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Rigorous Solutions for the One-Dimensional Hartmann Potential in the Quantum Phase-Space Representation

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The rigorous solutions of the Schrödinger equation with the one-dimensional Hartmann potential for a particle are solved and discussed within the framework of the quantum phase space representation established by Torres-Vega and Frederick. For a simple example, the uncertainty principle for the quantum probability density functions is revealed in phase space representation.

KEY WORDS: rigorous solutions; Schrödinger equation; quantum phase space representation.

1. INTRODUCTION

The relationship between classical mechanics and quantum mechanics is always a very interesting subject. In 1932, for quantum corrections to classical statistical mechanics, the first quasi-probability distribution function was introduced by Wigner (1932), then, a variety of quantum phase-space distribution functions have been proposed (Kirkwood, 1933; Husimi, 1940; Glauber, 1963a,b; Sudarshan, 1963) and extensive uses in many areas of physics and chemistry have also been found (Moyal, 1949; Glauber, 1965; Berry, 1977; Carruthers and Zachariasen, 1983; Lee, 1983; Takahashi, 1989; Schroeck, 1996). The other way to establish quantum phase space representation is to define quantum state functions directly in phase space, and to determine corresponding Schrödinger equations. In 1990s, a new scheme of quantum mechanics of phase space representation was established by Torres-Vega and Frederick (1990, 1993), and was just based on the following assumption: (a) There exists a set of complete basic functions $\Gamma(q, p)$,

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the quantum state $|\Psi\rangle$ can be represented in the phase space as

$$\langle \Gamma(q, p) \mid \Psi \rangle = \Psi(q, p), \tag{1}$$

(b) the dynamic variable operators $\hat{Q}$ and $\hat{P}$ in the quantum phase space representation may be directly represented as

$$\hat{Q} = \frac{q}{2} + i\hbar\frac{\partial}{\partial p}, \tag{2}$$

$$\hat{P} = \frac{p}{2} - i\hbar\frac{\partial}{\partial q}. \tag{3}$$

(c) the time-evolution equation of the wavefunction $\Psi(q, p)$ in the phase space representation has the similar form to the Schrödinger equation, i.e.,

$$i\hbar\frac{\partial}{\partial t}\Psi(q, p, t) = \left[\frac{1}{2\mu}\left(\frac{p}{2} - i\hbar\frac{\partial}{\partial q}\right)^2 + \hat{V}\left(\frac{q}{2} + i\hbar\frac{\partial}{\partial p}\right)\right]\Psi(q, p, t). \tag{4}$$

The energy eigenvalues and eigenfunctions in the phase space representation might be solved directly. And (d) the mean values of dynamic variables in the phase space representation might be computed just as those in general position or momentum representation (Li and Hu, 1995). However, the number of dimensions for a physical system in the phase space representation is double of that in general position space or momentum space of quantum mechanics, which makes the mathematical treatment for physical problems much more complicated than that in general position space or momentum space representation. Therefore, the wavefunctions in the quantum phase space representation are also more complicated in form than those in general position or momentum space representation of quantum mechanics.

As well known that the Hartmann potential function, as a special case to be the hydrogen atom potential, is first introduced by Hartmann for molecular interaction (Hartmann, 1972; Hartmann and Schuch, 1980; Kibler and Negadi, 1984) and the corresponding Schrödinger equation could be exactly soluble in general coordinate or momentum space of quantum mechanics. In this paper, the Schrödinger equation with one-dimensional Hartmann potential function will be strictly solved in the quantum phase space representation. The energy eigenvalues and eigenfunctions of this system in the phase space representation will be given in Section 2. In Section 3, the properties of the eigenfunctions are discussed and the Heisenberg uncertainty principle in the physical system is tried to interpret in the quantum phase space representation.

2. RIGOROUS SOLUTIONS IN PHASE SPACE

For any potential $V(q)$, the stationary-state Schrödinger equation in the quantum phase space can be written as follows,

$$\left[\frac{1}{2\mu}\left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)^2+\hat{V}\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)\right]\Psi\left(q,p\right)=E\Psi\left(q,p\right), \qquad (5)$$

where p and q are the classical momentum and coordinate variables, $E(<0)$ is an eigenenergy and $\Psi\left(q,p\right)$ is the eigenfunction corresponding to the eigenenergy E. By means of the following relations

$$\left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)^n=\exp\left(-ipq/2\hbar\right)\left(-i\hbar\frac{\partial}{\partial q}\right)^n\exp\left(ipq/2\hbar\right), \qquad (6)$$

$$\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)^n=\exp\left(ipq/2\hbar\right)\left(i\hbar\frac{\partial}{\partial p}\right)^n\exp\left(-ipq/2\hbar\right), \qquad (7)$$

$$\hat{V}\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)=\exp\left(-ipq/2\hbar\right)\hat{V}\left(q+i\hbar\frac{\partial}{\partial p}\right)\exp\left(ipq/2\hbar\right), \qquad (8)$$

and by putting

$$\Psi(p,q)=\exp\left(-ipq/2\hbar\right)\Phi(p,q), \qquad (9)$$

Equation (5) can be transform as

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2}+\hat{V}\left(q+i\hbar\frac{\partial}{\partial p}\right)\right]\Phi\left(q,p\right)=E\Phi\left(q,p\right). \qquad (10)$$

For the one-dimensional Hartmann potential

$$V\left(q\right)=-\frac{a}{|q|}+\frac{b}{q^2} \qquad (11)$$

where a and b are positive constants, for $q>0$, Equation (10) becomes

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2}-\frac{a}{q+i\hbar(\partial/\partial p)}+\frac{b}{\left(q+i\hbar(\partial/\partial p)\right)^2}\right]\Phi\left(q,p\right)=E\Phi\left(q,p\right) \qquad (12)$$

An attempted solution could be selected as

$$\Phi\left(q,p\right)=W\left(q\right)\left(q+i\hbar(\partial/\partial p)\right)^s e^{-\frac{1}{2}\left(q+i\hbar(\partial/\partial p)\right)}C\left(p\right) \qquad (13)$$

Here, making variable replacement

$$\xi=2\sqrt{-2\mu E}\left(q+i\hbar(\partial/\partial p)\right)/\hbar \qquad (14)$$

and putting

$$s\left(s-1\right)=\frac{2\mu b}{\hbar^2}, \qquad (15)$$

the Equation (12) can be transformed as

$$\xi \frac{d^2}{d\xi^2} W(\xi) + (2s - \xi) \frac{d}{d\xi} W(\xi) - \left(s - \frac{\mu a}{\sqrt{-2\mu E \hbar}} \right) W(\xi) = 0 \tag{16}$$

This is a confluent hypergeometric equation for variable ξ. Therefore, the solutions of Equation (16), satisfying the boundary conditions that the wave functions should be finite at the boundary of the phase space, can be obtained, i.e.,

$$W(\xi) = F\left(\left(s - \frac{\mu a}{\sqrt{-2\mu E \hbar}} \right), 2s, \xi \right) \tag{17}$$

and

$$s - \frac{\mu a}{\sqrt{-2\mu E \hbar}} = -n \quad n = 0, 1, 2, \ldots \tag{18}$$

Here n is a quantum number and determines an eigenenergy of this system in quantum phase space representation. It is clear that the eigenenergies are

$$E_n = -\frac{\mu a^2}{2\hbar^2 (n+s)^2} \tag{19}$$

and the corresponding eigenfunctions are

$$\begin{aligned} \Psi_n(p,q) = {} & N_n \exp(-ipq/2\hbar)\, F\left(-n, 2s, \frac{2\mu a}{\hbar^2 (n+s)} (q + i\hbar(\partial/\partial p)) \right) \\ & \times (q + i\hbar(\partial/\partial p))^s \exp\left(-\frac{(q + i\hbar(\partial/\partial p))}{2} \right) C(p) \end{aligned} \tag{20}$$

For $q < 0$, in a similar way, we can obtain the corresponding eigenfunctions. For the whole space, the corresponding eigenfunctions can be written as

$$\begin{aligned} \Psi_n(p,q) = {} & N_n \exp(-ipq/2\hbar)\, F\left(-n, 2s, \frac{2\mu a}{\hbar^2 (n+s)} |q + i\hbar(\partial/\partial p)| \right) \\ & \times (q + i\hbar(\partial/\partial p))^s \exp\left(-\frac{|q + i\hbar(\partial/\partial p)|}{2} \right) C(p) \end{aligned} \tag{21}$$

where N_n is the normalized constant for a given quantum number n. Actually,this set of complete solutions is not yet determined thoroughly due to the existence of arbitrary function $C(p)$. Considering the boundary conditions for p-coordinate, the $C(p)$ must be

$$\int_{-\infty}^{\infty} dp \left| \frac{d^k}{dp^k} C(p) \right| < \infty, \quad k = 0, 1, 2, \ldots \tag{22}$$

If letting constant $b = 0$, corresponding to $s = 0$, the eigenenergy and the corresponding eigenfunctions of one-dimensional hydrogen atom can be obtained.

3. DISCUSSION

In eigenfunction Equation (21), there is an arbitrary function, $C\,(p)$ of the momentum variable. It is not surprising that the solutions to the Schrödinger equation in quantum phase space are not unique, because the position and momentum variables are now used simultaneously in quantum phase space representation, the forms of solutions must be uncertain in order to satisfy the Heisenberg uncertainty principle. Certainly, the unique eigenfunctions in position or momentum space representation must still be obtained if the phase space eigenfunctions is projected into position or momentum space representation through the 'Fourier-like' projection transformation (Torres-Vega and Frederick, 1990, 1993).

The eigenfunctions Equation (21) are usually the complicated functions about variables q and p, but one simple case of $C\,(p)$ may be selected so as to discuss the physical meaning of the eigenfunctions. By putting

$$C\,(p) = \left(\frac{1}{\sigma}\right)^{\frac{1}{2}} \exp\left(-\frac{i2\pi kp}{\sigma}\right), \quad k = 0, \pm 1, \pm 2, \ldots \tag{23}$$

where $C\,(p)$ is the eigenfunctions about the operator $i\hbar\frac{\partial}{\partial p}$ that is restricted in the range of $\left(-\frac{\sigma}{2} \leq p \leq \frac{\sigma}{2}\right)$. Thus eigenfunction Equation (21) corresponding to Equation (23) in the phase space representation become

$$\Psi_n(p, q) = N_n \exp\left(-ipq/2\hbar\right) C\,(p) \left|\left(q + \frac{2\pi\hbar k}{\sigma}\right)\right|^s \exp\left(-\frac{\left|\left(q + \frac{2\pi\hbar k}{\sigma}\right)\right|}{2}\right)$$

$$\times F\left(-n, 2s, \left(\frac{2\mu a}{\hbar^2\,(n+s)}\right)\left|q + \frac{2\pi\hbar k}{\sigma}\right|\right) \tag{24}$$

Obviously, the variables q and p in the eigenfunctions Equation (24) can be separated from each other expect the phase factor.

As well known, the transform of wave functions from phase space representation to coordinate or momentum space representation is a simple Fourier project transform (Torres-Vega and Frederick, 1990, 1993). The solution Equation (24) is substituted into Fourier project transform formula and following equations is given:

$$\psi_n\,(q) = A \int_{-\frac{\sigma}{2}}^{\frac{\sigma}{2}} dp \Psi_n\,(q, p) \exp\left(\frac{ipq}{2\hbar}\right)$$

$$= N_n F\left(-n, 2s, \frac{2\mu a}{\hbar^2\,(n+s)}|q|\right) |q|^s \exp\left(-\frac{|q|}{2}\right) \tag{25}$$

and

$$\phi_n(p) = A' \int_{-\infty}^{\infty} dq \Psi_n(q, p) \exp\left(-\frac{ipq}{2\hbar}\right) \tag{26}$$

where we make use of following relation

$$\int_{-\frac{\sigma}{2}}^{\frac{\sigma}{2}} C_k(p) C_{k'}^*(p) dp = \delta_{k,k'} \tag{27}$$

Similar to coordinate or momentum space representation, the quantum probability density functions $\rho_n(q, p)$ can be defined in phase space representation

$$\begin{aligned}\rho_n(q, p) = |\Psi_n(q, p)|^2 = N_n \frac{1}{\sigma} \left(q + \frac{2\pi\hbar k}{\sigma}\right)^{2s} \exp\left|\left(q + \frac{2\pi\hbar k}{\sigma}\right)\right| \\ \times \left|F\left(-n, 2s, \left(\frac{2\mu a}{\hbar^2(n+s)}\right)\left|q + \frac{2\pi\hbar k}{\sigma}\right|\right)\right|^2\end{aligned} \tag{28}$$

If integrating $\rho_n(q, p)$ over the whole space of position q or over the whole space of momentum p, we obtain

$$\rho_n(p) = \frac{1}{\sigma} \tag{29}$$

or

$$\begin{aligned}\rho_n(q) = N_n \left|\left(q + \frac{2\pi\hbar k}{\sigma}\right)^2\right|^s \exp\left(q + \frac{2\pi\hbar k}{\sigma}\right) \\ \times \left|F\left(-n, 2s, \left(\frac{2\mu a}{\hbar^2(n+s)}\right)\left|q + \frac{2\pi\hbar k}{\sigma}\right|\right)\right|^2\end{aligned} \tag{30}$$

Obviously, Equations (29) and (30) are not the probability density functions in momentum or position space. So, the quantum probability density function $\rho_n(q, p)$ defined by Equation (28) do not satisfy the marginal conditions. It is coincident with the previous conclusion that the positive and the marginal conditions can not be satisfied simultaneously for any quantum phase space distribution functions (Wigner, 1971; O'Connel and Wigner, 1981).

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