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ONE-BODY STATES IN THE SCHRÖDINGER MODEL WITH HYPERBOLIC DOUBLE-WELL POTENTIALS

Wave one-body states in the model system describing by the one-dimensional Schrödinger equation with a hyperbolic double-well confining potential is considered. With the help of the transformation to confluent Heun equation we have obtained polynomial solutions, representing the wavefunctions of bound states. The requirements on the potential parameters providing existent of the coupled quantum states is analized.

1. Introduction

A small number of exact solutions to the Schrödinger equation were obtained historically in the genesis of quantum mechanics.[1–5]. More recently, other exactly-soluble systems have been found by both traditional means [6,7] and via the factorization techniques of supersymmetric quantum mechanics (SUSY).[8,9]. Conventionally, analytical solutions to the Schrödinger equation were found via a reduction to a hypergeometric equation,[10] an equation with three regular singular points, however recently a new solution via Heun's differential equation[11–14] has been reported.[15].

Heun's equation, a Fuchsian equation with four regular singular points, was initially studied by the German mathematician Karl Heun in the late 19th century.[16] It has several special or limiting cases of great importance in mathematical physics, namely the Lam´e, Mathieu and spheroidal differential equations.[17] However, it is only recently that its use in physics has become increasingly widespread,[18] with its solutions being used in works ranging from quantum rings[19] to black holes.[20] In this work, we report a class of confining potentials that can be transformed to the confluent Heun equation from the one-dimensional Schrödinger equation. One case, of a hyperbolic double-well, allows one to reduce the solution to simple polynomials for special values of the system parameters. The double-well problem has been studied extensively [21–23] and is of continued interest due to its importance as a toy model, from heterostructure physics[24] to the trapping of Bose-Einstein condensates.[25].

Please consider the following class of potentials, defined by two physical parameters V_0 and d, shaping the potential depth and width respectively, and with two class parameters, with $q = -2, 0, 2, 4, 6$ defining the 'family' and $p = 0$.

Most notable is the case $(q, p) = (2, 0)$, which describes the well-known P¨oschl-Teller potential.[4] In fact, all constituent potentials of the families $q = -2$, 0, 2 lead to Schr¨odinger equations of no more than three singular points after a transformation of independent variable to $\_ = 1/\cosh 2(x/d)$ or $\_ = \tanh(x/d)$, and so can be reduced to equations of the hypergeometric type. Termination of the

resultant hypergeometric functions leads to analytic expressions for the eigenvalues of the problem. However, when q = 4, 6 the same transformation variables lead to equations of the confluent Heun type. Now, two termination conditions must be satisfied in order to get a polynomial solution to the Schr¨odinger equation. The (4, p) family cannot be terminated due to the first condition, which imposes a simple relation on the physical parameters arising in the problem. The (6, p) family fulfill the first condition but not the second, more involved condition, which also must hold to abort the Taylor series solution. However, remarkably the special case of (6, 4) is an exception and does admit polynomial solutions for certain values of the physical parameters, which will be the main focus of this work. The rest of this work is as follows. We give a full derivation of our solution in terms of confluent Heun functions in Sec. II, along with details of the power series solution. In Sec. III we provide the eigenvalues of our hyperbolic double-well problem, along with examples of the wavefunctions found for the first few states. We provide numerical support to our analytic results in Sec. IV and finally, we draw some conclusions in Sec. V.

The atomic and electron structure of carbon nanotubes can be represented as, a two-dimensional carbon hexagonal structure rolling along a given direction and reconnecting the carbon bonds. Systems of carbon atoms can exist in several modifications: laminated graphite with a hexagonal structure, nite carbon, crystal diamond, the fullerenes C_{60}, C_{70}, C_{78}, C_8, and carbon nanotubes—two-dimensional extended structures rolled up in a single- or multiwall tube [1,2]. Carbon nanotubes were synthesized simultaneously with fullerenes and are more interesting structures because they model a one-dimensional system. Soliton states are known to be formed in such systems.

The property of nanotubes to absorb liquid metal, hydrogen, oxygen, methane, and other gases opens a prospect for constructing strong thin conducting lines of fuel elements and creating new types of fuel. The discovery of superconductivity in metal-doped C_{60} [3] feeds the hope to find the same phenomenon in nanotubes filled with metal or to modify the superconductivity of known superconductors by injecting them in a nanotube.

Electron spectrum of such structure is characterized by quantum numbers including the number of radial (n), azimuthal (m) and longitudinal (k) modes [4,5]. Its physical properties are considerably related to collective electron-phonon excitations and oscillations of electron density (plasmons or plasma oscillations).

The equations, describing such excitations, can be obtained on the basis the functional integral method with help of the variational derivatives of the expression for the effective action integral. We assume that a such approach allows most precisely to calculate polarizing function of the carbon nanotube in view of all features of its atomic structure.

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2. The effective action function of the system

The researched system consists of ions with charge Ze and degenerate electrons. Then the functional integral of the system in terms of spatial coordinates (x, y, z) and imaginary time (τ) can be represented as [4,5]

$$Z = \int D\psi^{+} D\psi \exp\left(S[\psi]\right), \qquad (1)$$

where the action $S[\psi]$ is determined by the expression

$$S[\psi] = \int_{0}^{\beta} dr \int dx \sum_{s} \psi_{s}^{+}(x,r) K(x,r) \psi_{s}(x,r) -$$

$$-\frac{e^2}{2} \int_{0}^{\beta} dr \int dx dy \rho(x,r) V(x-y) \rho(y,r) + \qquad (2)$$

$$+\int_{0}^{\beta} dr \sum_{l_a} \left[i p_{l_a}(r) \partial_r q_{l_a}(r) - \frac{p_{l_a}(r)}{2M_C} \right], \qquad a = \alpha, \beta.$$

Here s is an electron spin, $\psi_{s}(x,r)$ is the two-component wave function of the nanotube lattice (a, b)

$$\psi_{s}(x,\tau) = \begin{pmatrix} \psi_{as}(x,\tau) \\ \psi_{as}(x,\tau) \end{pmatrix},$$

p_{l_a}, q_{l_a} and $2M_C$ are a moment, a coordinate and the mass of an ion in l_a sublattice cite, $V(x-y) = 1/|x-y|$ is the operator of the Coulomb interaction. Beside, $K(x,r)$ is the operator of kinetic energy of the form

$$K(x,r) = \begin{pmatrix} K_a(x,r) & 0 \\ 0 & K_b(x,r) \end{pmatrix}, \quad K_{a,b}(x,r) = -\partial_r + \frac{\Delta_{a,b}}{2m_\varepsilon} + \mu_{a,b},$$

where $\partial_r = \partial/\partial_r$, $\Delta_a/(2m)$ is the kinetic energy for the a th sublattice, μ_a a chemical potential of the a th sublattice.

The charge density $\rho(x,r)$ is composed of ion ($\rho^{q}(x,r)$) and electron ($\rho^{e}(x,r)$) parts and equals $\rho(x,r) = \rho^{q}(x,r) - \rho^{e}(x,r)$, where

$$\rho^{q}(x,r) = \sum_{\alpha,\gamma} \rho^{q}_{\alpha\gamma}(x,r) \delta_{\alpha,\gamma}, \quad \rho^{e}(x,r) = \sum_{\alpha,\gamma} \rho^{e}_{\alpha\gamma}(x,r).$$

The summation on α and γ is carried out over all lattice sites a and b.

In the representation of the functional integral (1) can be rewritten as

$$Z[\psi,\varphi] = \int D\psi^{+} D\psi \int D\varphi \exp\left(S[\psi,\varphi]\right), \qquad (3)$$

where the action function $S[\psi,\varphi]$, which contains an electron influence, the field φ and its interaction, has the form

$$S[\psi] = -\frac{1}{2}\int_0^\beta dr \int dxdy \varphi(x,\tau)V^{-1}(x-y)\varphi(y,\tau)+$$

$$+\int_0^\beta d\tau \int dx \sum_s \psi_s^+(x,r)K'(x,r)\psi_s(x,r)+$$

$$+ie\int_0^\beta dr \int dx \rho^q(x,\tau)\varphi(x,\tau)+$$

$$+\int_0^\beta dr \sum_{l_a}\left[ip_{l_a}(r)\partial_r q_{l_a}(r) - \frac{p_l^2(r)}{2M_C}\right], \quad a = \alpha,\beta.$$

Here

$$K'(x,r) = \begin{pmatrix} K_a(x,r)-ie\varphi(x,\tau) & -ie\varphi(x,\tau) \\ ie\varphi(x,\tau) & K_b(x,r)-ie\varphi(x,\tau) \end{pmatrix}.$$

Integrating in (3) on Fermi fields [4] and using the known Liouville formulae, $\left(\lg\det A\right)' = \mathrm{Sp}\left((\ln A)'\right)$, where A is matrix, a prime denotes a first derivative, we can transform (3) to the form $Z = \int D\varphi \exp\left(S_{eff}[\varphi]\right)$. Here the effective action

$$S_{eff}[\varphi] = -\frac{1}{2}\int_0^\beta dr \int dxdy \varphi(x,\tau)V^{-1}(x-y)\varphi(y,\tau)+$$

$$+2\mathrm{SplnK'}(x,\tau)+ie\int_0^\beta d\tau \int dx \rho^q(x,\tau)\varphi(x,\tau)+$$

$$+\int_0^\beta dr \sum_{l_a}\left[ip_{l_a}(r)\partial_r q_{l_a}(r) - \frac{p_l^2(r)}{2M_C}\right], \quad a = \alpha,\beta, \tag{4}$$

allows to describe the system in collective variables.

The matrix Green function, $G = \|G_{\alpha,\beta}\|$ of the system is determined by the equation

$$K'(x,\tau)G(x,\tau_x;y,\tau_y) = \delta(x-y)\delta(\tau_x - \tau_y) \tag{5}$$

At presence only the effective field, V_{eff}, of single-electron model potential of carbon nanotube (see [Ah]) the Green function, $G_0 \| G_{0,\alpha\beta}\|$, is determined by the equation

$$K_0'(x,\tau)G_0(x,\tau_x;y,\tau_y) = \delta(x-y)\delta(\tau_x - \tau_y),$$

where $K_0(x,\tau_x) = K'(x,\tau_x)|_{\varphi=iV_{eff}}$.

Using the representation $K'(x,\tau_x) = K_0(x,\tau_x) + K_1(x,\tau_x)$, where the function $K_0(x,\tau_x) = (-ie\varphi(x,\tau_x) + eV_{eff}(x))\|c_{ik}\|$, $c_{ik} = 1$, $(i,k = 1,2)$ (5) can be rewritten in the form

$$G(x,\tau_x;y,\tau_y)=G_0(x,\tau_x;y,\tau_y)-$$
$$-\int_0^\beta d\tau_z\int dz G_0(x,\tau_x;z,\tau_z)K_1(z,\tau_z)G(z,\tau_z;y,\tau_y). \tag{6}$$

The obtained expressions for the effective action function together with the equation (6) for the Green function permit build the equations determining the field $\varphi(x,\tau_x)$.

3.   The equations for field functions

The equations describing states of the system are obtained by equating to zero the variational derivation of the effective action function (4) with respect to generalized coordinates $\varphi(x,\tau_x)$, q_{l_α}, p_{l_α} that give the system

$$\frac{\delta S_{eff}[\varphi]}{\delta(\varphi(x,\tau))}=0,\ \frac{\delta S_{eff}[\varphi]}{\delta(q_{l_\alpha}(\tau))}=0,\ \frac{\delta S_{eff}[\varphi]}{\delta(p_{l_\alpha}(\tau))}=0.$$

These three equality result in the system of the three equations

$$-\int dy V^{-1}(x-y)\varphi(y,\tau)+ie\rho^q(x,\tau)-$$
$$-2e\lim_{\substack{y\to k\\ \tau_y\to\tau_x-0}}\mathrm{Sp}\left\{G(x,\tau_x;y,\tau_y)\begin{pmatrix}1&1\\1&1\end{pmatrix}\right\}=0,$$
$$i\partial_\tau p_{l_\alpha}(\tau)-ieZ\int d^3x\varphi(x,\tau)\nabla\delta(x-q_{l_\alpha})=0, \tag{7}$$
$$i\partial_\tau q_{l_\alpha}(\tau)-\frac{p_{l_\alpha}(\tau)}{M_C}=0.$$

From the first equation of the system (7) follows that the field function

$$\varphi(z,\tau)=ie\int dx V(z-x)\rho^q(x,\tau)-4ie\int dx V(z-x)\times$$
$$\times\lim_{\substack{y\to k\\ \tau_y\to\tau_x-0}}\left(G_1(x,\tau_x;y,\tau_y)+G_2(x,\tau_x;y,\tau_y)\right), \tag{8}$$

means the electrical field of the electrical potential of ions and electrons. This quantity completely determines the interaction in the system and its collective excitations. Taking into account that $\Delta V(x-y)=-4\pi\delta(x-y)$, the equation (8) can be transformed to the form

$$\Delta\varphi(z,\tau)=4\pi e\rho^q(x,\tau)-$$
$$-16\pi e\lim_{\tau_y\to\tau_x-0}\left(G_1(x,\tau_x;y,\tau_y)+G_2(x,\tau_x;y,\tau_y)\right), \tag{9}$$

that together with the equation (6) consists the closed system. For solving this system we introduce the new notations the $\widetilde{G} = G_1 + G_2$ and $\widetilde{G}_0 = G_{01} + G_{02}$. Then taking into account that for statical ions

$$iV_{eff} = ie\int dzV(x-z)\rho^q(z,\tau) - 4ie\int dxV(z-x)\lim_{\substack{z_1\to z\\ \tau_{z_1}\to\tau_z-0}}\left(\widetilde{G}_0(z,\tau_z;z_1,\tau_{z_1})\right) \quad \text{and}$$

$$\widetilde{G} = \widetilde{G}_0 + 2ie\widetilde{G}_0(\varphi - iV)\widetilde{G} \approx \widetilde{G}_0 + 2ie\widetilde{G}_0(\varphi - iV)\widetilde{G}_0 + ...,$$

we can obtain the expression

$$\varphi(z,\tau) - iV_{eff} = 8e^2\int dzdz_1d\tau_{z_1}\, V(x-z)G_0(z,\tau;z_1,\tau_1)\times$$
$$\times\left(\varphi(z_1 - iV_{eff}(z_1))G_0(z,\tau;z_1,\tau_1)G_0(z_1,\tau_1;z,\tau) + ..., \quad \tau_z \to \tau,\right.$$

which describes plasma oscillations.

The second and third equations of the system (7) determine motion of carbon ions. The obtained self-consistent close system of equations describes the electron and vibrational subsystems via collective variations.

For calculation the electron density fluctuation induced by plasma vibration relative to the stationary ion lattice we will enter into (8) the polarization operator $P(x,\tau;z_1,\tau_1)$ which is determined by equality

$$\int dz_1 d\tau_1 V(x-z_1)\delta(\tau-\tau_1)\widetilde{G}(z_1,\tau_1;z',\tau') -$$
$$-\int dz_1 d\tau_1 P(x,\tau;z_1,\tau_1)\delta(\tau-\tau_1)\widetilde{G}_0(z_1,\tau_1;z',\tau').$$

Then the field function can represent in terms of the effective potential V_{eff} and polarization operator P in the form

$$\varphi(z,\tau) = iV_{eff}(z,\tau) - 4ie\int dz_1 d\tau_1\left(P(x,\tau;z_1,\tau_1) -\right.$$
$$\left. -V(x-z_1)\delta(\tau-\tau_1)\right)G_0(z_1,\tau_1;z',\tau')$$

The Green function obeys the matrix equation

$$\widetilde{G} = \widetilde{G}_0 + 8e^2\widetilde{G}_0\left(P-V\right)\widetilde{G}_0\widetilde{G} ,$$

whence applying the relation $V\widetilde{G} = P\widetilde{G}_0$ we can obtain the equation

$$P = V - 8e^2 V\widetilde{G}_0 P , \tag{10}$$

determining in the linear approximation the polarization P. The poles of the Fourier transform of the polarization function P determine plasma oscillations of the density relative to a ground stationary state.

Applying the Fourier transform to (10) we can obtain in the approximation of the second order in V the expression

$$P(q,\omega;q',\omega') = -\frac{4\pi}{q^2}\delta(q-q')\delta(\omega-\omega') \times$$

$$\times\left(1 + \frac{e^2}{2}\frac{4\pi}{q^2}\sum_{\substack{n,m,k;\\n_1,m_1,k_1}}\int dx\, G_{nmk}(x)G_{n_1m_1k_1}(-x)e^{-iqx}\delta(\omega - E_{nmk} + E_{n_1m_1k_1})\right),$$

where q and ω are coordinate and frequency components of the Fourier transform; Energy levels of stationary states of the electron subsystem are denoted as E_{nmk} (see [1]). The spectrum and intensity of the collective excitations are described by the diagonal part of $P(q,\omega;q',\omega')$.

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ЗАСТОСУВАННЯ МЕТОДУ АНАЛІТИЧНИХ МЕРЕЖ ДЛЯ ВИБОРУ ПРОГРАМНИХ ПРОДУКТІВ ДИСТАНЦІЙНОГО НАВЧАННЯ

The problem solution of software choice that are designed for use in the educational process when implementing of distance learning using the method of analytic networks was proposed.

Distance learning, software, task selection, problem solution.

Аналіз існуючих програмних засобів щодо побудови програмного забезпечення (ПЗ) систем дистанційного навчання (СДН) дозволили зробити висновок про наявність багатьох програмних продуктів, які розроблені для дистанційного навчання (ДН). Ці програмні продукти, поділяються на три класи: системи управління навчанням (СУН), авторські засоби розробки (АЗР) та засоби веб-комунікацій (ЗВК). Під час вибору зазначених