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Schrodinger Particle on Spheroidal Surfaces

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Abstract It is shown that the problem of a Schrödinger particle in stationary motion on prolate and oblate spheroidal surfaces has an exact solution. The constants of motion are explicitly identified, and the procedure to construct the eigenfunctions and energy eigenvalues is outlined. Illustrations of the energy spectra for spheroids of different eccentricities are presented.

1. INTRODUCTION

The problem of a point particle constrained to move on a M-sphere S^N under the action of a conservative central force, has been investigated and solved in its nonrelativistic, classical and quantum mechanical versions[1,2,3]. More recently, Ferreira and Palladino have shown that one relativistic and quantum mechanical version of the problem, namely, a Dirac particle constrained to move freely on a two-dimensional sphere S^2, admits exact solutions[4], As it was pointed out in ref. 4, possible extensions of such problems may involve other surfaces.

In this paper, we show that the problem of a Schrödinger particle constrained to move on a two-dimensional spheroidal surface embedded in a three-dimensional euclidean space has an exact solution. In section 2, we identify the constants of motion, in their classical and quantum versions, for the free particle in euclidean space in both prolate and oblate spheroidal coordinates, which is useful to show and to understand the separability and the solution of the Schrödinger

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+ Consultant of Instituto Nacional de Investigaciones Nucleares equation. In section 3, the constrain on the particle to move on a spheroidal surface is introduced, and the procedure to obtain its eigenfunctions and energy eigenvalues is outlined. In section 4, we present some illustrations of the energy spectra for both prolate and oblate spheroids of different eccentricities, and discuss their relations with the spectra of some other rotators.

2. CONSTANTS OF MOTION AND SEPARABILITY OF THE SCHRÖDINGER EQUAVION

In this section we follow Erkson and Hill[5] to identify the constants of motion and to understand the reason for the separability of the Schrödinger equation in both prolate and oblate spheroidal coordinates. In fact, the results of ref. 5 for the case of one-electron states of diatomic molecules can be directly applied to the case of the free particle in prolate spheroidal coordinates by taking thei nuclear charges equal to zero. For the sake of completeness and as a point of comparison, we treat the last case explicitly. Then we carry out the corresponding analysis for the free particle in oblate spheroidal coordinates pointing out the differences and similarities.

Let us first define the spheroidal coordinates. In the prolate case we take the foci 1 and 2 on the z-axis at distances f from the origin below and above the xy-plane, respectively. The position of a point in space can be defined by its distances r_1 and r_2 from the respective foci, and the angle between the xz-plane and the plane determined by the z-axis and the point itself. The prolate spheroidal coordinates are defined by

$$\xi = \frac{r_1 + r_2}{2f}, \quad \eta = \frac{r_1 - r_2}{2f}, \quad \phi \tag{1}$$

which are mutually orthogonal prolate spheroids of eccentricity $1/\xi$, two-sheet hyperboloids of eccentricity $1/\eta$, and planes containing the z-axis of revolution. In the oblate case, the foci form a circle in the xy-plane centered at the origin and with a radius f. Calling 1 and 2 the foci in the plane determined by the z-axis and the point under consideration, the position of the latter is again fixed by the distances r_1 and r_2, and the angle ϕ which that plane makes with the xz-plane. The oblate spheroidal coordinates can be defined through eqs. (1) with the appropriate distances r_1 and r_2, but we choose the alternative set

$$\zeta = \sqrt{\xi^2-1}\ , \quad \omega = \sqrt{1-\eta^2}\ , \ \phi \tag{2}$$

which are mutually orthogonal oblate spheroids of eccentricity $1/\sqrt{\zeta^2+1}$, one-sheet hyperboloids of eccentricity $1/\sqrt{1-\omega^2}$ and planes containing the z-axis of revolution. The choice of this alternative set of coordinates leads to a closer similarity of the equations of motion for the prolate and oblate cases.

For the free particle and for both systems of coordinates the energy E and the z-component of the angular momentum ℓ are immediately identified as constants of the motion. In both cases another constantof the motion can be identified, and we proceed to construct it following ref. 5. Let

$$\vec{\ell}_1 = \vec{r}_1\times\vec{p} = (\vec{r}+\vec{f})\times\vec{p} \tag{3a}$$

and

$$\vec{\ell}_2 = \vec{r}_2\times\vec{p} = (\vec{r}-\vec{f})\times\vec{p} \tag{3b}$$

be the orbital angular momenta of the particle relative to the respective foci 1 and 2. In the familiar case of spherical coordinates the focal semiaxis $\vec{f}$ vanishes and both angular momenta reduce to the angular momentum relative to the origin; in such a case, the square of the latter $\vec{\ell}.\vec{\ell} = (\vec{r}\times\vec{p}).(\vec{r}\times\vec{p})$ is known to be a constant of motion. This suggests one should analyze the quantity $\vec{\ell}_1.\vec{\ell}_2$ and its variation with time for the present case of spheroidal coordinates. It is straightforward to establish that

$$\frac{d}{dt}(\vec{\ell}_1.\vec{\ell}_2) = -2\left[\frac{d\vec{f}}{dt}\times\vec{p}\right].[\vec{f}\times\vec{p}]\ . \tag{4}$$

In the prolate case, $\vec{f} = \hat{k}f$ is a fixed vector, and therefore $\vec{\ell}_1.\vec{\ell}_2$ is a constant of the motion. The corresponding quantum symmetrized operator will be represented by

$$\hbar^2\hat{\Lambda}_p = \frac{1}{2}[\vec{\ell}_1.\vec{\ell}_2 + \vec{\ell}_2.\vec{\ell}_1] = \hat{\ell}^2 - (\vec{f}\times\vec{p}).(\vec{f}\times\vec{p})$$

$$= \hat{\ell}^2 - f^2(\hat{p}^2-\hat{p}_z^2) \tag{5a}$$

In the oblate case, the position vector of focus 2 is radial $\vec{f} = \hat{\rho} f$ and its time rate of change is $df/dt = \hat{\phi}\dot{\phi} f$. By using the cylindrical components of the linear momentum, $p_\rho = \mu\dot{\rho}$ and $p_\phi = \mu\rho\dot{\phi}$, and the e-components of angular momentum $\ell_z = \mu\rho^2\dot{\phi}$, eq. (4) can be written as

$$\frac{d}{dt}(\vec{\ell}_1 . \vec{\ell}_2) = 2(\vec{f}.\vec{p})(\vec{p} . \frac{d\vec{f}}{dt}) = 2f^2 p_\rho p_\phi \dot{\phi}$$

$$= 2f^2\mu^2\rho\dot{\rho}\dot{\phi}^2 = 2f^2\ell_z^2\dot{\rho}/\rho^3$$

$$= -\frac{d}{dt}\left(\frac{f^2\ell_z^2}{\rho^2}\right) \qquad (6)$$

Consequently, $\vec{\ell}_1 . \vec{\ell}_2 + (f^2\ell_z^2/\rho^2)$ is a constant of motion; the last term can be interpreted as arising from the rotation of the plane containing the foci 1 and 2. The corresponding quantum operator is

$$\hbar^2\hat{\Lambda}_0 = \frac{1}{2}\left[\vec{\ell}_1 . \vec{\ell}_2 + \vec{\ell}_2 . \vec{\ell}_1\right] + \frac{f^2\ell_z^2}{\rho^2}$$

$$= \hat{\ell}^2 - (\vec{f}\times\vec{p}) . (\vec{f}\times\vec{p}) + \frac{f^2\ell_z^2}{\rho^2} \qquad (5b)$$

The quantum operators representing the constants of tlie motion in prolate and oblate spheroidal coordinates can be written respectively as follows, The hamiltonian operators are

$$\hat{H}_p = -\frac{\hbar^2}{2\mu f^2}\left\{\frac{1}{\xi^2-\eta^2}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right] + \frac{1}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\phi^2}\right\} \qquad (6a)$$

$$\hat{H}_0 = -\frac{\hbar^2}{2\mu f^2}\left\{\frac{1}{\zeta^2+\omega^2}\left[\frac{\partial}{\partial\zeta}(\zeta^2+1)\frac{\partial}{\partial\zeta} + \frac{\partial}{\partial\omega}(1-\omega^2)\frac{\partial}{\partial\omega}\right] + \frac{1}{(\zeta^2+1)(1-\omega^2)}\frac{\partial^2}{\partial\phi^2}\right\} \qquad (6b)$$

The operators of eqs. (5) become

$$\hat{\Lambda}_p = \frac{\eta^2}{\xi^2-\eta^2}\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} - \frac{\xi^2}{\xi^2-\eta^2}\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} - \frac{\xi^2+\eta^2-1}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\phi^2} \qquad (7a)$$

$$\Lambda_0 = -\frac{\omega^2}{\zeta^2+\omega^2}\frac{\partial}{\partial\zeta}(\zeta^2+1)\frac{\partial}{\partial\zeta} - \frac{\zeta^2}{\zeta^2\ \omega^2}\frac{\partial}{\partial\omega}(1-\omega^2)\frac{\partial}{\partial\omega} - \frac{\zeta^2\ \omega^2}{(\zeta^2-1)(1-\omega^2)}\frac{\partial^2}{\partial\phi^2} \qquad (7b)$$

And the z-component of the angular momentum has the well-known form

$$\hat{\ell}_z = -i\hbar \frac{\partial}{\partial\phi} . \tag{8}$$

The operators $\hat{H}$, $\hat{\Lambda}$ and $\hat{\ell}_z$ commute with each other by pairs and consequently they have common eigenfunctions. We represent the respective eigenvalues by $E = \hbar^2 k^2/2\mu$, λ and $\hbar m$, where $m = 0, \pm 1, \pm 2, \ldots$. The eigenvalue equations for H and $\hat{\Lambda}$ are separable with eigenfunctions

$$\psi(\xi,\eta,\phi) = \Xi(\xi)H(\eta)\Phi(\phi) \tag{9a}$$

$$\psi(\zeta,\omega,\phi) = Z(\zeta)\Omega(\omega)\Phi(\phi) \tag{9b}$$

It is straightforward to obtain from either of those eigenvalue equations the corresponding separated ordinary differential equations

$$\left[\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi} - \frac{m^2}{\xi^2-1} + k^2f^2\xi^2 - \lambda\right]\Xi = 0 \tag{10a}$$

$$\left[\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta} - \frac{m^2}{1-\eta^2} - k^2f^2\eta^2 + \lambda\right]H = 0 \tag{11a}$$

and

$$\left[\frac{d}{d\zeta}(\zeta^2+1)\frac{d}{d\zeta} + \frac{m^2}{\zeta^2+1} + k^2f^2\zeta^2 - \lambda\right]Z = 0 \tag{10b}$$

$$\left[\frac{d}{d\omega}(1-\omega^2)\frac{d}{d\omega} - \frac{m^2}{1-\omega^2} + k^2f^2\omega^2 + \lambda\right]\Omega = 0 \tag{11b}$$

When we start from the Schrödinger equation, the constant of separation is λ. When we start from the eigenvalue equation for the operator $\hat{\Lambda}$, the constant of separation is k^2f^2. We have thus estahlished that the separability of the Schrödinger equation in prolate and oblate spheroidal coordinates is due to the existence of the respective constants of motion of eqs. (5a) and (5b), which leads to the commutation of the hamiltonian and $\hat{\Lambda}$ operators of eqs. (6) and (7), and to their common eigenfunctions.

3. THE EIGENVALUE PROBLEM ON SPHEROIDAL SURFACES

Now we follow ref. 4, starting with the equations of motion in the Euclidean three-dimensional space developed in the previoussection, and restricting ourselves from now on to the two-dimensional spheroidal surfaces defined by $\xi = \xi_0$ or $\zeta_0 = \sqrt{\xi_0^2-1}$. Correspondingly, in eqs.(10) we take

$$\Xi(\xi) = \Xi(\xi_0) = \text{constant}\ , \quad \frac{d\Xi}{d\xi} = 0 \tag{12a}$$

$$Z(\zeta) = Z(\zeta_0) = \text{constant}\ , \quad \frac{dZ}{d\zeta} = 0 \tag{12b}$$

and obtain the energy eigenvalues in terms of the other two constants of motion

$$E_{\lambda m} = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2}{2\mu f^2 \xi_0^2}\left[\lambda + \frac{m^2}{\xi_0^2-1}\right] \tag{13a}$$

$$E_{\lambda m} = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2}{2\mu f^2 \zeta_0^2}\left[\lambda - \frac{m^2}{\zeta_0^2+1}\right] \tag{13b}$$

The eigenfunctions of eqs. (9) can be rewritten as

$$\psi_{\lambda m}(\chi,\phi) = X(\chi)\,\Phi(\phi) \tag{14}$$

where χ equal η and ω for the prolate and oblate cases, respectively. Then eqs. (11a) and (11b) can be rewritten in the form

$$\left[-\frac{d}{d\chi}(1-\chi^2)\frac{d}{d\chi} + \frac{m^2}{1-\chi^2} \pm k^2 f^2 \chi^2\right]X = \lambda X \tag{15}$$

where the plus and minus signs apply to the respective cases. This equation and its solutions correspond to the angular spheroidal wave-functions[6]. For the sake of completeness we discuss a method, alternative to that of ref. 6, to obtain the solutions of this eigenvalue problem, which is the eigenvalue problem for the operator $\hat{\Lambda}$. Such a method consists of constructing the matrix of the operator $\hat{\Lambda}$ in an appropriate basis of functions and diagonalizing it[7]. The natural basis is that of associated Legendre polynomials $P_l^m(\chi)$, which are eigenfunctions of the first two terms inside the bracket in eq. (15) with eigenvalues $L(L+1)$. The eigenfunctions of eq. (14) can be written in the corresponding "spherical" harmonic basis as

$$\psi_{\lambda m} = \sum_L a_L Y_{Lm}(\theta,\phi) \tag{16}$$

where $\chi = \cos\theta$, and the matrix form of eq. (15) becomes

$$\begin{aligned}
&\langle Lm|(\hat{L}^2 \pm k^2f^2\chi^2 - \lambda)|L'm\rangle \\
&= \left\{ L(L+1) \pm k^2f^2 \frac{(2L-1)(L+1+m)(L+1-m) + (2L+3)(L+m)(L-m)}{(2L-1)(2L+1)(2L+3)} - \lambda \right\} \delta_{LL'} \\
&\pm k^2f^2 \left\{ \frac{1}{2L+3} \sqrt{\frac{(L+1+m)(L+2+m)(L+1-m)(L+2-m)}{(2L+1)\ (2L+5)}}\ \delta_{L+2,L'} \right. \\
&\quad \left. + \frac{1}{2L-1} \sqrt{\frac{(L+m)(L-m)(L-1+m)(L-1-m)}{(2L-3)\ (2L+1)}}\ \delta_{L-2,L'} \right\} = 0
\end{aligned} \tag{17}$$

For chosen values of m and k^2f^2, this matrix equation can be constructed and solved in a computer obtaining the coefficients a_L for the eigenfunctions in eq. (16) and the eigenvalues $\lambda(k^2f^2)$ to the desired accuracy.

The energy eigenvalues can be determined through eqs. (13a) and (13b), by finding the intersections of the curves $\lambda(k^2f^2)$ with the straightlines

$$y(k^2f^2) = \xi_0^2k^2f^2 - \frac{m^2}{\xi_0^2-1} \tag{18a}$$

and

$$y(k^2f^2) = \zeta_0^2k^2f^2 + \frac{m^2}{\zeta_0^2+1}\ , \tag{18b}$$

respectively.

4. ILLUSTRATION AND DISCUSSION OF ENERGY SPECTRA

In this section we present some graphical results to illustrate the solution of the eigenvalue problem, as outlined in section 3, and the energy spectra of the nonrelativistic quantum particle constrained to move on prolate and oblate spheroidal surfaces of different eccentricities,

Figures la, b, c and d are plots of the eigenvalue λ of eq. (15) versus k^2f^2 for prolate spheroids on the right and for oblate spheroids on the left, and for values of $m = 0,1,2$ and 3, respectively. Notice from eqs. (15) or (17) that the difference between the prolate and oblate cases is in the sign of the term $k^2f^2\chi^2$, resulting in the monotonic increase of the eigenvalues λ when going from left to right in the figures, In particular, when $f = 0$, corresponding to the spherical case, the eigenvalue λ reduces to $\ell(\ell+1)$, with $\ell = m,m+1,m+2,\ldots$ The numerical values of λ obtained from the diagonalization of the matrix in eq. (17) with a basis of twenty functions are as accurate as the ones in the tables of ref. 6 for $m = 0,1,2$. The same figures contain the plots of the straightlines of eqs. (18a) and (18b) for splieroids with eccentricities of 1/2, 1/1.25 and 1/1.1, respectively; notice the variations of the slopes and interceptions of those lines according to the values of ξ_0 and m. The energy eigenvalues are determined, according to eqs. (15), by the values of k^2f^2 at the intersections of the $\lambda(k^2f^2)$ curves and the straight line associated with each spheroid. If we take $\hbar^2/2\mu f^2$ as the unit of energy, then the energy eigenvalue are given directly the abscissae k^2f^2 of those intersections.

Figure 2 shows the energy spectra for the particle on prolate and oblate spheroids on the right and on the left, respectively, for eccentricity parameters of $\xi_0 = 2$, 1.25 and 1.1, grouping together the energy levels with common values of $m = 0,1,2$ and 3.

In order to discuss the characteristics of these energy spectra, we take the energy spectra of the rigid rotator $\hbar^2\ell(\ell+1)/2I$ and of the symmetric top

$$\hbar^2 \left\{ \frac{\ell(\ell+1)}{2I_1} + \frac{m^2}{2} \left(\frac{1}{I_3} - \frac{1}{I_1}\right) \right\}$$

as points of comparison[8]. The comparison can be made more directly by

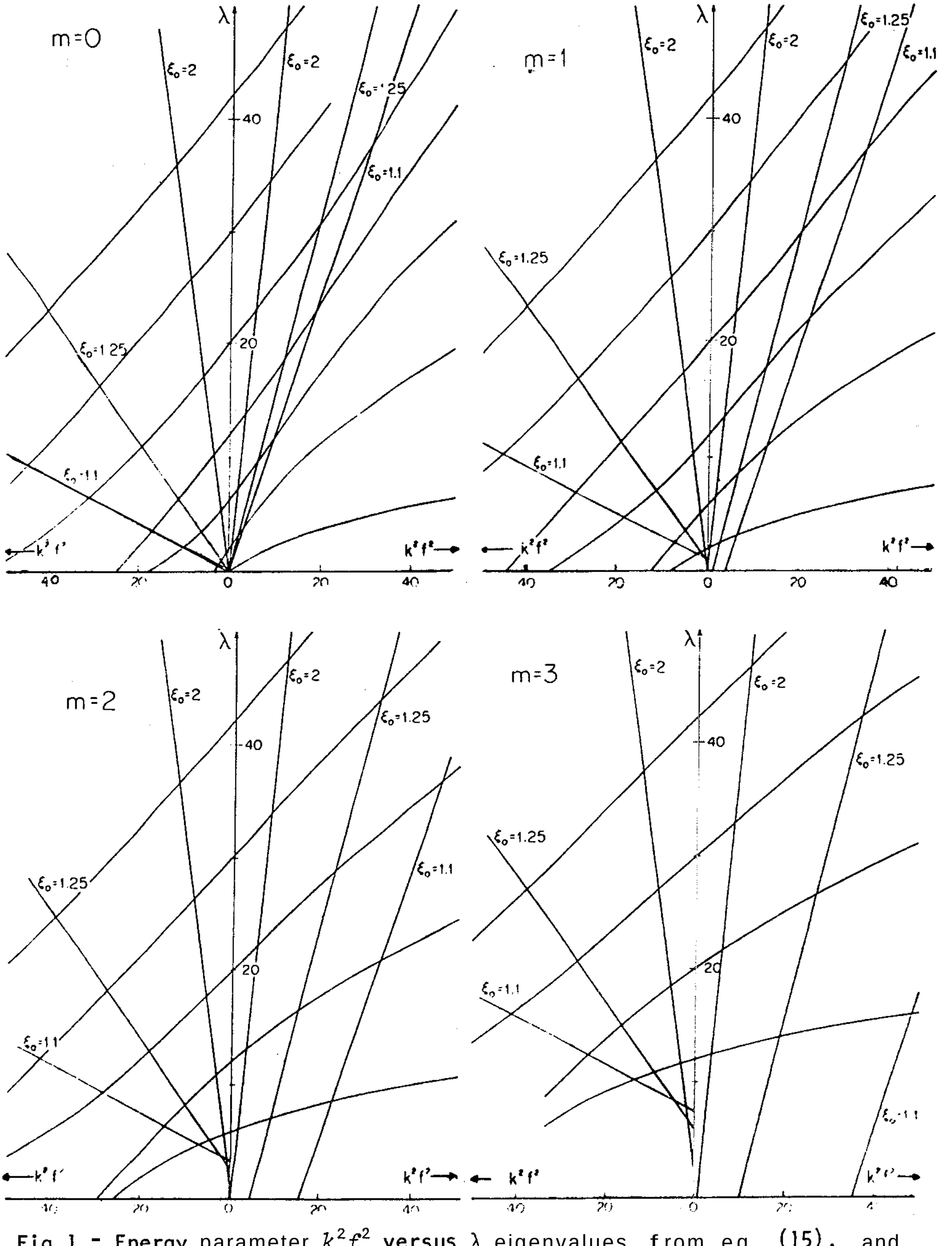

Fig.1 - Energy parameter k^2f^2 versus λ eigenvalues from eq. (15), and straightlines of eqs, (18) for prolate (oblate) spheroids on the right (left) side, for a) m = 0, b) m = 1, c) m = 2 and d) m = 3.

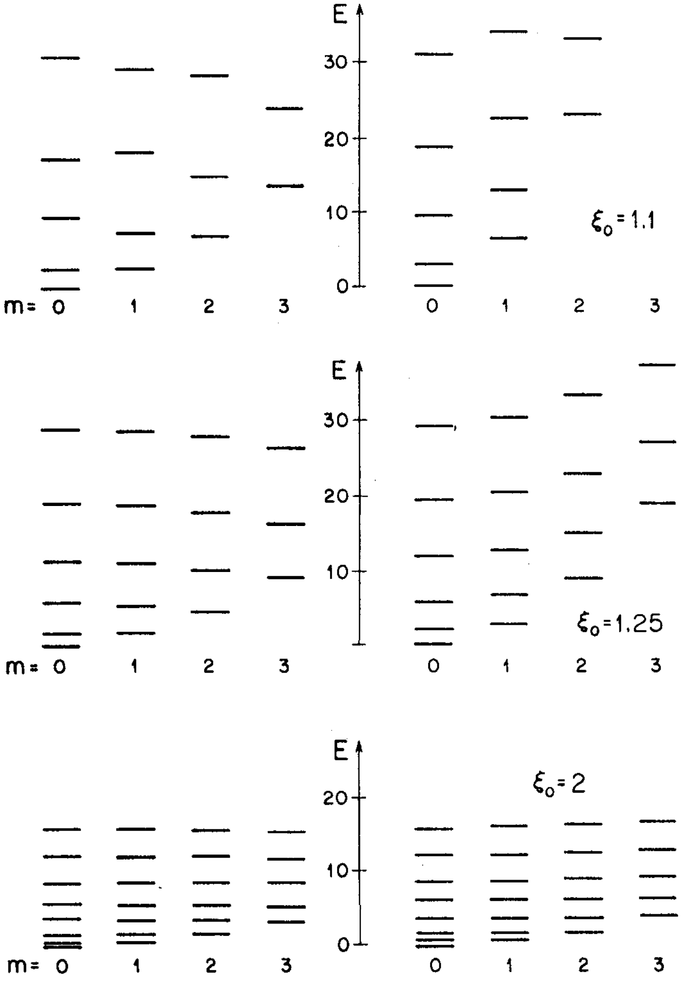

Fig. 2 - Energy spectra, with $\hbar^2/2\mu f^2$ as the energy unit, for particle constrained to move on prolate (oblate) spheroidal surfaces of eccentricity $1/\xi_0$ on the right (left) side.

rewriting eqs. (13a) and (13b) in terms of the major and minor semiaxes of the spheroids $a = f\xi_0$ and $b = f\zeta_0$ in the respective forms

$$E_{\lambda m} = \frac{\hbar^2\lambda}{2\mu a^2} + \frac{\hbar^2 m^2}{2\mu}\left[\frac{1}{b^2} - \frac{1}{a^2}\right] \qquad (13a')$$

$$E_{\lambda m} = \frac{\hbar^2\lambda}{2\mu b^2} + \frac{\hbar^2 m^2}{2\mu}\left[\frac{1}{a^2} - \frac{1}{b^2}\right] \qquad (13b')$$

Notice that the major (minor) axis is the symmetry axis for the prolate (oblate) spheroid, and $I_3 = \mu b^2$ (μa^2) and $I_1 = \mu a^2$ (μb^2) play the roles of the moments of inertia relative to the symmetry axis and a transversal axis, respectively. Then the difference between the energy levels of the particle constrained to move on the spheroidal surface and the energy levels of the symmetric top consists of the difference between the values of λ and $\ell(\ell+1)$. As the top and the surfaces become spherical $I_3 \to I_1, b \to a$, $f \to 0$, $\lambda \to \ell(\ell+1)$, and the energy spectra of both systems tend to that of the rigid rotator. The departure from sphericity removes the $(2\ell+1)$ - fold degeneracy of the rigid-rotator energy levels, and a two-fold degeneracy remains for the states with $m = \pm 1, \pm 2, \ldots$. The energy levels are shifted up (down) as the shape becomes elongated (flattened).

In the case of spheroidal surfaces of small eccentricity, i.e., large values of ξ_0, the energy spectra are very close to that of the rigid rotator, as it can be appreciated graphically in figs. 1 where the corresponding straight lines tend to become vertical and their intersections with the A curves are close to $A = \ell(\ell+1)$; also the terms of eqs. (13) depending on m^2 tend to become negligible. In fig. 2 it can be seen that even for spheroids with $\xi_0 = 2$, in which the eccentricity is not too small, the energy spectra for the particle on both prolate and oblate spheroidal surfaces resemble the one of the rigid rotator, and the tendency of the energy levels with different values of m to remain degenerate is still apparent.

As the spheroids become more elongated and flattened, the corresponding energy spectra depart more and more from each other and from the one of the rigid rotator. This can be appreciated in figs. 1 since the slopes of the straight lines become smaller as the eccentricity increases, approaching the values of one and zero for the respective limiting cases of bar-shaped and disc-shaped spheroids. Figure: 2 shows that for ξ_0 = 1.25, there is a systematicshifting up (down) of the energy levels with the increasing values of m for the prolate (oblate) case, illustrating a situation analogous to that of the symmetric top. In the same fig. 2 one can appreciate that the fairly simple ordering of the energy levels observed in the two previous cases starts to be replaced by more complex ones for ξ_0 = 1.1, which already show the trend of the energy spectra for the limiting cases of bar-shaped and disc-shaped spheroidal surfaces.

Just like in ref. 4, the nonrelativistic particle on spheroidal surfaces admits an exact quantum solution if the hamiltonian contains a potential funstion $V(\Lambda,\ell_z)$ of the commuting operators $\hat{\Lambda}$ and ℓ_z. We are also investigating the solutions for the Dirac particle on spheroidal surfaces.

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Resumo

Mostra-se que o problema de uma partícula de Schrödinger em movimento estacionário sobre superfícies esferoidais prolatas e oblatas tem uma solução exata. Identificam-se as constantes de movimento explicitamente, e esquematiza-se o procedimento para construir as auto-funções e os auto-valores da energia. Apresentam-se ilustrações dos espectros de energia para esferoides de diferentes excentricidades.