{3.8}$$

Note that this is exactly the same as Eq. (2.4), except that m^2 has been replaced by l^2. The three equations (3.5), (3.7), and (3.8) may be solved analytically by choosing the potentials suitably.

As an illustration, we consider the potential

$$V_1(r,\theta,\phi)=\frac{\omega^2}{4}r^2+\frac{\delta}{r^2}+\frac{C}{r^2\sin^2\theta}+\frac{D}{r^2\cos^2\theta}+\frac{G}{r^2\sin^2\theta\sin^2 p\phi}+\frac{F}{r^2\sin^2\theta\cos^2 p\phi}, \tag{3.9}$$

where ω, δ, C, D, G, F, and p are parameters, with p being an integer as before. There are some restrictions on the other parameters (to be given later) arising from the acceptability of the wave function. Comparing Eqs. (3.9) and (3.1), we obtain the Pöschl–Teller potential hole that is solved in Flügge's text,[2]

$$U(\phi)=G\operatorname{cosec}^2 p\phi+F\sec^2 p\phi. \tag{3.10}$$

Note that this potential is highly singular at $\phi=0$ and $p\phi=\pi/2$. Thus the range for $K(\phi)$ is $0\leq p\phi\leq\pi/2$ with the boundary conditions [cf. Eq. (2.8)]

$$K(\phi=0)=0=K(p\phi=\pi/2). \tag{3.11}$$

With the above boundary condition in mind, it is natural to take the form

$$K(\phi)=(\sin p\phi)^{\alpha}(\cos p\phi)^{\beta}R(\phi), \tag{3.12}$$

in Eq. (3.5) with $U(\phi)$ given by Eq. (3.10). Here, α and β are real positive constants and $R(\phi)$ is a smooth function which is finite and nonzero at $\phi=0$ and $p\phi=\pi/2$. This fixes α and β

$$\alpha=\tfrac{1}{2}+\tfrac{1}{2}(1+4G/p^2)^{1/2},\qquad \beta=\tfrac{1}{2}+\tfrac{1}{2}(1+4F/p^2)^{1/2}. \tag{3.13}$$

The complete eigenspectrum is now given by $(n_1=0,1,2,\ldots)$

$$\frac{m^2}{p^2}=[2n_1+\alpha+\beta]^2. \tag{3.14}$$

The unnormalized wave function in the ϕ coordinate is given in terms of the Jacobi polynomial $P_{n_1}^{\alpha-1/2,\beta-1/2}$ of degree n_1,

$$K(\phi)=(\sin p\phi)^{\alpha}(\cos p\phi)^{\beta}P_{n_1}^{\alpha-1/2,\beta-1/2}(\cos 2p\phi). \tag{3.15}$$

Having solved the eigenvalue m^2 of the ϕ part, the Schrödinger equation (3.7) for the θ variable can be taken up. Again, comparing Eqs. (3.1) and (3.9), we see that

$$V(\theta)=C\operatorname{cosec}^2\theta+D\sec^2\theta. \tag{3.16}$$

The Schrödinger equation for $H_1(\theta)$ is

$$-\frac{d^2H}{d\theta^2}+[(C+m_1^2-1/4)\operatorname{cosec}^2\theta+D\sec^2\theta]H=l^2H. \tag{3.17}$$

Note that as in the ϕ case, this potential $V_1(\theta)$ is singular at $\theta=0$ and $\theta=\pi/2$. Thus Eq. (3.17) is solved in the range $0\leq\theta\leq\pi/2$ with the boundary conditions

$$H(\theta=0)=H(\theta=\pi/2)=0. \tag{3.18}$$

Since Eq. (3.17) and the boundary conditions (3.18) are identical to those discussed for the ϕ variable, the eigenvalue spectrum and the eigenfunctions can be written down immediately. These are given by

$$l^2=[2n_2+\tilde{\alpha}+\tilde{\beta}]^2, \tag{3.19}$$

with $n_2=0,1,2,\cdots$. In the above equation,

$$\tfrac{1}{2}\tilde{\alpha}=+(C+m^2)^{1/2},\qquad \tilde{\beta}=\tfrac{1}{2}+\tfrac{1}{2}(1+4D)^{1/2}, \tag{3.20}$$

and

$$H_{n_2}(\theta)=(\sin\theta)^{\alpha}(\cos\theta)^{\beta}P_{n_2}^{\tilde{\alpha}-1/2,\tilde{\beta}-1/2}(\sin 2\theta). \tag{3.21}$$

Note that in general there is no degeneracy in l except for $C=0$, and then it is given by

Table I. The three solvable potentials $U(\phi)$ are given in column (1). The eigenvalues m^2 of Eq. (3.5) are listed in column (2), and the corresponding eigenstates in column (3). Case (i) is discussed in detail in the text.

$U(\phi)$	m^2	$K(\phi)$
(i) $G\,\mathrm{cosec}^2(p\phi)+F\,\sec^2(p\phi)$ $p=1,2,3,\cdots$	$p^2(\alpha+\beta+2n_1)^2$ $2\alpha = 1+\sqrt{1+4G/p^2}$ $2\beta = 1+\sqrt{1+4F/p^2}$	$(\sin p\phi)^{\alpha}(\cos p\phi)^{\beta}$ $\times P_{n_1}^{(\alpha-1/2,\beta-1/2)}(\cos 2p\phi)$ $n_1=0,1,2,\cdots$
(ii) $G\,\mathrm{cosec}^2(p\phi)+F\,\cot(p\phi)$ $p=1,2,3,\cdots$	$p^2\left[(\alpha+n_1)^2-\dfrac{\lambda^2}{(\alpha+n_1)^2}\right]$ $2\alpha = 1+\sqrt{1+4G/p^2}$ $2\lambda=\dfrac{F}{p^2}$	$(\sin p\phi)^{(\alpha+n_1)}e^{\gamma p\phi}$ $\times P_{n_1}^{(-\alpha-n_1-i\gamma,-\alpha-n_1+i\gamma)}(i\cot p\phi)$ $\gamma=\dfrac{\lambda}{(\alpha+n_1)}$
(iii) $G\,\mathrm{cosec}^2(p\phi)$ $-F\,\cot(p\phi)\mathrm{cosec}(p\phi)$ $p=1,3,5,\ldots$	$(A+n_1p)^2$ $G=A^2+B^2-Ap$ $F=B(2A-p)$	$(1-\cos p\phi)^{(s-\lambda)/2}(1+\cos p\phi)^{(s+\lambda)/2}$ $\times P_{n_1}^{(s-\lambda-1/2,s+\lambda-1/2)}(\cos p\phi)$ $s=A/p,\ \lambda=B/p$

$$l^2=p(2n_1+1)+(2n_2+1)+\sqrt{D+1/4}+\sqrt{F+p^2/4}+\sqrt{G+p^2/4}. \tag{3.22}$$

Finally, the radial Schrödinger Eq. (3.8)

$$-\frac{d^2u}{dr^2}+\left(\frac{\omega^2r^2}{4}+\frac{\delta+l^2-1/4}{r^2}\right)u=Eu \tag{3.23}$$

is to be solved, and this is exactly of the same form as Eq. (2.4). The solutions may be labeled by the radial quantum number n, and the angular quantum numbers n_1 and n_2 that define l^2 in Eq. (3.19)

$$u_{n,n_1,n_2}(r)=r^{(\sqrt{\delta+l^2}+1/2)}\exp(-\tfrac{1}{4}\omega r^2)L_n^{\sqrt{\delta+l^2}}(\tfrac{1}{2}\omega r^2). \tag{3.24}$$

The corresponding eigenvalues are given by

$$E_{n,n_1,n_2}=[(2n+1)+(\delta+l^2)^{1/2}]\omega, \tag{3.25}$$

where l^2 is given explicitly as

$$l^2=\left[(2n_2+1)+\sqrt{D+\frac{1}{4}}+\left\{C+\left(\sqrt{F+\frac{p^2}{4}}+\sqrt{G+\frac{p^2}{4}}+p(2n_1+1)\right)^2\right\}^{1/2}\right]^2. \tag{3.26}$$

Thus the complete eigenfunction of the noncentral potential (3.9) is given by the form (3.3), with $u(r)$, $H(\theta)$, $K(\phi)$ as defined by Eqs. (3.24), (3.21), and (3.15), respectively. Note that there is degeneracy in the problem when either δ or C (or both) are zero. The maximum degeneracy is obtained when both δ and C are zero, and the eigenspectrum then reduces to the form

$$E_{n,n_1,n_2}=(2n+l+1)\omega,$$

where

$$l=\left[(2n_2+1)+\sqrt{D+\frac{1}{4}}+\sqrt{F+\frac{p^2}{4}}+\sqrt{G+\frac{p^2}{4}}+p(2n_1+1)\right]. \tag{3.27}$$

Since degeneracy is usually associated with some symmetry in the system, it would be interesting to enquire about the extra symmetry in the problem. For the case $p=1$ (and $\delta=C=0$), the symmetry is clear. In such a case, the potential is simply the spherically symmetric harmonic oscillator, with the perturbations of the form F/x^2, G/y^2, and D/z^2. However, in general, for any other p, the symmetry is not obvious.

Table II. The three potentials $V(\theta)$ are shown in column (1). The eigenvalues l^2 of Eq. (3.7) are given in column (2), and the corresponding eigenstates in column (3). Case (i) is treated in detail in the text.

$V(\theta)$	l^2	$H(\theta)$
(i) $C\,\mathrm{cosec}^2\,\theta+D\,\sec^2\,\theta$	$(\tilde{\alpha}+\tilde{\beta}+2n_2)^2$ $\tilde{\alpha} = \frac{1}{2}+\sqrt{C+m^2}$ $\tilde{\beta} = \frac{1}{2}+\frac{1}{2}\sqrt{(1+4D)}$	$(\sin\theta)^{\tilde{\alpha}}(\cos\theta)^{\tilde{\beta}}$ $\times P_{n_2}^{\tilde{\alpha}-1/2,\tilde{\beta}-1/2}(\cos 2\theta)$ $n_2=0,1,2,\cdots$
(ii) $C\,\mathrm{cosec}^2\,\theta+D\,\cot\,\theta$	$(\tilde{\alpha}+n_2)^2-\dfrac{\lambda^2}{(\tilde{\alpha}+n_2)^2}$ $\tilde{\alpha} = \frac{1}{2}+\sqrt{(C+m^2)}$ $\lambda=D/2$	$(\sin\theta)^{\tilde{\alpha}+n_2}e^{\gamma\theta}$ $\times P_{n_2}^{-\tilde{\alpha}-n_2-i\gamma,-\tilde{\alpha}-n_2+i\gamma}(i\cot\theta)$ $\gamma=\dfrac{\lambda}{(\tilde{\alpha}+n_2)}$
(iii) $C\,\mathrm{cosec}^2\,\theta$ $+D\,\mathrm{cosec}\,\theta\cot\,\theta$	$(A_1+n_2+\frac{1}{2})^2$ $A_1^2+B_1^2=m^2+C$ $2A_1B_1=D$	$(1-\cos\theta)^{[(A_1+B_1+1/2)/2]}(1+\cos\theta)^{[(A_1-B_1+1/2)/2]}$ $\times P_{n_2}^{(A_1+B_1,A_1-B_1)}(\cos\theta)$

Table III. The two solvable radial potentials for the eigenvalue Eq. (3.8). The eigenenergy E [see Eq. (3.25)] and the corresponding eigenfunction $u(r)$ are displayed in columns (2) and (3), respectively.

$U(r)$	E	$u(r)$
(i) $\frac{\omega^2}{4}r^2+\delta/r^2$	$(2n+B_2+\frac{3}{2})\omega$	$r^{B_2+1}e^{-wr^2/4}L_n^{B_2+1/2}(\frac{1}{2}\omega r^2)$
	$B_2 = -\frac{1}{2}+\sqrt{\delta+l^2}$	$n=0,1,2,\ldots$
(ii) $-\frac{e^2}{r}+\frac{\delta}{r^2}$	$\frac{e^4}{4(n+B_2+1)^2}$	$y^{B_2+1}\exp(-\frac{1}{2}y)L_n^{2B_2+1}(y)$
	$B_2 = -\frac{1}{2}+\sqrt{\delta+l^2}$	$y=\frac{e^2r}{(n+B_2+1)}$, $n=0,1,2,\ldots$

IV. DISCUSSION

The potentials for which solutions were found in the earlier sections are highly singular at $\theta=0,\ \pi/2,\ldots$, and at $(p\phi)=0,\ \pi,\ldots$. This resulted in solutions that were restricted in angular ranges, e.g., $(0\leqslant\theta\leqslant\pi/2)$, and $(0\leqslant\phi\leqslant\pi/p)$. In general, there is no physical way of connecting these disjointed solutions in the different angular regions. However, for the two dimensional case, when a mapping is done to the corresponding three-body problem, the different angular regions corresponded to distinct ordering of the particles. No such physical interpretation is apparent in the three dimensional case.

After having dealt with the potential given by Eq. (3.9) in detail, we may search for other examples of solvable noncentral potentials in spherical polar coordinates in three dimensions. One way to answer this question is to go through the list of the analytically solvable potentials in one dimension as given in the standard texts on quantum mechanics.[1,2] It is found that there are three possible forms for $U(\phi)$ and $V(\theta)$ and two possible forms for $\tilde{U}(r)$ for which the corresponding Schrödinger equations are solvable. In Tables I to III we give the possible forms for $U(\phi)$, $V(\theta)$, $\tilde{U}(r)$, and the corresponding eigenvalues and eigenfunctions which have been calculated by following the same procedure as given above. Of course, due attention has to be paid to the restrictions on the parameters arising from the physical acceptibility of the wave function. It is worth pointing out that for all the 18 examples, the energy eigenvalues and eigenfunctions may also be obtained algebraically by using the property of shape invariant potentials within the formalism of supersymmetric quantum mechanics.[5,14] In fact, in constructing the Tables I–III, we have taken advantage of the list of shape-invariant potentials given in Ref. 15. This aspect of the problem will not be discussed here. The interested reader may also look up Ref. 16, where supersymmetry has been exploited to solve algebraically the three-body problem in one dimension for many other examples.

It is also clear from the above discussion that in two dimensions there will be six exactly solvable noncentral potentials in spherical polar coordinates corresponding to the various choices for $\tilde{U}(r)$ and $U(\phi)$.

The main results can be summarised as follows:

(i) It is seen from the three tables that 18 different noncentral potentials in spherical polar coordinates may be constructed in three dimensions by taking various combinations of $\tilde{U}(r)$, $V(\theta)$, and $U(\phi)$ for which the energy eigenvalues and eigenfunctions can be obtained analytically. Each of these 18 noncentral potentials may have up to 7 independent parameters, as in the example given by Eq. (3.9).

(ii) For all the 18 potentials, the eigenfunctions are given by

$$\psi(r,\theta,\phi)=u_n(r)H_{n_2}(\theta)K_{n_1}(\phi),$$

where n, n_1, n_2 can take integral values $0,1,2,3\cdots$. Depending on the form and choice of the parameters in the angle-dependent potentials, some degeneracy in the spectrum may arise.

(iii) For the nine noncentral potentials where $\tilde{U}(r)$ is taken to be the Coulomb potential, one also has a continuous spectrum over and above the discrete one. It would be interesting to obtain the phase shifts for these noncentral potentials.

(iv) As mentioned already, for all the 18 noncentral potentials, one may obtain the spectrum algebraically without solving the Schrödinger equation. This is also related to Schrödinger's factorization method.[17]

(v) Generalization of our technique to noncentral potentials in other standard orthogonal coordinate systems is straightforward. For example, one could instead consider the Schrödinger equation in the cylindrical coordinates and obtain other examples of the noncentral potentials with seven parameters. The spectra may again be written down by using the well known results for the analytically solvable potentials in one dimension in each of the coordinates ϕ, ρ, and z, where $\rho=\sqrt{x^2+y^2}$. Other systems of coordinates, or higher dimensions may similarly be considered.

(vi) For noncentral potentials in two dimensions, there are interesting applications in many-body problem, as discussed in Sec. II. However, it is not clear if the noncentral potentials in three dimensions, discussed in Sec. III, are of any physical interest.

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Collinear H+H–H reaction. Computer simulation of quasiclassical trajectories

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An undergraduate computer project, suitable for a computational physics or applied numerical analysis course, is presented. The equations of motion for the three H atoms of the collinear H+H–H system are set up in the Hamiltonian formalism. They are then solved numerically, using the analytical Porter–Karplus potential energy function and the Runge–Kutta algorithm. The program is used to illustrate several types of motion: nonlinear oscillations of the H_2 molecule, atom–molecule inelastic collisions, reactive collisions. Results are displayed either as internuclear distances versus time or as the motion of a point in configuration space.

I. INTRODUCTION

Since several years, the Physics Department of our University requires undergraduates to complete a semester course on Applied Numerical Analysis. As part of the course work, students must write at least one computer project. The program should simulate some interesting physical phenomenon, for which analytical study is either impossible or very lengthy. Students are given a short (one or two pages) text describing a mathematical model of a physical system and are asked to select and implement a suitable numerical method and to explore properties of the model. The required level of mathematical ability is roughly intermediate between what is expected of the reader by Gould and Tobochnik[1] and by Koonin.[2] In this context, we have found that an investigation of reactive collisions between simple atomic systems provides an interesting challenge, requiring a working knowledge of Lagrangian or Hamiltonian dynamics and of numerical methods for solving initial value differential problems. Further, the current intense research interest in similar problems may motivate students. We offer this account in the belief that it may be useful to other Physics instructors.

The system $H+H_2$ (and its isotopic variations, such as $D+H_2$) is the simplest and best known reactive system.[3–7] It has been the subject of so many experimental and theoretical investigations that even review papers are too numerous to be all cited here. The theoretical approach is usually divided in two parts. One first determines, through quantum mechanical calculations in the framework of the Born–Oppenheimer approximation, the energy of the system, as a function of the nuclear distances. This step yields a so-called potential energy surface (PES). Once the PES has been obtained, the dynamics of the nuclei can be investigated. Two courses are then open to the investigator: either the nuclei are

