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Analytical solution to position dependent mass for 3D-Schrödinger equation

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Abstract: We have derived an analytical solution of the 3D Schrödinger equation where the mass varies with position. Our solution is a general solution for any massive particle with a position dependent mass $m(\mathbf{r})$ scattered by an arbitrary potential $\mathcal{V}(\mathbf{r})$

1. Introduction

The concept of position dependent massodinger equation (PDMSE), applied to different physical systems [1–9], has attracted great attention in the past few decades. Owing to its application from bulk semiconductors to quantum fluids have motivated the researchers to investigate the dynamics of these systems. To solve this problem analytically, different approaches have been employed [10–17].

From elementary quantum mechanics we know that if two operators do not commute with each other then their relative ordering is very important. In case of position dependent mass, the ordering of the momentum and the position dependent mass to define the kinetic energy becomes crucial because of their non-commutativity. The choice of the ordering should be such that the kinetic energy operator is Hermitian. O. von Roos [18] was the first to suggest the following generalized form of the kinetic energy operator for position-dependent mass model

$$T = \frac{1}{4}(m^{\eta}\mathbf{p}m^{\epsilon}\mathbf{p}m^{\rho} + m^{\rho}\mathbf{p}m^{\epsilon}\mathbf{p}m^{\eta}), \tag{1}$$

where $m = m(\mathbf{r})$ is the position-dependent mass. The constants η, ϵ and ρ, which are also known as the von Roos ambiguity parameters can be assumed to be arbitrary but they obey the constraint equation $\eta + \epsilon + \rho = -1$. It can be easily verified that the kinetic energy operator T is Hermitian. Before von Roos several forms of operator T has been used to solve this problem [19–22]. Some of the forms are

$$T = \tfrac{1}{4}\left[\tfrac{1}{m}p^2 + p^2\tfrac{1}{m}\right], (\eta = -1, \epsilon = 0, \rho = 0), \tag{2}$$

$$T = \tfrac{1}{2}\left[\mathbf{p}\tfrac{1}{m}\mathbf{p}\right], (\eta = 0, \epsilon = -1, \rho = 0), \tag{3}$$

$$T = \tfrac{1}{2}\left[\tfrac{1}{\sqrt{m}}p^2\tfrac{1}{\sqrt{m}}\right], (\eta = -1/2, \epsilon = 0, \rho = -1/2). \tag{4}$$

In some cases vanishing wave function at the hetero-junction boundary, puts an additional constraint on the von Roos parameters, i.e $\eta = \rho$.

Recently we have explored this problem analytically [23] and obtained an approximate solution which is in excellent agreement with the numerical simulations. In this article we have extended the approach from 1-D [23] to 3-D. The main

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result of this paper is the analytical solution given by Eq.(25). The structure of the paper is as follows. In section II, we will briefly summarize the approach used for 1-D and show how well our approximate solution works in comparison with the numerical simulations [see Fig (2)]. In section III, we extended this approach to find an analytical solution for PDMSE for 3D variation of mass and potential function.

2. Analytical solution for 1D-position dependent mass SchrodingerSchrödinger equation

Let us first recall the approach for the 1D problem. The mass variable Schrodinger equation describing the evolution of the wavefunction for an incident beam of particles with variable mass $m(x)$ moving in one dimension with kinetic energy $\mathcal{E}$, interacting with potential $\mathcal{V}(x)$ is given by

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left[\frac{1}{m(x)}\frac{d\Psi(x)}{dx}\right]+\mathcal{V}(x)\Psi(x)=\mathcal{E}\Psi(x). \tag{5}$$

Here the mass function $m(x)=m_0\varrho(x)$. By using the following scaling parameters

$$E=\mathcal{E}/\mathcal{E}_0,\quad V(x)=\mathcal{V}(x)/\mathcal{E}_0,\quad z=\left(\sqrt{2m_0\mathcal{E}_0}/\hbar\right)x. \tag{6}$$

$\mathcal{E}_0$ is a scaling energy, Eq.(5) becomes

$$\left\{\frac{d^2}{dz^2}-2\zeta(z)\frac{d}{dz}+\xi(z)\right\}\Psi(z)=0, \tag{7}$$

where

$$\zeta(z) = \frac{\varrho'(z)}{2\varrho(z)}, \tag{8}$$

$$\xi(z)=\varrho(z)[E-V(z)]. \tag{9}$$

Eq.(7) can be solved by transforming it into a Ricatti-type equation

$$f'^2-2\zeta(z)f(z)+\xi(z)=0, \tag{10}$$

where we have used the formal substitution

$$\Psi(z)=e^{\int f(\tilde{z})d\tilde{z}}. \tag{11}$$

For an adiabatic variation of the potential and the mass we can neglect the contribution of $f'(z)$ in Eq.(10) and obtain

$$f_0(z)=\zeta(z)\pm i\sqrt{\xi(z)-\zeta(z)^2}. \tag{12}$$

The adiabatic solution for the Schrödinger equation with position dependent mass Eq.(7) is then given by

$$\Psi(z)=A_1e^{\varphi(z)+i\theta(z)}+A_2e^{\varphi(z)-i\theta(z)}, \tag{13}$$

where

$$\varphi(z)=\int_{z_0}^{z}\zeta(\tilde{z})d\tilde{z}, \tag{14}$$

$$\theta(z)=\int_{z_0}^{z}\sqrt{\xi(\tilde{z})-\zeta(\tilde{z})^2}d\tilde{z}. \tag{15}$$

To go beyond the adiabatic approximation we assume,

$$f_1(z)=f_0(z)+\epsilon_1(z). \tag{16}$$

We then obtain

$$f_0'(z)+\epsilon_1'(z)+2f_0(z)\epsilon_1(z)-2\zeta(z)\epsilon_1(z)=0, \tag{17}$$

where we have neglected the term $\propto\epsilon^2(z)$. The general solution to Eq(7) is given by

$$\Psi(z)=A_1exp\left[\varphi(z)+i\theta(z)-\phi_+(z)\right] \tag{18}$$

$$+A_2\text{exp}\left[\varphi(z)-i\theta(z)-\phi_-(z)\right], \tag{19}$$

$$\tag{20}$$

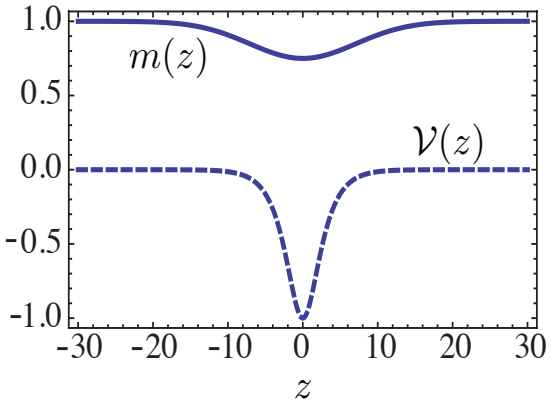

Figure 1 The hyperbolic potential $V(z) = -\text{sech}(\alpha z)$ and the Gaussian-mass variation $m(z) = 1 - 0.25\text{exp}\left(-\beta^2 z^2\right)$. For numerical simulation $\alpha = 1/2, \beta = 0.1$

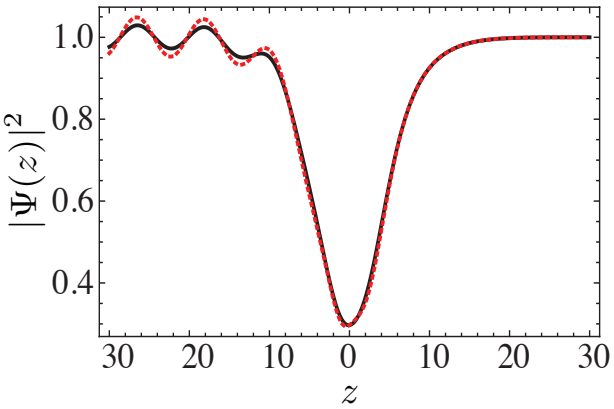

Figure 2 (Color Online) $|\Psi(z)|^2$ versus z for the energy E=0.14, the hyperbolic potential and Gaussian-mass variation. Dashed line represents the exact solution and solid line is the solution from Eq.(18)

where $f_{\pm}(z), \varphi(z), \theta(z)$ is given by Eq.(12), Eq.(14a) and Eq.(14b), respectively, and $\phi_{\pm}(z)$ is defined as

$$\phi_{\pm}(z) = \int_{z_0}^{z} \left\{ \int_{z_0}^{\tilde{z}} \left[f'_{\pm}(\tilde{z}) e^{\pm 2i[\theta(\tilde{z}) - \theta(\tilde{z})]} d\tilde{z} \right] \right\} d\tilde{z}. \tag{21}$$

Here, A_- and A_+ are the complex amplitudes determined from the boundary conditions. Let us now compare our approximate analytical solution with the exact solution for a physical problem. As an example, we study the scattering of a particle by a 1-D hyperbolic potential and a Gaussian mass function (see Fig1):

$$V(z) = -\text{sech}(\alpha z), \tag{22}$$
$$m(z) = 1 - 0.25\text{exp}\left(-\beta^2 z^2\right). \tag{23}$$

Fig. (2) shows the plot of the the probability density $|\Psi(z)|^2$ against z. The dashed line is the numerical solution of the PDMSE Eq.(7), obtained by standard numerical techniques using the commercial software "mathematica", while the solid line is the solution from Eq.(18). Figure 2 shows that the approximate analytical solution is nearly identical to the exact solution. Our analytical solution gives an accurate solution to the Schrödinger equation with position dependent mass $m(x)$ for a particle scattered by a potential $\mathcal{V}(x)$.

3. Analytical solution for 3D-position dependent mass Schrödinger equation

In this section we will extend the approach used earlier to solve the PDMSE problem for the 3D case. The 3D-position dependent mass Schrödinger equation can be written in general as

$$\left[\overrightarrow{\mathbf{p}}\frac{1}{m}\overrightarrow{\mathbf{p}}+V(\overrightarrow{\mathbf{r}})\right]\Psi(\overrightarrow{\mathbf{r}})=E\Psi(\overrightarrow{\mathbf{r}}), \tag{24}$$

where $\overrightarrow{\mathbf{p}}=-i\hbar\overrightarrow{\nabla}$.

Introducing $\overrightarrow{F}=\overrightarrow{\nabla}\phi$, we choose ϕ so that $\overrightarrow{F}//\overrightarrow{\nabla}m$, we can then transform PDMSE to the generalized Ricatti equation:

$$\overrightarrow{\nabla}\cdot\overrightarrow{F}-\frac{\left(\overrightarrow{\nabla}m\right)\cdot\overrightarrow{F}}{m}+\overrightarrow{F}^2+\frac{2m}{\hbar^2}(E-V)=0, \tag{25}$$

where the boundary condition can be given for example far from the potential as the plane wave solution:

$$\Psi(\overrightarrow{r})\overrightarrow{r}\rightarrow-\infty\rightarrow e^{ikx}, \tag{26}$$

where $k=\frac{p}{\hbar}$. Using the technique developed in [24,25,23], we can write

$$\overrightarrow{F}=\overrightarrow{F}_0+\overrightarrow{\eta}, \tag{27}$$

where $\overrightarrow{F_0}$ satisfies the following equation:

$$-\frac{\left(\overrightarrow{\nabla}m\right)\cdot\overrightarrow{F_0}}{m}+\overrightarrow{F_0}^2+\frac{2m}{\hbar^2}(E-V)=0, \tag{28}$$

with the solution

$$\overrightarrow{F_0}=\left[\frac{1\pm\frac{1}{\left|\overrightarrow{\nabla}m\right|}\sqrt{\left(\frac{\overrightarrow{\nabla}m}{m}\right)^2-\frac{8m}{\hbar^2}(E-V)}}{m}\right]\overrightarrow{\nabla}m. \tag{29}$$

Using the transformation:

$$\overrightarrow{\chi}(\overrightarrow{r})=\exp\left[\int\left(2\overrightarrow{F_0}-\frac{\left(\overrightarrow{\nabla}m\right)}{m}\right)\cdot d\overrightarrow{r}\right]\overrightarrow{\eta}\left(\overrightarrow{r}\right), \tag{30}$$

and following the same calculation procedure as in [24,25,23] we obtain

$$\overrightarrow{\eta}\left(\overrightarrow{r}\right)= \tag{31}$$

$$\frac{-\exp\left[-\int\left(2\overrightarrow{F_0}(\overrightarrow{r}')-\frac{\overrightarrow{\nabla}m(\overrightarrow{r}')}{m(\overrightarrow{r}')}\right)\cdot d\overrightarrow{r}'\right]}{4\pi}\times$$

$$\int\{\exp[-\int\left(2\overrightarrow{F_0}(\overrightarrow{r}")-\frac{\overrightarrow{\nabla}m(\overrightarrow{r}")}{m(\overrightarrow{r}")}\right)\cdot d\overrightarrow{r}"]$$

$$\overrightarrow{\nabla}.\overrightarrow{F_0}(\overrightarrow{r}')\}\frac{\overrightarrow{r}-\overrightarrow{r}'}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}d^3\overrightarrow{r}'. \tag{32}$$

The expression of the wave function solution to 3D PDMSE is then

$$\psi(\overrightarrow{r})=A_+\exp\left[\int\left(\overrightarrow{F_{0+}}+\overrightarrow{\eta_+}\right)\right]$$

$$+A_-\exp\left[\int\left(\overrightarrow{F_{0-}}+\overrightarrow{\eta_-}\right)d\overrightarrow{r}\right], \tag{33}$$

where $A_{\pm}$ are the complex amplitudes that can be determined from the boundary conditions

$$\overrightarrow{F_{0\pm}} = \left[\frac{1 \pm \frac{1}{\left|\frac{\overrightarrow{\nabla} m}{m}\right|} \sqrt{\left(\frac{\overrightarrow{\nabla} m}{m}\right)^2 - \frac{8m}{\hbar^2}(E-V)}}{m} \right] \overrightarrow{\nabla} m, \tag{34}$$

and

$$\begin{aligned} \overrightarrow{\eta_{\pm}}(\overrightarrow{r}) \; = \; & \left[\frac{-\exp\left[-\int \left(2\overrightarrow{F_{0\pm}}(\overrightarrow{r}') - \frac{\overrightarrow{\nabla} m(\overrightarrow{r}')}{m(\overrightarrow{r}')} \right) \cdot d\overrightarrow{r}' \right]}{4\pi} \right] \times \\ & \int \{ \exp[-\int \left(2\overrightarrow{F_{0\pm}}(\overrightarrow{r}") - \frac{\overrightarrow{\nabla} m(\overrightarrow{r}")}{m(\overrightarrow{r}")} \right) \cdot \\ & d\overrightarrow{r}"] \overrightarrow{\nabla} . \overrightarrow{F_{0\pm}}(\overrightarrow{r}') \} \frac{\overrightarrow{r} - \overrightarrow{r}'}{\left|\overrightarrow{r} - \overrightarrow{r}'\right|} d^3\overrightarrow{r}'. \end{aligned} \tag{35, 36}$$

4. conclusion

To conclude, in this paper we have derived an analytical solution for the position-dependent mass Schrödinger equation in 3D. Our approach can be easily extended to find bound states.The developed approach can be applied to study several effects in nano-systems such as scattering of electrons and holes, carbon nano-tubes and quantum dots.

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