Zeitschrift: Helvetica Physica Acta

Band: 72 (1999)

Heft: 5-6

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DOI: https://doi.org/10.5169/seals-117181

Helv. Phys. Acta 72 (1999) 295 - 300
0018-0238/99/050295-06 $ 1.50+0.20/0

Helvetica Physica Acta

Impurity at the boundary of two quantum wires: 1D Schrödinger equations with an asymmetric Coulumb potential.

By

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Abstract. In the momentum space we find the bound eigenenergies and eigenfunctions of the 1D Schrödinger equation for an asymmetric Coulomb potential. We find that eigenfunctions in the configuration space are expressed in terms of fractional derivatives. Our approach could provide qualitative features of the electronic states of an impurity located between two different quantum wires.

1 Introduction

In general, asymmetry in nature produces exciting physical phenomena. For instance, in the study of artificial heterostructures there is recent experimental and theoretical interest in the effects of asymmetry in quantum systems such as wells [1]-[5], wires [6] and dots [7].

The stationary states of the one-dimensional (1D) Schrödinger equation describing the 1D hydrogen atom (1D H atom) have attracted a great deal of interest [8, 9, 10, 11]. This equation is related to the exciton problem in the effective mass approximation in the study of high temperature superconductors[12], semiconductor quantum wires [13, 14, 15, 16], polymers [17, 18], and due to the existence of image forces on 1D electron gas at the helium surface, is also related to the Wigner crystal [19, 20].

A general characteristic of some 1D calculations is that the Frobenius series method was employed to solve the 1D Schrödinger equation in real space, and this was done only for the symmetric potential $1/|x|$. To our knowledge the 1D asymmetric potential $\lambda_1/|x|$ for $x > 0$ and $\lambda_2/|x|$ for $x < 0$ with $\lambda_1 \neq \lambda_2$ has not been investigated before. We believe that our approach is illustrative since there are not many problems of this type suitable to be solved in the momentum space.

Clearly, our 1D Hamiltonian does not describe a physical problem since real systems always exhibit finite thickness. However, due to recent advances in the fabrication and study of the physical properties of semiconductor heterostructures [13] it is now feasible to construct and study a system formed by a fixed impurity of total charge Ze located between two different semiconductor very thin quantum wires (QW) -with transverse thickness of the order of nanometers. Hopefully, our results could exhibit some qualitative features of the behaviour of such real system in the case of highly-confined electrons -for which $x >> y, z$ almost always if the system is oriented along the x-direction. Electrons experience asymptotic Coulomb potentials $Ze/\epsilon_i r$ to the right and to the left where ϵ_i $(i = 1, 2)$ are screening dielectric constants and $r = \sqrt{x^2 + y^2 + z^2}$, which is similar to our potential $Ze/\epsilon_i |x|$. On the other hand, in a highly-confined real system electrons practically move in 1D since its wavefunction can be written as $f(y, z)e^{ikx}$. That is, an electron is free in the x-direction and in the y- and z-directions it has its lowest energy when $f(y, z)$ corresponds to the transverse confinement groundstate.

2 Momentum space equation

The 1D Schrödinger equations with attractive asymmetric Coulomb potential to be considered here are given by

$$\frac{d^2\psi}{dx^2} + \left(\frac{\gamma g}{|x|} - \mathcal{E}\right)\psi = 0, \tag{2.1}$$

where $\gamma = 2mZe^2/\hbar^2$, $\mathcal{E} = -\epsilon\Updownarrow\mathcal{E}/\zeta^{\epsilon}$ and $g = 1/\epsilon_1$ for $x > 0$ and $g = 1/\epsilon_2$ for $x < 0$. Here m and e are the mass and electric charge of the electron and Z is a positive integer. We restrict our work to consider just the bounded states associated to Eq.(2.1) for which their corresponding wave functions are square integrable in the whole space. For such states the Laplace transform $\mathcal{L}$ exists for both the positive and negative parts of the real axis, defined by

$$\phi(s) = \mathcal{L}[\psi(\S)] = \int_{/}^{\infty} \lceil\S\psi(\S)\rceil^{-/\S}, \tag{2.2}$$

and can be performed by using the property [21] $\mathcal{L}[\psi(\S)/\S] = \int_{\surd}^{\infty} \phi(\int)\lceil\int$ valid when $\lim_{x->0}\psi(x)/x$ is well defined. It should be remarked that it can be directly shown form Eq.(2.1) that $\psi(x)$

does satisfy this condition. Here s is understood as $s = ip/\hbar$. Taking the Laplace transform of Eq.(2.1) gives

$$\left(-s^2 + \mathcal{E}\right)\frac{dG}{ds} + \frac{\gamma}{\epsilon_1}\left(G(s) - G(\infty)\right) - \frac{d\psi}{dx}(0^+) = 0, \tag{2.3}$$

where $G(s) = \int_0^p \phi(s')ds'$ and $d\psi(0^+)/dx$ is the right hand side limit of $\psi(x)$ at $x = 0$. By solving this equation for $G(s)$ and rewriting the resulting expression in terms of p, we arrive at

$$G(s) - G(\infty) - \frac{\epsilon_1}{\gamma}\frac{d\psi}{dx}(0^+) = A_1\left(\frac{\sqrt{\mathcal{E}} - s}{\sqrt{\mathcal{E}} + s}\right)^{\frac{\gamma}{2\epsilon_1\sqrt{\mathcal{E}}}}, \quad x > 0 \tag{2.4}$$

where A_1 is an arbitrary constant to be determined by normalization. Using the same procedure but for the negative part of the real axis, we obtain

$$G(s) - G(-\infty) - \frac{\epsilon_2}{\gamma}\frac{d\psi}{dx}(0^-) = A_2\left(\frac{\sqrt{\mathcal{E}} - s}{\sqrt{\mathcal{E}} + s}\right)^{\frac{\gamma}{2\epsilon_2\sqrt{\mathcal{E}}}}, \quad x < 0, \tag{2.5}$$

where A_2 is an arbitrary constant to be determined by normalization. By integrating Eq.(2.1) one time with respect to x, it can be shown that the condition $\lim_{x->0}\psi_2(x)/x < 0$, leads to $d\psi(0^+)/dx = d\psi(0^-)/dx$. Thus by evaluating Eqs.(2.4) and (2.5) at ∞ and $-\infty$, respectively, the continuity of the derivative allows to write $(A_1/\epsilon_1)e^{i\gamma\pi/\left(2\epsilon_1\sqrt{\mathcal{E}}\right)} = (A_2/\epsilon_2)e^{-i\gamma\pi/\left(2\epsilon_2\sqrt{\mathcal{E}}\right)}$, which yields the eigenenergy spectrum; $E_n = -(1/\epsilon_1 + 1/\epsilon_2)^2 mZ^2e^4/\left(8\hbar^2n^2\right)$ with n an integer. Taking the derivative of G_n for a particular n yields

$$\frac{dG(s)}{ds} = -\frac{A}{\sqrt{\mathcal{E}}}\frac{\left(\sqrt{\mathcal{E}} - s\right)^{\frac{\gamma}{2\epsilon_1\sqrt{\mathcal{E}}}-1}}{\left(\sqrt{\mathcal{E}} + s\right)^{\frac{\gamma}{2\epsilon_1\sqrt{\mathcal{E}}}+1}}, \tag{2.6}$$

or written in terms of p, we have after manipulation

$$\phi_n(p) = \frac{dG_n}{dp} = A\frac{\hbar^2 e^{4ing(\epsilon_1\epsilon_2/(\epsilon_1+\epsilon_2))\arctan\left(p\hbar n\epsilon_1\epsilon_2/mZe^2(\epsilon_1+\epsilon_2)\right)}}{p^2 + \left[(1/\epsilon_1 + 1/\epsilon_2)mZe^2/\hbar n\right]^2}, \tag{2.7}$$

where $A = \gamma A_1/\epsilon_1 = \gamma A_2/\epsilon_2$. The corresponding probability densities associated to each n-eigenfunction can be calculated from $P_n(p) = |dG_n/dp|^2$ yielding $P_n(p) = A_n^2/(\mathcal{E} + \sqrt{\ }^{\epsilon})^{\epsilon}$ where A_n is a normalization constant. Notice that for a given n, $P_n(p)$ has the same form as that of the only bound state of an attractive delta potential, that is to say, we could adjust the strength of the delta potential in such way that we could reproduce $P_n(p)$ for any n.

3 Wavefunctions in real space

To obtain the eigenfunctions in real space $\psi_n(x)$, we take the inverse Laplace transform of dG_n/dp or Bromwich integral for both the positive and negative parts of the real axis, defined by

$$\psi_n(x) = \mathcal{L}^{-\infty}\left[\phi(\int)\right] = \frac{\infty}{\in\pi\rangle}\oint_{\nabla-\rangle\infty}^{\nabla+\rangle\infty} \lceil \int\phi(\int)\rceil^{\int\S}. \tag{3.1}$$

Here the integration contour is a vertical line in the complex plane which may be closed by an infinite semicircle in the left hand semiplane, r is a constant to be chosen so that all the singularities of $\phi(s)$ are on the left hand side of the vertical line. Substitution Eq.(2.6) into the last definition and integrating by parts, we have

$$\psi_n(x) = \frac{A_n x}{2\pi i}\oint_{r-i\infty}^{r+i\infty}\frac{ds}{g}\left(\frac{\sqrt{\mathcal{E}}-s}{\sqrt{\mathcal{E}}+s}\right)^{\frac{g\gamma}{2\sqrt{\mathcal{E}}}} e^{sx}, \tag{3.2}$$

and if we introduce the dimensionless variable $z = (s+\sqrt{\mathcal{E}})/(s-\sqrt{\mathcal{E}})$, Eq.(3.2) can be expressed as the contour integral in the complex unit circle $|z| < 1$ given by

$$\psi_n(x) = \frac{A_n'\zeta e^{\zeta}}{2\pi i}\oint_C dz\frac{e^{-2\zeta z/(1-z)}}{z^{\frac{g\gamma}{2\sqrt{\mathcal{E}}}}(1-z)^2}, \tag{3.3}$$

where $\zeta \equiv \sqrt{\mathcal{E}}x$. It is convenient to rewrite the contour integral of Eq.(3.3) in terms of the variables $w - \zeta \equiv 2\zeta z/(1-z)$, to obtain

$$\begin{aligned}\psi_n(x) &= A_n'\frac{\zeta^{-1}e^{\zeta}}{2\pi i}\oint dw\frac{w^{ng\alpha+1}e^{-w}}{(w-\zeta)^{ng\alpha+1}}\\ &= \frac{\zeta^{-1}e^{\zeta}}{\Gamma(ng\alpha+1)}\frac{d^{ng\alpha}}{d\zeta^{ng\alpha}}\left(\zeta^{ng\alpha+1}e^{-\zeta}\right),\end{aligned} \tag{3.4}$$

where $\alpha = 2\epsilon_1\epsilon_2/(\epsilon_1+\epsilon_2)$. With this transformation the new contour encloses the point $w = \zeta$ in the w plane. In Eq.(3.4) we have used the Osler-Nekrassov definition for the fractional derivative [22], given by

$$\frac{1}{2\pi i}\oint_C dw\frac{h(w)}{(w-\zeta)^{\eta+1}} = \frac{1}{\Gamma(\eta+1)}\frac{d^{\eta}h(w)}{d\zeta^{\eta}}$$

for any function $h(w)$ and real number η. Here $\Gamma(n)$ is the Gamma function . To expand Eq.(3.4) we use the Leibnitz rule's generalization

$$\frac{d^{ng\alpha}[fg]}{d\zeta^{ng\alpha}} = \sum_{k=0}^{\infty}\binom{ng\alpha}{k}\frac{d^{ng\alpha-k}f}{d\zeta^{ng\alpha-k}}\frac{d^k g}{d\zeta^k}, \tag{3.5}$$

valid for arbitrary value of q, and the formulae [23]

$$\frac{d^{ng\alpha-k}\zeta^{ng\alpha+1}}{d\zeta^{ng\alpha-k}} = \frac{\Gamma(ng\alpha+2)}{\Gamma(k+2)}\zeta^{k+1}, \tag{3.6}$$

$$\frac{d^k e^{-\zeta}}{dx^k} = \frac{e^{-\zeta}}{\zeta^k}\Gamma(-k,-\zeta), \tag{3.7}$$

where $\Gamma(c,\zeta)$ is the incomplete Gamma function defined by [24]

$$\Gamma(c,\zeta) = \frac{\zeta^{-c}}{\Gamma(c)}\int_0^{\zeta} t^{c-1}e^{-t}dt. \tag{3.8}$$

By substituting the above expressions into Eq.(3.4) we write $\psi_n(\zeta)$ as

$$\psi_n(\zeta) = 2\pi A_n\zeta e^{-\zeta}\sum_{k=0}^{\infty}\binom{ng\alpha}{k}\frac{\Gamma(ng\alpha+2)}{\Gamma(ng\alpha+1)\Gamma(k+2)}\Gamma(-k,-\zeta). \tag{3.9}$$

Finally, we shall exhibit explicitly the asymptotic behavior of $\psi_{1,n}(\zeta)$ for both small ζ and large values of ζ. From Eq.(3.8) we have $\Gamma(c,0) = 1/\Gamma(c+1)$, and thus we can approximate $\psi_{1,n}(\zeta)$ around the origin as

$$\psi_{1,n}(\zeta) \approx 2\pi A_n\zeta F(n), \tag{3.10}$$

where $F(n)$ is a finite positive constant given by

$$F(n) = \sum_{k=0}^{\infty}\binom{ng\alpha}{k}\frac{ng\alpha+1}{\Gamma(k+2)\Gamma(1-k)}. \tag{3.11}$$

On the other hand, using the fact that $\Gamma(-c,\zeta) \approx \zeta^c$ for large values of ζ we obtain the following asymptotic expression

$$\psi_n(\zeta) = 2\pi A_n\zeta e^{-\zeta}\sum_{k=0}^{\infty}\binom{ng\alpha}{k}\frac{ng\alpha+1}{\Gamma(k+2)}\zeta^k. \tag{3.12}$$

In summary, we have obtained the 1D bound states of an asymmetric Coulomb potential which to our knowledge has not been investigated before. We found the eigenergies and gave expressions of the eigenfunctions in terms of fractional derivatives which in turn can be written in terms of incomplete Gamma functions. Also we provided analytical asymptotic expressions of these eigenfunctions for small and large arguments. We hope that this paper may stimulate further work on the study of asymmetric quantum problems with Coulomb-type and related singular potentials.

Acknowledgments

We acknowledge useful discussions with C. I. Mendoza and support by DGAPA-UNAM and CONACYT- México through grants Nos. IN–114498 and 3042PE, respectively.

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