СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E4-99-297

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ON QUANTUM MOTION OF PARTICLE IN LINEAR POTENTIAL BOUNDED BY PERFECTLY REFLECTING PLANE AND PARABOLIC SURFACES

1999

Покотиловский Ю.Н. E4-99-297

О квантовом движении частицы в линейном потенциале, ограниченном идеально отражающей плоской и параболической поверхностями

Рассмотрено квантовое движение частицы в линейном потенциале, ограниченном наклонной плоскостью или параболической поверхностью. Численно получены квантовые моды (собственные энергии и собственные функции) методом разделения переменных.

Работа выполнена в Лаборатории нейтронной физики им. И.М.Франка ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна, 1999

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On Quantum Motion of Particle in Linear Potential Bounded by Perfectly Reflecting Plane and Parabolic Surfaces

The motion of particle in linear potential bounded by inclined plane or parabolic surfaces is considered. The quantization of energy and wave functions are obtained numerically by the separation of variables method.

The investigation has been performed at the Frank Laboratory of Neutron Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna, 1999

1 Introduction

Confined quantum systems or localized quantum wave packets are produced in many physical situations in molecular, atomic, and condensed matter physics. The last twenty years the most interesting applications of confined quantum systems are quantum dots, wires, and wells.

The subject of this consideration is the particle in linear potential, which is bounded by a ideally reflecting parabolic surface. It is nonlinear quantum system, which is characterized by dependence of the period of motion on the energy. We consider here the case of the infinitely high potential of the boundary, which is simplification of the realistic quantum model. The realistic boundary is the potential of finite height. It may be neutral atom, bouncing in gravitational field [1]. The boundary in this case is produced by exponential potential of atom interaction with electromagnetic (optical) evanescent wave [2]. In [3] the results for ideal reflecting plane (infinitely high potential wall) and the realistic (exponential) one were considered and compared from the point of view of quantum dynamics and quantum revivals of the initial state.

In the case of flat horizontal mirror the particle motion in gravitational field is infinite in horizontal direction along the mirror plane. Therefore the parabolic concave reflecting surface, when the confinement region is restricted in transverse direction, is practically more interesting. In [4] the classical motion of atom in cavity consisting of a horizontal concave parabolic mirror in gravitational field is considered as well as quantum mechanical problem in paraxial approximation.

Review of confined quantum systems is contained in [6], which presents also the detailed consideration of parabolically confined hydrogen atom.

Another possible example of confining surface is potential

step for very slow neutron, bouncing in gravitational field from reflecting horizontal mirror, consisting of nuclei with positive coherent neutron scattering length.

The examples considered here are typical three-dimensional Schrödinger problems allowing separation of variables into three ordinary differential equations. The type of boundary is simply presented in parabolic coordinates for they are surfaces of constant coordinate and are therefore the most natural boundaries.

The first example is the inclined plane, which is simple generalization of the case [5] of horizontal plane as a boundary for linear potential. This example may be interesting in view of possible experimental demonstration of quantum levels for massive particle in gravitational field in vicinity of reflecting plane. The second and the third cases are linear potential bounded by parabolic cylinder and by paraboloid of revolution.

2 The particle in a linear potential bounded by the perfectly reflecting inclined plane

For the sake of concreteness we assume the uniform field to be gravitational one along the y' axis, g being the gravitational acceleration value. The Schrödinger equation is given by:

$$-\frac{\hbar^2}{2M}\Delta'\psi + (Mgy' - E)\psi = 0\,. \qquad (1)$$

This problem is separable in the turned by the angle α coordinates (x,y), in which the y axis is normal to the inclined plane surface,

$$x' = x \cdot cos\alpha - y \cdot sin\alpha, \quad y' = x \cdot sin\alpha + y \cdot cos\alpha :$$

$$-\frac{\hbar^2}{2M}\Delta\psi + [Mg(y \cdot cos\alpha + x \cdot sin\alpha) - E]\psi = 0. \qquad (2)$$

Representing $\psi = X(x)Y(y)$, dividing by XY, and separating variables we obtain two equations:

$$-\frac{\hbar^2}{2M}Y'' + [Mgy \cdot cos\alpha - (E - \gamma)]Y = 0, \qquad (3)$$

and

$$-\frac{\hbar^2}{2M}X'' + (Mgx \cdot sin\alpha + \gamma)X = 0. \qquad (4)$$

with γ as the constant of separation. Introducing:

$$2M^2g \cdot cos\alpha/\hbar^2 = 1/l^3, \qquad \text{and} \qquad 2M(E-\gamma)/\hbar^2 = \lambda/l^2 \quad (5)$$

for the equation (3), and

$$2M^2g \cdot sin\alpha/\hbar^2 = 1/s^3, \qquad \text{and} \qquad 2M\gamma/\hbar^2 = \mu/s^2 \quad (6)$$

for the equation (4) we have:

$$d^2Y/d\xi^2 - \xi Y = 0, \qquad (7)$$

where $\xi = y/l - \lambda$, with boundary conditions $Y(\xi = -\lambda) = 0$, $Y(\xi \to \infty) \to 0$, and

$$d^2X/d\zeta^2 - \zeta X = 0, \qquad (8)$$

where $\zeta = x/s + \mu$, and boundary condition $X(\zeta \to \infty) \to 0$.

The solutions of these equations which are evanescent at the infinity are Airy functions, and Dirichlet boundary conditions for (7) give the spectrum of stationary states. The total energy E is not quantized in this situation, but the part of energy $(E - \gamma)$, corresponding to the motion normal to the surface of the inclined plane is quantized in accordance to (5) and (7). The solution of the equation (8) describes the wave, moving in the uniform field with changing energy γ.

Recently the planned experiment was advertised on the measurement of energy quantization of neutrons in vicinity of perfectly reflecting horizontal plane in the presence of gravitational field [7]. One of the main experimental problems is very small energy (and respectively space) separation of energy levels ~ several microns. In [8] it was proposed to use the vertical gradient of the magnetic field to compensate gravitational force and in this way to increase the separation of levels for one of the neutron spin components.

It is seen from (5) that rotation of the plane around the horizontal z-axis changes the energies of the quantum levels for motion in the direction along the y-axis and respectively the space separation of the maxima in the neutron wave density profiles in respect to reflecting surface.

3 The particle in a linear potential bounded by the perfectly reflecting parabolic cylinder

In this case we use the following coordinates of parabolic cylinder (u, v, z):

$$x = \pm uv, \; y = (u^2 - v^2)/2,$$
$$\rho = (x^2 + y^2)^{1/2}, \; u = (\rho + y)^{1/2}, \; v = (\rho - y)^{1/2}, \qquad (9)$$

where $0 \leq u, v < \infty$, $-\infty < z < \infty$. Laplacian in these coordinates is:

$$\Delta = \frac{1}{u^2 + v^2}\Big(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\Big) + \frac{\partial^2}{\partial z^2}. \qquad (10)$$

The Schrödinger equation with linear potential $V = Mgy$ gradient of which is directed normally to horizontal z-axis of parabolic cylinder has the form:

$$\frac{1}{u^2+v^2}\Big(\frac{\partial^2\psi}{\partial u^2}+\frac{\partial^2\psi}{\partial v^2}\Big)-\frac{2M^2g}{\hbar^2}\Big(\frac{u^2-v^2}{2}\Big)\psi+\frac{2ME}{\hbar^2}\psi+\frac{\partial^2\psi}{\partial z^2}=0. \tag{11}$$

We present $\psi = f_1(u)f_2(v)f_3(z)$, and after dividing by $f_1f_2f_3$ and multiplying by u^2+v^2 we obtain:

$$\frac{f_1''(u)}{f_1(u)}+\frac{f_2''(v)}{f_2(v)}+\frac{f_3''(z)}{f_3(z)}-\frac{M^2g}{\hbar^2}(u^4-v^4)+\frac{2ME}{\hbar^2}(u^2+v^2)=0. \tag{12}$$

The motion along the $z-$axis is infinite, corresponding wave function $f_3(z) = exp(ikz)$, therefore we omit it from futher consideration. Separation of coordinates gives two one-dimensional equations:

$$f_1''-\Big(\frac{M^2gu^4}{\hbar^2}-\frac{2MEu^2}{\hbar^2}\Big)f_1=\gamma f_1, \tag{13}$$

and

$$f_2''+\Big(\frac{M^2gv^4}{\hbar^2}+\frac{2MEv^2}{\hbar^2}\Big)f_2=-\gamma f_2. \tag{14}$$

Now we introduce:

$$M^2g/\hbar^2 = 1/l^6, \quad 2ME/\hbar^2 = \lambda/l^4,$$

and have equations in the new variables: $\xi = u/l$, and $\eta = v/l$:

$$f_1''+(-\xi^4+\lambda\xi^2)f_1=\gamma f_1 \tag{15}$$

and

$$f_2''+(\eta^4+\lambda\eta^2)f_2=-\gamma f_2. \tag{16}$$

We have two one-dimensional Schrödinger problems: for the function $f_1(\xi)$ the potential $U(\xi) = \xi^4-\lambda\xi^2$, and for the function $f_2(\eta)$ the potential is $V(\eta) = -\eta^4-\lambda\eta^2$, with boundary condition $f_2(\eta=\eta_0) = 0$.

If initially the parabolic cylinder in Cartesian coordinates has the form $y = ax^2+b$, after transformation:

$$x' = (2a)^{1/2}\eta_0 x, \quad y' = y-\frac{\eta_0^4}{2}-b \quad \text{we have} \quad y' = \frac{x'^2}{2\eta_0^2}-\frac{\eta_0^4}{2},$$

which corresponds to $\eta = \eta_0$ in coordinates of parabolic cylinder.

We did not try to find the eigenvalues for this problem in the form of roots of some explicit function (it is possible that such solution exists), but solved Eqs. (15-16) together numerically with boundary conditions:

$$f_1(\xi\to\infty)\to 0; \quad f_2(\eta=\eta_0=1)=0,$$

which corresponds in Cartesian coordinates to confining boundary parabolic cylinder $y = (x^2-l^4)/2l^2$.

The graphic method of finding energy eigenvalues λ for these equations is shown in Fig. 1 in which these eigenvalues are located at the intersections of curves presenting the common for these two equations eigenvalues γ as a function of energy λ. The figures indicate the corresponding quantum number of the energy state for each equation.

The stationary states exist only in the case of parabolic cylinder with its top directed downward (along the direction of external force); equation of this surface is $\eta = \eta_0$. There is no stationary state for the inverted parabolic cylinder $\xi = \xi_0$ with its top directed upward. It is interesting to note that classically the state exists (not stable to perturbations in the classical sense, however) for a particle bouncing strongly vertically from the top of the inverted parabolic cylinder.

Fig. 2 shows spatial distribution for some of the stationary quantum states for confining parabolic cylinder described by equation $\eta = \eta_0 = 1$. The eigenstates are labelled according to the number of nodes of eigenfunctions for the equations (15) and (16) respectively.

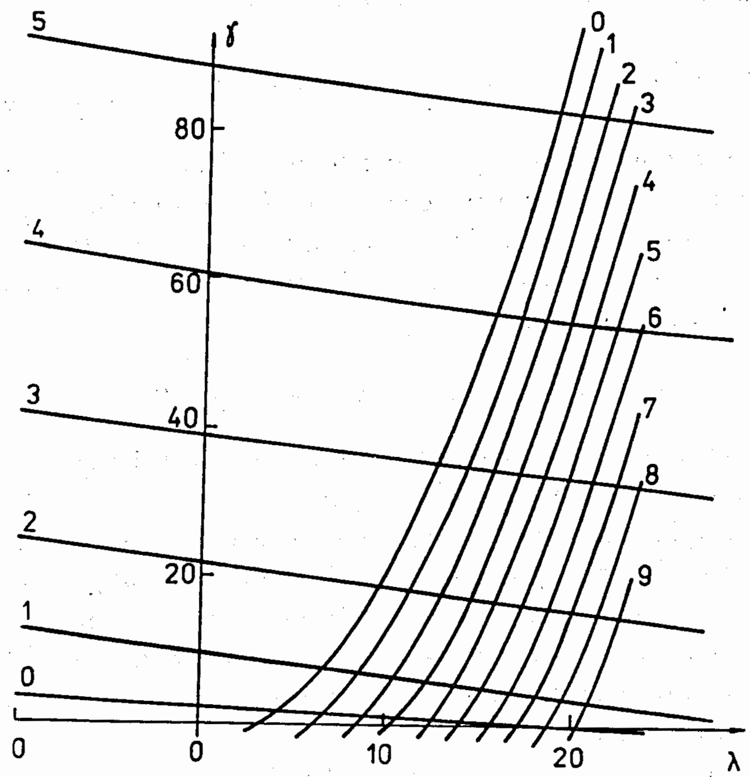

Fig. 1 Graphic method of obtaining the eigenvalues λ for the joint solution of eigenvalue problem for the Eqs. (15) and (16). The curves (0-9) show the eigenvalue γ as a function of λ for the Eq.(15), and the curves (0-5) show the eigenvalue γ as a function λ for the Eq. (16). The intersection points give simultaneous energy eigenvalues λ for the system of equations (15-16).

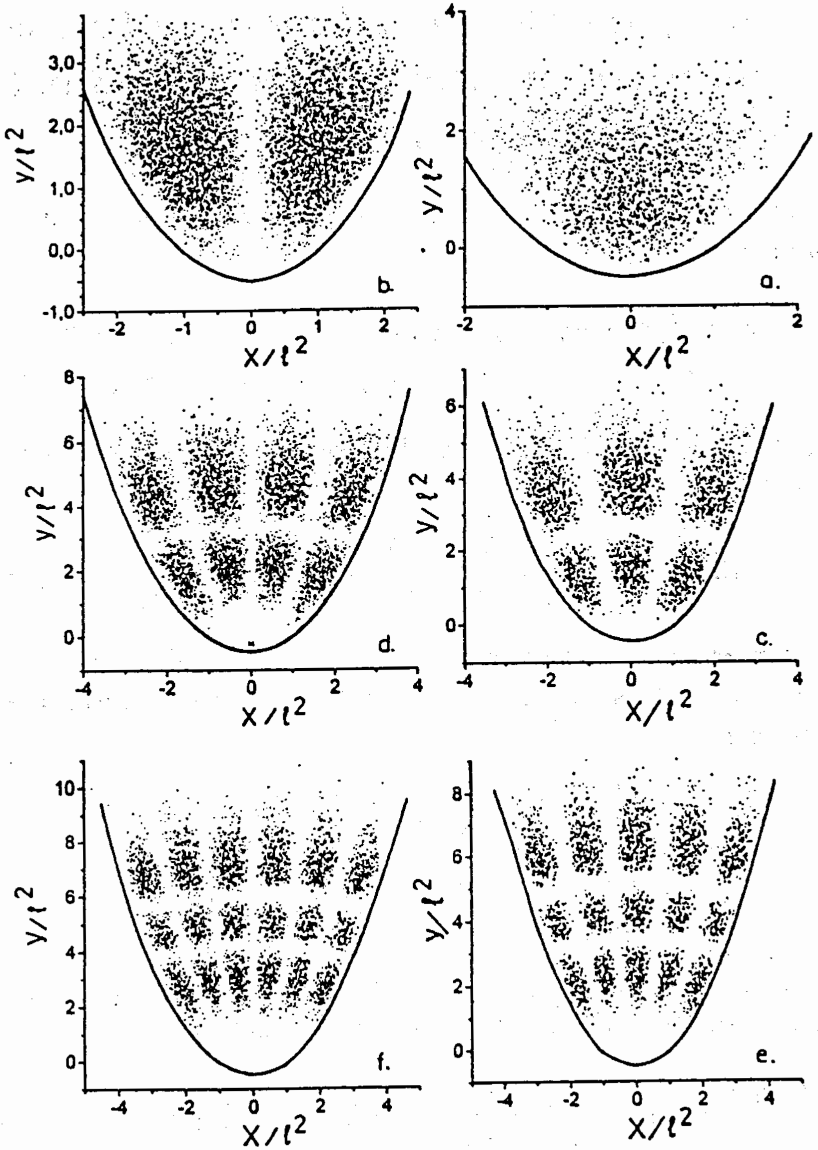

Fig.2 Density plots in Cartesian coordinates for some low energy eigenstates in vicinity of perfectly reflecting cylindrical paraboloid. a: ψ_{00}, $\lambda = 4.08$; b: ψ_{01}, $\lambda = 6.71$; c: ψ_{12}, $\lambda = 11.22$; d: ψ_{13}, $\lambda = 14.15$; e: ψ_{24}, $\lambda = 18.28$; f: ψ_{25}, $\lambda = 21.25$.

4 The particle in a linear potential bounded by the perfectly reflecting paraboloid of revolution

In this case we use the coordinates of paraboloid of revolution ξ, η and φ:

$$x = \sqrt{\xi\eta} \cdot cos\varphi, \quad y = \sqrt{\xi\eta} \cdot sin\varphi, \quad z = (\xi - \eta)/2;$$
$$\xi = r + z, \quad \eta = r - z, \quad r = (\xi + \eta)/2, \quad \varphi = arctan(y/x), \tag{17}$$

where $0 \leq \xi, \eta < \infty$, $0 \leq \varphi \leq 2\pi$. Laplacian in these coordinates has the form:

$$\Delta = \frac{4}{\xi + \eta}\Big[\frac{\partial}{\partial \xi}(\xi\frac{\partial}{\partial \xi}) + \frac{\partial}{\partial \eta}(\eta\frac{\partial}{\partial \eta})\Big] + \frac{1}{\xi\eta}\frac{\partial^2}{\partial \varphi^2}. \tag{18}$$

The Schrödinger equation with linear potential directed along the z-axis (which is the axis of paraboloid) in these coordinates has the form:

$$\Big[\frac{\partial}{\partial \xi}(\xi\frac{\partial \psi}{\partial \xi}) + \frac{\partial}{\partial \eta}(\eta\frac{\partial \psi}{\partial \eta})\Big] + \frac{\xi + \eta}{4\xi\eta}\frac{\partial^2 \psi}{\partial \phi^2} +$$
$$+ \frac{(\xi + \eta)M}{2\hbar^2}\Big[-\frac{Mg}{2}(\xi - \eta) + E\Big]\psi = 0. \tag{19}$$

Introducing $\psi = f_1(\xi) \cdot f_2(\eta) \cdot e^{im\varphi}$, dividing by $f_1 f_2 \cdot exp(im\varphi)$, and separating the variables we have two equations:

$$\frac{d}{d\xi}\left(\xi\frac{df_1(\xi)}{d\xi}\right) + \Big[\frac{ME\xi}{2\hbar^2} - \frac{m^2}{4\xi} - \frac{M^2 g\xi^2}{4\hbar^2} + \beta/l\Big]f_1(\xi) = 0, \tag{20}$$

and

$$\frac{d}{d\eta}\left(\eta\frac{df_2(\eta)}{d\eta}\right) + \Big[\frac{ME\eta}{2\hbar^2} - \frac{m^2}{4\eta} + \frac{M^2 g\eta^2}{4\hbar^2} - \beta/l\Big]f_2(\eta) = 0 \tag{21}$$

with β/l - the separation constant. After substituting:

$$\frac{M^2 g}{4\hbar^2} = 1/l^3, \quad \frac{ME}{2\hbar^2} = \lambda/l^2, \quad u = \xi/l, \quad v = \eta/l$$

we have two equations:

$$\frac{d}{du}\left(u\frac{df_1(u)}{du}\right) + \Big[\lambda u - \frac{m^2}{4u} - u^2 + \beta\Big]f_1(u) = 0, \tag{22}$$

and

$$\frac{d}{dv}\left(v\frac{df_2(v)}{dv}\right) + \Big[\lambda v - \frac{m^2}{4v} + v^2 - \beta\Big]f_2(v) = 0. \tag{23}$$

Introducing: $\chi_1(u) = f_1(u) \cdot u^{1/2}$ and $\chi_2(v) = f_2(v) \cdot v^{1/2}$ we have two one-dimensional Schrödinger equations:

$$\chi_1''(u) + \left(\lambda + \frac{\beta}{u} - u + \frac{1 - m^2}{4u^2}\right)\chi_1(u) = 0, \tag{24}$$

and

$$\chi_2''(v) + \left(\lambda - \frac{\beta}{v} + v + \frac{1 - m^2}{4v^2}\right)\chi_2(v) = 0, \tag{25}$$

with the potentials respectively:

$$U(u) = -\frac{\beta}{u} + u + \frac{m^2 - 1}{4u^2}, \tag{26}$$

and

$$V(v) = \frac{\beta}{v} - v + \frac{m^2 - 1}{4v^2}. \tag{27}$$

Again as in the case of parabolic cylinder the stationary states exist only in the case of paraboloid of revolution with its top directed downward (in the direction of external force); the equation of this paraboloid is $v = v_0$. There is no stationary state for the inverted paraboloid $u = u_0$ with its top directed upward. In this case the classical state for a massive particle bouncing strongly

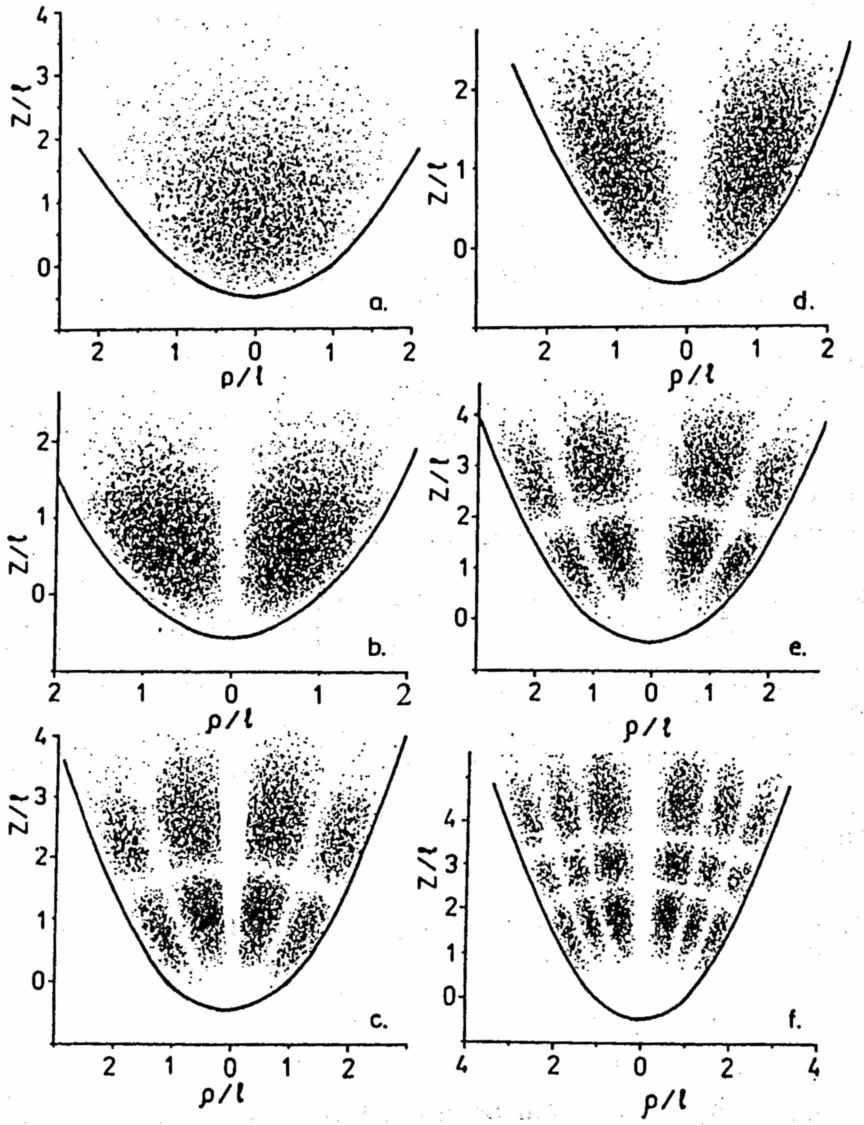

Fig.3 Space distribution probabilities for some low energy eigenstates in vicinity of perfectly reflecting paraboloid of revolution. a: ψ_{000}, $\lambda = 3.05$; b: ψ_{011}, $\lambda = 3.79$; c: ψ_{131}, $\lambda = 7.80$; d: ψ_{012}, $\lambda = 4.96$; e: ψ_{132}, $\lambda = 4.91$; f: ψ_{252}, $\lambda = 12.8$.

vertically from the top of the inverted paraboloid has no quantum mechanical analog.

The eigenvalues and eigenvectors were obtained with the method similar to the case of cylindrical paraboloid. Fig.3 shows spatial distribution in Cartesian coordinates of some of the stationary quantum states for confining paraboloid of revolution described by equation $v = v_0 = 1$. The wave functions are labelled according to the number of nodes in eigenfunctions of equations (24) and (25) respectively, and rotational quantum number m (the third quantum number).

Author is grateful to Mrs. G.F.Gareeva for her help in preparation of Figs. 2 and 3.

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Received by Publishing Department
on November 12, 1999.