THE EXACTLY RESOLVED MODEL OF A QUANTUM PARTICLE WITH SINGULAR AND PERIODIC POSITION DEPENDENT MASS

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ТОЧНО РОЗВ'ЯЗУВАНА МОДЕЛЬ КВАНТОВОЇ ЧАСТИНКИ З СИНГУЛЯРНОЮ І ПЕРІОДИЧНО ЗАЛЕЖНОЮ ВІД КООРДИНАТ МАСОЮ

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Abstract

One special case of the quantum particle with the effective mass which depends on the coordinate has been considered. The coordinate dependence of the particle mass is expressed in terms of trigonometric functions, namely, inverse square of the cosine. The model we have chosen has the following main features: (1) position dependent mass is periodic function of the coordinate; (2) the coordinate dependence has singular points of inverse squares type which can be classified as the centres of falling; (3) the eigenfunctions in their explicit exact form can be established.

Having determined the eigenfunctions by applying procedure of regulazation proposed in the given article and Flock's theorem the equation for eigenvalues has been found. Its approximate solution allows to find and analyse the law of dispersion that, as it turned out, is continuous in function of wave number and forms a continuous spectrum.

Key words: position dependent mass, eigenfunctions, law of dispersion.

Анотація

Тут розглянуто один спеціальний випадок квантової частинки з ефективною масою, яка залежить від координат. Координатна залежність маси частинки виражена у термінах тригонометричних функцій обернено пропорційність квадрату косинуса. Розглянута тут модель відзначається такими основними особливостями: 1) координатна залежність маси виражена періодичною функцією; 2) цій функції властива наявність сингулярних точок, які можна кваліфікувати як центри падіння; (3) модель допускає можливість встановити власні функції у їх точній і явній формі.

Застосуванням процедури регуляризації, запропонованої в даній роботі, і теореми Флоке одержано рівняння на власні значення, наближене розв′язання якого показує, що закон дисперсії, як функція хвильового числа, формує неперервний спектр.

Ключові слова : координатно залежна маса, власні функції, закон дисперсії.

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Introduction

Quantum mechanics of a particle with an effective mass dependent on coordinates. for a long time yet is a subject of considerable number of studies. This fact is due to some nearly obvious circumstances. Let's note, among them, one of the most important and closely related to the fundamental quantum mechanics problem of accordance among dynamic variables such as kinetic energy and momentum linear from the one side and their quantum counterpart, from the another. In due time the creators of quantum theory which was elaborated and developed for particles with the position independent mass, dedicated their attention to this problem of the canonical variables quantization. In case of a mass dependent on coordinates when the particle motion can be treated as the movement of particle with variable mass in uniform space or can be interpreted as Hamilton's system, moving in curvilinear space whose metrics depends on coordinates, in arrangement of the particle mass and the operator of momentum linear a certain ambiguity appears.

This, in turn, leads to ambiguity in ordering of non-commuting operators of momentum and kinetic energy when the Hamilton's operator has to be written in its explicit form. Although the problem of ordering non-commutating operators in quantization of dynamic systems was thoroughly investigated by the creators of quantum physics, such as Bourne, Jordan, Weil, von Neumann, it is still far from being solved completely and exhaustively [1].

Another circumstance that has revived interest for studying the dynamics of a quantum particle with coordinate-dependent mass transfers the problem from a purely academic area on a practical plane. This concerns the study of quantum regularities associated with the coordinate dependence of effective mass of charge carriers, which is significantly stimulated by the creation and wide applications of gradient doped semiconductors, delta profiled layers, as well as advances in the heterojunctions synthesis.

Once more notable factor is the intensive development of nanotechnology, especially such its branches as the energy zones engineering, quantum dots, quantum wires fabrication that is a prerequisite for the creation of materials with demanded and predicted properties, which often are determined by the effective mass, in particular, the density of states, the coefficient of optical absorption, mobility and other mass-sensible kinetic coefficients.

Along with the above mentioned fundamental problem of ordering non-commuting operators, a number of studies, focused on solving the Schrödinger equation for some special model assumptions about the mass coordinate dependence, has been recently intensified. In this context two peculiarities can be pointed out. The first, presented by the extensive bibliography [2-5], concerns the development of algorithms for selecting models and model potentials that would admit existing of exact solutions. Equally important is the second peculiarity, which has also accumulated considerable bibliography [6-10] and is dedicated precisely to the search for these exact solutions. Searching of exact eigenfunctions and eigenvalues of energy is interesting not in itself but is also important for the development of various methods of perturbation theory. One of such models, which, as it turns out, allows to find exact and explicit solutions, is the object of study in this paper.

1. Model

Here we consider one-dimensional motion of a particle with a mass that depends on the coordinate accordingly to the general formula:

$$m(x) = \frac{m_0}{f(x)} \tag{1}$$

The model is specified in two stages. First of all, it is necessary to write down explicitly the function $f(x)$ that will be done in the following text. Beside it in the connection with the above-mentioned problem of non-commutability of the momentum linear $\hat{p}_x = -i\hbar\partial_x$ operator and mass $m(x)$, there is a need for an unambiguous choice of ordering these dynamic variables in order to the kinetic energy operator can be determined in its acceptable form. Putting attention to the researches represented by various authors [2-9] in this paper we will prefer the approach proposed by von Roos [11,12] and applied by a number of research groups. The Hamilton von Roos is as follows

$$\hat{H}_c = \frac{1}{4}\left[m^{\eta}(x)\hat{p}_x m^{\varepsilon}(x)\hat{p}_x m^{\rho}(x) + m^{\rho}(x)\hat{p}_x m^{\varepsilon}(x)\hat{p}_x m^{\eta}(x)\right]$$

where the parameters ε , ρ , η must satisfy to the condition $\varepsilon + \rho + \eta = -1$. In this paper, we accept the following values $\varepsilon = -1$, $\rho = 0$, $\eta = 0$ [13]. Such a choice not only considerable simplifies analytic form of Hamilton's operator but also shows its efficiency confirmed by a lot of authors, for example [4, 6-8,14] and references represented there. It makes sense to point out that with this set of parameters Hamiltonian retains its hermitian form. Regarding the Schrödinger's equation it due to the formula (1) assumes the form:

$$-\frac{\hbar^2}{2m_0}\partial_x(f\partial_x\Psi) = E\Psi \tag{2}$$

To choice a function $f(x)$, we use the method of variable change proposed in [9]. So, let's pass to the new variable by the formula

$$y = y(x) \tag{3}$$

:we come up to the equation

$$\frac{\partial}{\partial y}\left(f\frac{\partial y}{\partial x}\frac{\partial\Psi}{\partial y}\right)\frac{\partial y}{\partial x} + k^2\Psi = 0 \tag{4}$$

where $k-$is the wave number determined in the standard way, that is

$$k^2 = 2m_0E/\hbar^2 \tag{5}$$

Wave equation (4) assumes the most simple but non trivial structure if, as it is done in the model under study, we choose a function $f(x)$ and a new variable y so that the condition:

$$f\frac{\partial y}{\partial x} = C \tag{6}$$

could be satisfied. Here $C-$ is so far an arbitrary constant that only renormalizes the effective mass, and which will be set later. With the replacement of the variable proposed by formula (6), the wave equation is as follows:

$$\frac{\partial^2\Psi}{\partial y^2}C\frac{\partial y}{\partial x} + k^2\Psi = 0 \tag{7}$$

Now, finally, we choose the new variable y as the solution of the equation

$$y'_x = \frac{1}{a}(y^2+1) \tag{8}$$

where $a-$is the characteristic length that sets the scale of the significant mass change with the coordinate. By integrating equation (8), we obtain:

$$y = tg\left(\frac{x}{a}\right) \tag{9}$$

Joint consideration of equations (6) and (9) allows us to find $f(x)$ and write the mass as explicit function of the coordinate. Thus, one of the basic assumptions of this work, given by the formula (1), can be specified as follows:

$$m(x) = m_0 Cos^{-2}\left(\frac{x}{a}\right) \tag{10}$$

here for the constant C, we assumed the value $C = 1/a$. Summarizing the discussion of the model considered in this paper, we point out its main features: first, the kinetic energy operator is chosen as was proposed in [13]; second, the mass of a particle changes with the coordinate in accordance with formula (10).

2. The wave equation and its solution

After substituting (8) into (7) and taking in account the choice of constant $C = 1/a$, the wave equation can be represented by to below given expression:

$$(y^2+1)\frac{\partial^2\Psi}{\partial y^2} + (ka)^2\Psi = 0 \tag{11}$$

To transform the equation (11) to one of the standard and well-described in a number of sources form, it is convenient to introduce an imaginary variable, namely $y = -i\xi$, and a new unknown function Φ, expressing it by the relation:

$$\Psi = (\xi^2 - 1)\Phi \tag{12}$$

For the above introduced function, we have the equation

$$(\xi^2 - 1)\partial_\xi^2\Phi + 4\xi \cdot \partial_\xi\Phi + [(ka)^2 + 2)\Phi = 0 \tag{13}$$

The fundamental solutions of equation (13) accordingly to the books [15,16] can be expressed in terms of the associated Legendre functions of the first $P_\nu^1(\xi)$ and the second $Q_\nu^1(\xi)$ kind by the formulas

$$\Phi_{1\nu}(\xi) = (\xi^2 - 1)^{-1/2} P_\nu^1(\xi) \tag{14}$$

$$\Phi_{2\nu}(\xi) = (\xi^2 - 1)^{-1/2} Q_\nu^1(\xi) \tag{15}$$

where the degree ν of Legendre functions is equal to one of the solutions of the equation

$$\nu(\nu+1) = (ka)^2 + 2$$

that is

$$\nu_{1,2} = -1/2 \pm \sqrt{1/4 - (ka)^2} \tag{16}$$

Considering the definitions (12), relations (14) and (15), we write the general solution of the wave equation in the form of a linear combination:

$$\Psi = w(\xi)[AP_\nu^1(\xi) + BQ_\nu^1(\xi)] \equiv A\Psi_1 + B\Psi_2 \tag{17}$$

3. Main results: eigenvalues of the Schrödinger equation

The “potential” of a wave equation is a periodic function with a main period equal to πa. Therefore, the wave function must satisfy Floke's conditions [17] (Bloch's theorem).Before writing down these conditions, it should be noted that the singular nature of "potential" requires a certain regularization procedure. Here we perform the regularization according to the following scheme: we choose two infinitely close points symmetrically located at distances $\mp a\varepsilon$ on each side of the singular point $x_s = \pi a/2$ and write the Flock’s boundary conditions. These conditions conduct to appearing of equations for unknown coefficients A and B. The dispersion equation is then obtained in a standard manner. The regularization procedure will be ended by the performing of limit transition $\varepsilon \to 0$.

It is convenient to use, depending on the context, notation

$$f(0\mp) \equiv f[\xi(x)]\big|_{x=x_s \mp a\varepsilon} \equiv (f)_{0\mp} \tag{18}$$

which permit to represent the further calculations more compact form. Returning to the above mentioned boundary conditions, we write

$$\begin{cases} A\Psi_1(0-) + B\Psi_2(0-) = e^{iqa}[A\Psi_1(0+) + B\Psi_2(0+)] \\ \dfrac{1}{m(0-)}\left[A\left(\dfrac{\partial}{\partial\xi}\Psi_1\dfrac{\partial\xi}{\partial x}\right)_{0-} + B\left(\dfrac{\partial}{\partial\xi}\Psi_2\dfrac{\partial\xi}{\partial x}\right)_{0-}\right] = \\ = e^{iqa}\dfrac{1}{m(0+)}\left[A\left(\dfrac{\partial}{\partial\xi}\Psi_1\dfrac{\partial\xi}{\partial x}\right)_{0+} + B\left(\dfrac{\partial}{\partial\xi}\Psi_2\dfrac{\partial\xi}{\partial x}\right)_{0+}\right] \end{cases} \tag{19}$$

Non-trivial solutions of a homogeneous system of equations (19) exist if its determinant is equal to zero. The pointed out condition leads to the equation:

$$\begin{aligned}
&[\Psi_1(0-)-e^{iqa}\Psi_1(0+)]\left[\left(\frac{\partial}{\partial\xi}\Psi_2\frac{\partial\xi}{\partial x}\right)_{0-}-e^{iqa}\left(\frac{\partial}{\partial\xi}\Psi_2\frac{\partial\xi}{\partial x}\right)_{0+}\right]-\\
&-[\Psi_2(0-)-e^{iqa}\Psi_2(0+)]\left[\left(\frac{\partial}{\partial\xi}\Psi_1\frac{\partial\xi}{\partial x}\right)_{0-}-e^{iqa}\left(\frac{\partial}{\partial\xi}\Psi_1\frac{\partial\xi}{\partial x}\right)_{0+}\right]=0
\end{aligned}\tag{20}$$

Writing the equation (20), we took in account that the singular factors $m(0-)$ and $m(0+)$ in the second equation of the system (19) which are equal to $m_0 / Sin^2\varepsilon$, in the regularization scheme applied here can be reduced. Equation (20) contains another singular factor, namely the derivative $\partial\xi / \partial x$. Because of the relation $\xi = i \cdot tg(x / a)$ for the derivative $\partial\xi / \partial x$ results

$$\frac{\partial\xi}{\partial x}=\frac{i}{a}Cos^{-2}(x/a)\tag{21}$$

By substituting here the values $x = x_s \mp a\varepsilon$ we obtain

$$\left(\frac{\partial\xi}{\partial x}\right)_{0\mp}=\frac{i}{a}Sin^{-2}\varepsilon\tag{22}$$

Each of the equation (20) terms contains the same factor (22). Therefore we omit these sources of singularity. Than equation (20) assumes the following form:

$$\begin{aligned}
&e^{iqa}\left[\Psi_1(0+)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0+}-\Psi_2(0+)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0+}\right]+\\
&+e^{-iqa}\left[\Psi_1(0-)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0-}-\Psi_2(0-)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0-}\right]=\\
&=\Psi_1(0+)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0-}+\Psi_1(0-)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0+}-\\
&-\Psi_2(0+)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0-}-\Psi_2(0-)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0+}
\end{aligned}\tag{22}$$

The further transformations of the secular equation (22) which represented in Appendices B are based on the well-known [16,18] properties and asymptotics of the joined LeGendre's functions.

As the result we came up to the equation for eigen values of the following form

$$e^{iqa} + e^{-iqa} = \frac{e^{i\pi\nu} + e^{-i\pi\nu}}{2\nu + 1} \qquad (23)$$

deduced in Appendices B.

Now we consider two cases

1) First of them corresponds to the energy segment $0 \le E \le E_s = \hbar^2/(8m_0a^2)$.For such energy values the parameter η,which we define by relation $\eta = \sqrt{1/4 - (ka)^2}$, is real and satisfies to the conditions $0 \le \eta = \sqrt{1/4 - (ka)^2} \le 1/2$. However paying attention to the equation (16) we can modify it to the form $\nu_{1,2} = -1/2 \pm \eta$. By combining the last expression with the equation (23) we find the secular equation in unexpectedly simple form, namely:

$$e^{iqa} + e^{-iqa} = \frac{Sin\pi\eta}{\eta} \qquad (24)$$

Now we assume a complex form for a wave number that is:

$$q = u + iv \qquad (25)$$

The representation of the wave vector in a complex form is a standard approach to the study of wave phenomena and description the decaying or increasing modes in waveguide theory [19]. In addition, it is also a common way to pass to a complex zone structure in order to study the spectrum of elementary excitations in solids. In due time expanding the dispersion law on complex values of wave vector some type of surface states (Tamm's states) [20] with energy localized inside of a forbidden zone have been interpreted. The imaginary part of wave number assumes responsibility for wave function exponential decreasing with a distance from the crystal surface. It should be noted that in the passing to a complex zone structure with using of representation (25), the problem is reduced to expressing the imaginary part of a quasi-wave vector in terms of model parameters. As for our problem. after separating the real and imaginary parts in equation (24), we come to the equations

$$\begin{cases} Sinua \cdot Shva = 0 \\ Chva \cdot Cosua = \dfrac{Sin\pi\eta}{2\eta} \end{cases} \tag{26}$$

The solutions of the first equation are $u = \pi n/a$ either $v = 0$. By substituting of the first of them into the second equation of the system we obtain

$$(-1)^n Chva = \frac{Sin\pi\eta}{2\eta} \tag{27}$$

Since the parameter η varies from 0 to $1/2$, the right-hand side of equation (27) changes between $\pi/2$ and 1, and therefore for all even values of n the solutions exists and it can be given in the following implicit form

$$v = \frac{1}{a}\ln\left[\frac{Sin\pi\eta}{2\eta} \pm \sqrt{\left(\frac{Sin\pi\eta}{2\eta}\right)^2 - 1}\right] \tag{28}$$

Putting $v = 0$ in the second equation of system (26), we get the equation:

$$\frac{Sin\pi\eta}{2\eta} = Cosua$$

which has only solution $u = 2\pi n/a$ if $\eta = 1/2$ that corresponds to the energy equal to zero and is absorbed by the relation (28).

2) The second case corresponds to energy eigenvalues belonging to the interval: $E_s \le E < \infty$. For this case, both values of v are complex and can be written as: $v_{1,2} = -1/2 \pm i\eta$ where we use the notice $\eta = \sqrt{(ka)^2 - 1/4} \ge 0$. The equation (24) is equivalent to the system:

$$\begin{cases} Sinua \cdot Shva = 0 \\ Chva \cdot Cosua = \dfrac{Sh\pi\eta}{2\eta} \end{cases} \tag{29}$$

Considerations similar to those, used in the analysis of the above described first case, give us the dispersive law

$$v = \pm\frac{1}{a}\ln\left[\frac{Sh\pi\eta}{2\eta} + \sqrt{\left(\frac{Sh\pi\eta}{2\eta}\right)^2 - 1}\right] \quad , \qquad u = \pi n/a \tag{30}$$

which covers both of the possible values of ν .

The dispersion law given by expressions (28) and (30) as the results of numerical calculations which determinate undimensional energy in function of wave number νa is represented by Fig.1. The interval $[0 \le \nu a < 1)$ corresponds to Eq(28) while the segment $(1 < \nu a < \infty)$ refers to Eq(30). The same Fig.1 also includes for comparing the dispersion law for free particle with mass equal to m_0. There is clearly visible significant difference between two graphics for the same values of wave number.

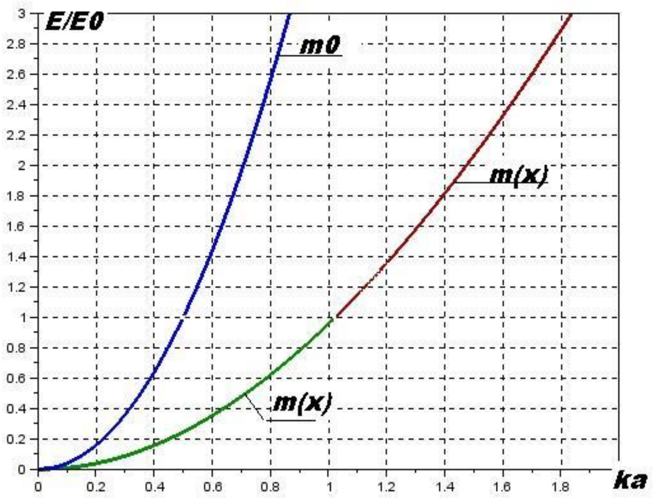

Fig. 1. Graphic of the undimensional dispersion law in function of wave number.

Appendices A

The nontrivial peculiarity of the model under study, as it can be seen from formula (10), follows from the fact that the mass of a particle shows the singularity of the inverse squares type, at points

$$x_s = \frac{\pi a}{2}(2s+1), \text{ where } s \in \mathbb{Z} . \tag{A1}$$

Some conclusion of Classical dynamics of the particle is established by Hamilton equations

$$\begin{cases} \dot{p} = \dfrac{p^2}{2m^2(x)} m' \\ \dot{x} = \dfrac{p}{m(x)} \end{cases} \tag{A2}$$

associated with the Hamiltonian

$$H = \frac{p^2}{2m(x)} \tag{A3}$$

Accordingly to the second equation of the system (A2) the linear momentum has to be given as $p = m(x)\dot{x}$. Then the first of these equations after simple rearrangement can be reduced to the form:

$$\ddot{x} + \frac{1}{2}\cdot(\dot{x})^2[\ln m(x)]' = 0 \tag{A4}$$

which admits exact integration.

Due to relation (10) the Eq (A4) assumes the following explicit form

$$\ddot{x} + \frac{(\dot{x})^2}{a} tg\left(\frac{x}{a}\right) = 0 \tag{A5}$$

which is accompanied with the initial conditions $x\big|_{t=0} = \pi s a$ and $p_x = p_0 = const$.

It is convenient to introduce non dimensional variable ξ using for it the definition:

$$a\xi = x \tag{A6}$$

In term of he new variable the equation (A5) becomes as

$$\ddot{\xi} Cos\xi + (\dot{\xi})^2 Sin\xi = 0 \tag{A7}$$

The Eq (A7) has integrating factor$1/Cos^2\xi$. Hence the first integral of (A7) is

$$\frac{\dot{\xi}}{Cos\xi} = C \tag{A8}$$

where accordingly to the initial conditions the constant $C = v_0 / a$. Being integrated the Eq (A8) conducts to the formula:

$$\ln \frac{tg(\xi/2)+1}{tg(\xi/2)-1} = \frac{v_0 t}{a} \tag{A9}$$

Inverting the Eq (A9) allows to find the following final result:

$$x(t) = \pi s a + 2a \cdot arctg\left[th\left(\frac{p_0 t}{a m_0}\right)\right]. \tag{A10}$$

Beginning from the initial point at the moment $t = 0$ the particle moves to the singular point achieving it when the time tends to infinity. The forces as well as acceleration at this point become equal to zero. Hence the classical motion of the particle with position dependent singular mass can be interpreted as falling into the center.

Appendices B

The factors in the square brackets of Eq(22) are nothing but a Wronskian $W(x)$ of the differential equation (2) determined to the right and left of the singular point. Given (8), we obtain

$$W[\xi(x)] = \begin{Vmatrix} wP_\nu^1(\xi) & wQ_\nu^1(\xi) \\ P_\nu^1(\xi)\partial_\xi w + w\partial_\xi[P_\nu^1(\xi)] & Q_\nu^1(\xi)\partial_\xi w + w\partial_\xi[Q_\nu^1(\xi)] \end{Vmatrix} \tag{B1}$$

The calculation of the Wronski determinant (B1) leads us to the expression:

$$W[\xi(x)] = \begin{Vmatrix} wP_\nu^1(\xi) & wQ_\nu^1(\xi) \\ w\partial_\xi[P_\nu^1(\xi)] & w\partial_\xi[Q_\nu^1(\xi)] \end{Vmatrix} = w^2 W[P_\nu^1(\xi), Q_\nu^1(\xi)] \tag{B2}$$

where $W[P_\nu^1(\xi), Q_\nu^1(\xi)]-$is the Wronskian built on associated Legendre functions for which there is the following relation [16];

$$W[P_\nu^\mu(\xi), Q_\nu^\mu(\xi)] = \frac{e^{i\pi\mu}2^{2\mu}}{(1-\xi^2)} \frac{\Gamma\left(\frac{\nu+\mu+2}{2}\right)\Gamma\left(\frac{\nu+\mu+1}{2}\right)}{\Gamma\left(\frac{\nu-\mu+2}{2}\right)\Gamma\left(\frac{\nu-\mu+1}{2}\right)} \tag{B3}$$

Here $\mu-$is the order of the associated Legendre functions and $\Gamma(x)-$is the Euler's gamma function. Substituting in (B3) of the value $\mu = 1$ conducts us to the result:

$$W[P_\nu^1(\xi), Q_\nu^1(\xi)] = \frac{2^2}{(\xi^2-1)} \frac{\nu(\nu+1)}{2\cdot 2} \frac{\Gamma\left(\frac{\nu+1}{2}\right)\Gamma\left(\frac{\nu}{2}\right)}{\Gamma\left(\frac{\nu+1}{2}\right)\Gamma\left(\frac{\nu}{2}\right)} = \frac{\nu(\nu+1)}{(\xi^2-1)} \tag{B4}$$

Thus, the Wronskian $W(x)$ is independent of the coordinate and can be expressed by the relation:

$$W(x) = \nu(\nu+1) \tag{B5}$$

Consequently, the left-hand side (LHS) of the equation (22) assumes the form

$$e^{iqa}\left[\Psi_1(0+)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0+}-\Psi_2(0+)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0+}\right]+$$
$$+e^{-iqa}\left[\Psi_1(0-)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0-}-\Psi_2(0-)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0-}\right]=\nu(\nu+1)\left(e^{iqa}+e^{-iqa}\right) \tag{B6}$$

As for the right-hand side (RHS) of the equation (22), by substituting the wave functions and their derivatives, we obtain:

$$\Psi_1(0+)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0-}+\Psi_1(0-)\left(\frac{\partial\Psi_2}{\partial\xi}\right)_{0+}-\Psi_2(0+)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0-}-\Psi_2(0-)\left(\frac{\partial\Psi_1}{\partial\xi}\right)_{0+}=$$
$$=\nu(\nu+1)\Big\{w(0+)\left[P_\nu^1(-ictg\varepsilon)Q_\nu(ictg\varepsilon)-Q_\nu^1(-ictg\varepsilon)P_\nu(ictg\varepsilon)\right]+ \tag{B7}$$
$$+w(0-)\left[P_\nu^1(ictg\varepsilon)Q_\nu(-ictg\varepsilon)-Q_\nu^1(ictg\varepsilon)P_\nu(-ictg\varepsilon)\right]\Big\}$$

Further simplifications are carried out on the basis of passing from negative to positive values of the Legendre function argument. The corresponding relationships are given by the following well-known [16] formulas, namely:

$$P_\nu^1(-ictg\varepsilon)=e^{-i\pi\nu}P_\nu^1(ictg\varepsilon)-\frac{2Sin\pi\nu}{\pi}Q_\nu^1(ictg\varepsilon) \tag{B8}$$

$$P_\nu(-ictg\varepsilon)=e^{-i\pi\nu}P_\nu(ictg\varepsilon)-\frac{2Sin\pi\nu}{\pi}Q_\nu(ictg\varepsilon) \tag{B9}$$

$$Q_\nu^1(-ictg\varepsilon)=-e^{i\pi\nu}Q_\nu^1(ictg\varepsilon) \tag{B10}$$

$$Q_\nu(-ictg\varepsilon)=-e^{i\pi\nu}Q_\nu(ictg\varepsilon) \tag{B11}$$

Substitution of formulas (B8) - (B11) in (B7) gives:

$$RHS=\nu(\nu+1)\times$$
$$\times\Big\{w(0+)\left[\left(e^{-i\pi\nu}P_\nu^1(ictg\varepsilon)-\frac{2}{\pi}Sin\pi\nu Q_\nu^1(ictg\varepsilon)\right)Q_\nu(ictg\varepsilon)\right]+$$
$$+w(0+)\left[e^{i\pi\nu}Q_\nu^1(ictg\varepsilon)P_\nu(ictg\varepsilon)\right]-$$
$$-w(0-)\left[\left(e^{-i\pi\nu}P_\nu(ictg\varepsilon)-\frac{2}{\pi}Sin\pi\nu Q_\nu(ictg\varepsilon)\right)Q_\nu^1(ictg\varepsilon)\right]-$$
$$-w(0-)\left[e^{i\pi\nu}Q_\nu(ictg\varepsilon)P_\nu^1(ictg\varepsilon)\right]\Big\} \tag{B12}$$

The right-hand side of the secular equation, as well as the determinant of Wronski, contain expressions $P_\nu^1(\xi)Q_\nu(\xi)+(-1)^n P_\nu(\xi)Q_\nu^1(\xi)$, in which for Wronskian it is necessary to put $n=1$, and for relation (B12) - $n=0$. To calculate these expressions, we use the Legendre function definitions in terms of Gaussian hyper geometric functions[16], namely

$$\begin{aligned}
P_\nu^\mu(\xi) &= \frac{2^{-\nu-1}\pi^{-1/2}\Gamma(-1/2-\nu)\xi^{-\nu+\mu-1}}{(\xi^2-1)^{\mu/2}\Gamma(-\nu-\mu)}\times \\
&\times F\left(1/2+\nu/2-\mu/2, 1+\nu/2-\mu/2; \nu+3/2; \xi^{-2}\right)+ \\
&+\frac{2^{\nu}\pi^{-1/2}\Gamma(1/2+\nu)\xi^{\nu+\mu}}{(\xi^2-1)^{\mu/2}\Gamma(1+\nu-\mu)}\times \\
&\times F\left(-\nu/2-\mu/2, 1/2-\nu/2-\mu/2; 1/2-\nu; \xi^{-2}\right)
\end{aligned} \tag{B13}$$

and

$$\begin{aligned}
Q_\nu^\mu(\xi) &= e^{i\pi\mu}\frac{2^{-\nu-1}\pi^{1/2}\Gamma(\nu+\mu+1)\xi^{-\nu-\mu-1}}{\Gamma(\nu+3/2)}(\xi^2-1)^{\mu/2}\times \\
&\times F\left(1+\nu/2+\mu/2, 1/2+\nu/2+\mu/2; \nu+3/2; \xi^{-2}\right)
\end{aligned} \tag{B14}$$

Considering the limit $|\xi|\to\infty$, we get

$$P_\nu^1(\xi)\approx\frac{2^{-\nu-1}\pi^{-1/2}\Gamma(-1/2-\nu)\xi^{-\nu}}{(\xi^2-1)^{1/2}\Gamma(-\nu-1)}+\frac{2^{\nu}\pi^{-1/2}\Gamma(1/2+\nu)\xi^{\nu+1}}{(\xi^2-1)^{1/2}\Gamma(\nu)} \tag{B15}$$

$$P_\nu(\xi)\approx\frac{2^{-\nu-1}\pi^{-1/2}\Gamma(-1/2-\nu)\xi^{-\nu-1}}{\Gamma(-\nu)}+\frac{2^{\nu}\pi^{-1/2}\Gamma(1/2+\nu)\xi^{\nu}}{\Gamma(1+\nu)} \tag{B16}$$

$$Q_\nu^1(\xi)=-\frac{2^{-\nu-1}\pi^{1/2}\Gamma(\nu+2)\xi^{-\nu-2}}{\Gamma(\nu+3/2)}(\xi^2-1)^{1/2} \tag{B17}$$

$$Q_\nu(\xi)=\frac{2^{-\nu-1}\pi^{1/2}\Gamma(\nu+1)\xi^{-\nu-1}}{\Gamma(\nu+3/2)} \tag{B18}$$

By substituting the above given asymptotes in the recently written expression we find the result:

$$P_\nu^1(\xi)Q_\nu(\xi)+(-1)^n P_\nu(\xi)Q_\nu^1(\xi)\approx$$
$$\approx\left[\frac{2^{-\nu-1}\pi^{-1/2}\Gamma(-1/2-\nu)\xi^{-\nu}}{(\xi^2-1)^{1/2}\Gamma(-\nu-1)}+\frac{2^{\nu}\pi^{-1/2}\Gamma(1/2+\nu)\xi^{\nu+1}}{(\xi^2-1)^{1/2}\Gamma(\nu)}\right]\times$$
$$\times\frac{2^{-\nu-1}\pi^{1/2}\Gamma(1+\nu)\xi^{-\nu-1}}{\Gamma(\nu+3/2)}- \tag{B19}$$
$$-(-1)^n\left[\frac{2^{-\nu-1}\pi^{-1/2}\Gamma(-1/2-\nu)\xi^{-\nu-1}}{\Gamma(-\nu)}+\frac{2^{\nu}\pi^{-1/2}\Gamma(1/2+\nu)\xi^{\nu}}{\Gamma(1+\nu)}\right]\times$$
$$\times\frac{2^{-\nu-1}\pi^{1/2}\Gamma(2+\nu)\xi^{-\nu-2}}{(\xi^2-1)^{-1/2}\Gamma(\nu+3/2)}$$

After opening the brackets and regrouping the terms we obtain the following relation

$$P_\nu^1(\xi)Q_\nu(\xi)+(-1)^n P_\nu(\xi)Q_\nu^1(\xi)\approx$$
$$\approx\frac{2^{-2(\nu+1)}\Gamma(-1/2-\nu)\Gamma(1+\nu)\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}\Gamma(-\nu-1)\Gamma(\nu+3/2)}-(-1)^n\frac{2^{-2(\nu+1)}\Gamma(-1/2-\nu)\Gamma(2+\nu)\xi^{-2\nu-3}}{\Gamma(-\nu)(\xi^2-1)^{-1/2}\Gamma(\nu+3/2)}+$$
$$+\frac{\Gamma(1/2+\nu)\Gamma(1+\nu)}{2(\xi^2-1)^{1/2}\Gamma(\nu)\Gamma(\nu+3/2)}-(-1)^n\frac{\Gamma(1/2+\nu)\Gamma(\nu+2)(\xi^2-1)^{1/2}\xi^{-2}}{2\Gamma(1+\nu)\Gamma(\nu+3/2)} \tag{B20}$$

Some obvious simplifications give us:

$$P_\nu^1(\xi)Q_\nu(\xi)+(-1)^n P_\nu(\xi)Q_\nu^1(\xi)\approx$$
$$\approx\frac{2^{-2(\nu+1)}\Gamma(-1/2-\nu)\Gamma(1+\nu)}{\Gamma(-\nu-1)\Gamma(\nu+3/2)}\left[\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}+(-1)^n(\xi^2-1)^{1/2}\xi^{-2\nu-3}\right]+ \tag{B21}$$
$$+\frac{\nu}{(\xi^2-1)^{1/2}(2\nu+1)}-(-1)^n\frac{(\nu+1)(\xi^2-1)^{1/2}\xi^{-2}}{(2\nu+1)}$$

For $n=1$ in the main order relative to the inverse powers of the variable ξ, we get the result

$$P_\nu^1(\xi)Q_\nu(\xi)-P_\nu(\xi)Q_\nu^1(\xi)\approx\frac{1}{(\xi^2-1)^{1/2}}+o(\xi^{-2\nu-2}) \tag{B22}$$

which in an independent way allows us to confirm the known [16] relation (17).

To $n=0$ we get:

$$P_\nu^1(\xi)Q_\nu(\xi)+P_\nu(\xi)Q_\nu^1(\xi)\approx$$
$$\approx\frac{2^{-2(\nu+1)}\Gamma(-1/2-\nu)\Gamma(1+\nu)}{\Gamma(-\nu-1)\Gamma(\nu+3/2)}\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}\left(2-\frac{1}{\xi^2}\right)+ \tag{B23}$$
$$+\frac{1}{(\xi^2-1)^{1/2}(2\nu+1)}\left[\nu-(\nu+1)\left(1-\frac{1}{\xi^2}\right)\right]$$

Now we pick out from the formula (B12) the following expression

$$\Delta=Cos\pi\nu[P_\nu^1(\xi)Q_\nu(\xi)+Q_\nu^1(\xi)P_\nu(\xi)]-\frac{2}{\pi}Sin\pi\nu Q_\nu^1(\xi)Q_\nu(\xi) \tag{B24}$$

By combining (B24) with the recently specified asymptotics (B17), (B18) and (B23) we obtain:

$$\Delta\approx Cos\pi\nu\frac{2^{-2(\nu+1)}\Gamma(-1/2-\nu)\Gamma(1+\nu)}{\Gamma(-\nu-1)\Gamma(\nu+3/2)}\left[\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}+(\xi^2-1)^{1/2}\xi^{-2\nu-3}\right]+$$
$$+Cos\pi\nu\left[\frac{\nu}{(\xi^2-1)^{1/2}(2\nu+1)}-\frac{(\nu+1)(\xi^2-1)^{1/2}\xi^{-2}}{(2\nu+1)}\right]+ \tag{B25}$$
$$+\frac{2Sin\pi\nu}{\pi}\frac{2^{-2(\nu+1)}\pi\Gamma(\nu+2)\Gamma(1+\nu)}{\Gamma(\nu+3/2)\Gamma(\nu+3/2)}(\xi^2-1)^{1/2}\xi^{-2\nu-3}$$

We regroup the terms in (B25) accordingly to the formula:

$$\Delta\approx\frac{2^{-2(\nu+1)}\Gamma(1+\nu)}{\Gamma(\nu+3/2)}\left\{Cos\pi\nu\frac{\Gamma(-1/2-\nu)}{\Gamma(-\nu-1)}\left[\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}+(\xi^2-1)^{1/2}\xi^{-2\nu-3}\right]+\right.$$
$$\left.+\frac{2(1+\nu)Sin\pi\nu\Gamma(1+\nu)}{\Gamma(\nu+3/2)}(\xi^2-1)^{1/2}\xi^{-2\nu-3}\right\}+ \tag{B26}$$
$$+Cos\pi\nu\left[\frac{\nu}{(\xi^2-1)^{1/2}(2\nu+1)}-\frac{(\nu+1)(\xi^2-1)^{1/2}\xi^{-2}}{(2\nu+1)}\right]$$

We rewrite the relation (B26) as follows:

$$\Delta \approx \frac{2^{-2(\nu+1)}\Gamma(1+\nu)}{\Gamma^2(\nu+3/2)\Gamma(-\nu-1)}\{Cos\pi\nu\Gamma(-1/2-\nu)\Gamma(\nu+3/2)\times$$
$$\times\left[\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}+(\xi^2-1)^{1/2}\xi^{-2\nu-3}\right]+2(1+\nu)Sin\pi\nu\Gamma(1+\nu)\Gamma(-\nu-1)(\xi^2-1)^{1/2}\xi^{-2\nu-3}\}+$$
$$+Cos\pi\nu\left[\frac{\nu}{(\xi^2-1)^{1/2}(2\nu+1)}-\frac{(\nu+1)(\xi^2-1)^{1/2}\xi^{-2}}{(2\nu+1)}\right] \tag{B27}$$

The Euler's gamma functions products can be simplified with using of the well known [16] identities as it is described below, i.e:

$$\Gamma(-1/2-\nu)\Gamma(\nu+3/2)=\Gamma[1-(\nu+3/2)]\Gamma(\nu+3/2)=$$
$$=-(\nu+3/2)\Gamma[-(\nu+3/2)]\Gamma(\nu+3/2)=\frac{\pi}{Sin\pi(\nu+3/2)}=-\frac{\pi}{Cos\pi\nu} \tag{B28}$$

$$\Gamma(-1-\nu)\Gamma(1+\nu)=-\frac{\pi}{(1+\nu)Sin\pi(1+\nu)}=\frac{\pi}{(1+\nu)Sin\pi\nu} \tag{B29}$$

Then by combining (B28) - (B29) with relation (B27), we obtain

$$\Delta \approx \frac{2^{-2(\nu+1)}\Gamma(1+\nu)}{\Gamma^2(\nu+3/2)\Gamma(-\nu-1)}\pi\left[(\xi^2-1)^{1/2}\xi^{-2\nu-3}-\frac{\xi^{-2\nu-1}}{(\xi^2-1)^{1/2}}\right]+$$
$$+Cos\pi\nu\left[\frac{\nu}{(\xi^2-1)^{1/2}(2\nu+1)}-\frac{(\nu+1)(\xi^2-1)^{1/2}\xi^{-2}}{(2\nu+1)}\right] \tag{B30}$$

The expression in the first line of formula (B30) is in order of $o(\xi^{-2\nu-4})$, whereas the expression in the second line is proportional to ξ^{-1}. Thus, keeping the terms of the main order we come to the result:

$$\Delta \approx -\frac{Cos\pi\nu}{(\xi^2-1)^{1/2}(2\nu+1)}+o(\xi^{-3}) \tag{B31}$$

Accordingly to the rule of determination of univalue branch of LeGendre functions [18] the relation

$$w(0+)=-w(0-)=-(\xi^2-1)^{1/2} \tag{B32}$$

takes place. By combining Eqs (B6), (B12), (B31) and (B32) we finally obtain the equation (23)

$$e^{iqa} + e^{-iqa} = \frac{e^{i\pi\nu} + e^{-i\pi\nu}}{2\nu + 1}$$

for eigenvalues of energy if particle position dependent mass is given by expression (10).

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