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Fisher information for the position-dependent mass Schrödinger system

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ABSTRACT

This study presents the Fisher information for the position-dependent mass Schrödinger equation with hyperbolic potential $V(x) = -V_0\text{csch}^2(ax)$. The analysis of the quantum-mechanical probability for the ground and exited states $(n = 0, 1, 2)$ has been obtained via the Fisher information. This controls both chemical and physical properties of some molecular systems. The Fisher information is considered only for $x > 0$ due to the singular point at $x = 0$. We found that Fisher-information-based uncertainty relation and the Cramer–Rao inequality holds. Some relevant numerical results are presented. The results presented show that the Cramer–Rao and the Heisenberg products in both spaces provide a natural measure for anharmonicity of $-V_0\text{csch}^2(ax)$.

1. Introduction

In recent years, there has been a great interest in studying information theoretic measures for different quantum systems. This is due to the fact that information theory of quantum-mechanical systems is related to the modern quantum communications, computation and the density functional methods [1]. According to the density functional theory (DFT) initiated by Hohenberg and Kohn [2], the one-particle position and momentum probability densities are the basic elements for describing the physical and chemical properties of some molecular systems. The quantum information theory plays an important role in the measure of uncertainty and other quantum parameters of the system. The main measures of quantum information are the Shannon entropy [3] and Fisher information [4]. They are functions of a characteristic probability density. They are traditionally used in engineering, physics, applied mathematics, condensed physics, chemical and other related areas.

The Fisher information was introduced by Fisher as a measure of intrinsic accuracy in statistical estimation theory but its basic properties are not completely well known yet, despite its early origin in 1925 [5]. The importance of this was noticed by Sears et al. [6]. The authors found that the quantum mechanical kinetic energy can be considered as a measure of the information distribution. Fisher information has been very useful and has been applied in different areas. For example using the principle of minimum Fisher information [7], one can obtain the equations of non-relativistic quantum mechanics [8], the time-independent Kohn–Sham equations and the time-dependent Euler equation of DFT [9]. Its local character is the main difference with respect to Shannon information which is global information measure. It is defined as the expectation value of the logarithmic gradient of density or as the gradient functional of density. So the Fisher information is given by [5]

$$I_F = \int_{-\infty}^{\infty} \rho(x) \left[\frac{d}{dx} \ln \rho(x)\right]^2 dx = \int_a^b \frac{\left[\rho'(x)\right]^2}{\rho(x)} dx. \quad (1)$$

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If the probability density is defined as $\rho_n(x) = |\psi_n(x)|^2$, then

$$I_F = \int_a^b |\psi(x)|^2 \left[\frac{d}{dx}\ln|\psi(x)|^2\right]^2 dx = 4\int_a^b \left[\psi'(x)\right]^2 dx, \tag{2}$$

which is not totally independent. There is an inequality which involves Fisher information and variance $V = \langle x^2\rangle - \langle x\rangle^2$. It is called the Cramer–Rao uncertainty relation:

$$I_F \cdot V \geq 1. \tag{3}$$

The Fisher information is a derivative functional of the density, so that it is very sensitive to local rearrangements of $\rho_n(x)$. In this paper we present the Fisher information of the position-dependent mass Schrödinger equation with hyperbolic potential.

The study of the Schrödinger equations with a position-dependent mass (PDM) is a very useful model of interest since the early days of solid state physics and in many applied branches of quantum physics such as condensed matter physics, material science, nuclear physics, etc. Special application of principal concept of PDM is found in the investigation of electronic properties of semiconductors, quantum dots and wells, etc. [10].

The rest part of this work is organized as follows: In Section 2, we give a brief review of the position-dependent mass Schrödinger equation. A particular case of the hyperbolic potential is presented. In Section 3, we first present the normalized wave function in position space and then calculate the Fisher Information I_F, the Heisenberg uncertainty product and Cramer–Rao product of hyperbolic cosecant potential for various values of potential parameter a and for few states $n = 0, 1, 2$. Finally, we give some concluding remarks in Section 4.

2. Calculation of the wave functions

The Schrödinger equation with the position-dependent mass for an arbitrary potential $V(x)$ can be expressed as [10–13]

$$\nabla_x\left(\frac{1}{m(x)}\nabla_x\psi(x)\right) + 2m_0\left[E - V(x)\right]\psi(x) = 0, \tag{4}$$

where E is the energy spectrum and solitonic smooth effective mass distribution $(m(x))$ is taken as $m(x) = m_0(x)\mathrm{sech}^2(ax)$, which has been used widely in condensed matter and low-energy nuclear physics. Taking $\psi(x) = \cosh^\tau(ax)\mathcal{F}(ax)$ and then substitute it into equation (4), we have

$$\mathcal{F}''(ax) + 2a(1+\tau)\tanh(ax)\mathcal{F}'(x) + \frac{\mathrm{sech}^2(ax)}{2}\left\{a^2\tau(\tau+2)\cosh(2ax) + \left[4m_0\left(E - V(x)\right) - a^2\tau^2\right]\right\}\mathcal{F}(ax) = 0. \tag{5}$$

Further substitution of $\delta = 2m_0/a^2$ and $\gamma = ax$ into equation (5) gives

$$\mathcal{F}''(\gamma) + 2(1+\tau)\tanh(\gamma)\mathcal{F}'(\gamma) + \left\{\tau(\tau+2)\tanh^2(\gamma) + \left[\tau + \sigma\left(E - V(y)\right)\right]\mathrm{sech}^2(\gamma)\right\}\mathcal{F}(\gamma) = 0. \tag{6}$$

Considering a new relation of the form $\mathrm{sech}(\gamma) = \cos(z)$ and $\tanh(\gamma) = \sin(z)$, which transform the boundary condition of the wave function from $(-\infty, \infty)$ to $(-\pi/2, \pi/2)$ and taking $\tau = -1/2$, then the above equation (6) can be simplified further as

$$-\mathcal{F}''(z) + \mathcal{V}(z)\mathcal{F}(z) = \varepsilon\mathcal{F}(z) \ \text{ with } \ \mathcal{V}(z) = \frac{3}{4}\tan^2(z) + \sigma V(z) + \frac{1}{2}, \quad \varepsilon = \delta E. \tag{7}$$

In recent study [14], the Shannon entropy for the position-dependent Schrödinger equation for a particle with a nonuniform solitonic mass density is evaluated in the case of a trivial null potential. It was found that the negative Shannon entropy exists for the probability densities that are highly localized. In this work, we consider a special squared hyperbolic cosecant potential $V(ax) = -V_0\mathrm{csch}^2(ax)$ and then analyze its quantum-mechanical probability cloud for the ground and excited states by means of local (Fisher information) information-theoretic measure. Now, substituting this potential into equation (7) and recalling the relation $\mathrm{sech}(\gamma) = \cos(z)$, one has $\mathcal{V}(z) = 3\tan^2(z)/4 - \delta V_0\cot^2(z) + 1/2$. It is interesting to note that this family of potentials represents different potentials in z space. For example, for $\mathcal{V}_0 = \delta V_0 > 0$, they look like infinitely deep funnels and behave like the potential $1/x$, while for $\mathcal{V}_0 < 0$ they become infinite double-wells and if $\mathcal{V}_0 = 0$ they become the infinite single-well.

In order to obtain exact solution to this system, we take the following wave function ansatz:

$$\mathcal{F}(z) = \sin^\mu(z)\cos^\nu(z)\mathcal{G}(z), \tag{8}$$

where the parameters μ and ν are calculated by considering the behaviors of the wave functions at $z \sim 0$ and $z \sim \pi/2$ as $\mu = 1/2 + \sqrt{1 - 4\mathcal{V}_0}/2$ and $\nu = 3/2$ respectively. The function $\mathcal{G}(z)$ satisfies the following differential equation

$$\mathcal{G}''(z) + 2\left[\mu\cot(z) - \nu\cot(z)\right]\mathcal{G}'(z) + (\varepsilon - \mu - \nu - 2\mu\nu)\mathcal{G}(z) = 0. \tag{9}$$

Using a change of variable $\xi = \sin^2(z)$, the equation is transformed to

$$\xi(1-\xi)\mathcal{G}''(\xi) + \left[\mu + \frac{1}{2} - (1+\mu+\nu)\xi\right]\mathcal{G}'(\xi) + \frac{1}{4}\left(\varepsilon - \frac{1}{2} - \mu - \nu - 2\mu\nu\right)\mathcal{G}(\xi) = 0, \tag{10}$$

whose solution is given by hypergeometric function ${}_2F_1(a, b; c; \xi)$ with the parameters

$$a = \frac{\mu}{2} + \frac{\nu}{2} - \frac{1}{2}\sqrt{\varepsilon + \frac{1}{4} - \mathcal{V}_0}, \quad b = \frac{\mu}{2} + \frac{\nu}{2} + \frac{1}{2}\sqrt{\varepsilon + \frac{1}{4} - \mathcal{V}_0}, \quad c = \mu + \frac{1}{2}. \tag{11}$$