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1999 J. Phys. A: Math. Gen. 32 139

(http://iopscience.iop.org/0305-4470/32/1/015)

J. Phys. A: Math. Gen. **32** (1999) 139–146. Printed in the UK PII: S0305-4470(99)94828-X

Morse oscillator in a quantum phase-space representation: rigorous solutions

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Received 2 June 1998, in final form 21 September 1998

Abstract. Within the framework of the phase-space representation of quantum mechanics recently developed by Torres-Vega and Frederick we have solved for the exact solutions of the Schrödinger equation of a Morse oscillator whose structures reveal the special complexity.

Since the first quantum distribution function in phase-space was introduced by Wigner [1] for quantum correction to classical statistical mechanics, a variety of phase-space representations of quantum mechanics have been proposed and found extensive uses in many areas of physics and chemistry [2]. Development along this line has provided not only phase-space frameworks to perform quantum mechanics but also profound insight into the relationship between quantum and classical mechanics. Recently, a new scheme of quantum mechanical representation in phase-space has been developed [3]. This formulation was based on the fundamental operator mapping for Q and P : $\hat{Q} \to \frac{q}{2} + \mathrm{i}\hbar\frac{\partial}{\partial p}$, $\hat{P} \to \frac{p}{2} - \mathrm{i}\hbar\frac{\partial}{\partial q}$. This representation in phase-space presents a remarkably similar formulation of quantum mechanics to the usual one in position or momentum space, for the evolution equation of the phase-space quantum wavefunction $\Phi(q, p)$ is of the Schrödinger type. Although there are still issues to be clarified concerning this formulation, it provides a useful and interesting framework for constructing the Schrödinger evolution equation, eigenfunction equations, probability conservation equations and wavepacket dynamics directly in phase-space. In this paper we attempt to solve strictly for the Schrödinger equation of a Morse oscillator in the phase-space representation of quantum mechanics developed by Torres-Vega and Frederick [3] so as to contribute an exactly solvable model. It might seem that the process of solving it would be trivial, but the structure of solutions of the Morse oscillator displayed in quantum phase-space are worthy of further investigation. Here, we only consider the case of one degree of freedom.

For any potential $V(x)$ which may be expanded in a series with a finite number of negative powers and an infinite number of positive powers, the stationary-state Schrödinger equation in the phase-space representation reads [3]

$$\left\{\frac{1}{2\mu}\left(\frac{p}{2} - \mathrm{i}\hbar\frac{\partial}{\partial x}\right)^2 + V\left(\frac{x}{2} + \mathrm{i}\hbar\frac{\partial}{\partial p}\right)\right\}\psi(p, x) = E\psi(p, x) \tag{1}$$

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where p and x are the classical momentum and coordinate (real numbers); $E(<0)$ is an eigenenergy and $\psi(p,x)$, which belongs to $L^2(2)$ with number 2 denoting two independent variables, is the eigenfunction corresponding to the eigenenergy E. Using the relations

$$\begin{aligned} \mathrm{e}^{\mathrm{i}px/2\hbar}\left(\mathrm{i}\hbar\frac{\partial}{\partial p}\right)^n \mathrm{e}^{-\mathrm{i}px/2\hbar} &= \left(\frac{x}{2}+\mathrm{i}\hbar\frac{\partial}{\partial p}\right)^n \\ \mathrm{e}^{-\mathrm{i}px/2\hbar}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x}\right)^n \mathrm{e}^{\mathrm{i}px/2\hbar} &= \left(\frac{p}{2}-\mathrm{i}\hbar\frac{\partial}{\partial x}\right)^n \end{aligned} \tag{2}$$

and letting $\psi(p,x)=\mathrm{e}^{-\mathrm{i}px/2\hbar}\phi(p,x)$, we can change equation (1) into another useful form

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}+V\left(x+\mathrm{i}\hbar\frac{\partial}{\partial p}\right)\right\}\phi(p,x)=E\phi(p,x). \tag{3}$$

For the potential of a Morse oscillator, $V(x)=D(\mathrm{e}^{-2\beta x}-2\mathrm{e}^{-\beta x})$ in position representation with D and β being parameters, equation (3) gives

$$\left\{-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}+D(\mathrm{e}^{-2\beta x}\hat{T}^2-2\mathrm{e}^{-\beta x}\hat{T})\right\}\phi(p,x)=E\phi(p,x). \tag{4}$$

Here, we regard $\hat{T}=\mathrm{e}^{-\mathrm{i}\hbar\beta\frac{\partial}{\partial p}}$ as the momentum displacement operator. This equation can be solved analytically by means of the conventional procedures [4].

Making variable replacement $\xi=2\sqrt{2\mu D}/\hbar\beta\mathrm{e}^{-\beta x}$, and placing $s_n=\sqrt{-2\mu E}/\hbar\beta$, $n=\sqrt{2\mu D}/\hbar\beta-(s_n+\frac{1}{2})$ and $\phi(p,x)=\phi(p,\xi)$, in equation (4), we obtain

$$\left\{\xi^2\frac{\partial^2}{\partial\xi^2}+\xi\frac{\partial}{\partial\xi}+\left[\left(n+s_n+\frac{1}{2}\right)\xi\hat{T}-\left(\frac{\xi\hat{T}}{2}\right)^2-s_n^2\right]\right\}\phi(p,\xi)=0 \tag{5}$$

which is analogous in form to that in position representation but the operator $\hat{T}$ is involved. In view of the boundary conditions met by $\phi(p,x)$ for x-coordinate, choosing a trial solution

$$\phi(p,x)=\phi(p,\xi)=\xi^{s_n}\mathrm{e}^{-\xi\hat{T}/2}u(p,\xi) \tag{6}$$

and noting that $[\xi,\hat{T}]=0$ because $[x,\mathrm{i}\hbar\partial/\partial p]=0$, then equation (5) can be converted to

$$\left\{\xi\frac{\partial^2}{\partial\xi^2}+(2s_n+1-\xi\hat{T})\frac{\partial}{\partial\xi}+n\hat{T}\right\}u(p,\xi)=0. \tag{7}$$

This is a confluent hypergeometric equation for variable ξ. If we expand $u(p,\xi)$ in a series about ξ,

$$u(p,\xi)=\sum_{k=0}^{\infty}C_k(p)\xi^k \tag{8}$$

then the solution to equation (7) satisfying the boundary condition for x-coordinate are such generalized Laguerre (or Sonine) polynomials

$$u_n(p,\xi)=L_n^{2s_n}(\xi\hat{T})C_0(p) \qquad (n=0,1,2,\ldots) \tag{9}$$

with n being a quantum number and determining an eigenenergy of the Morse oscillator in quantum phase-space. $C_0(p)$ may be an arbitrarily reasonable function of p-variable on which we discuss some restrictions in the following. It is clear that the formula of the energy levels is still [4]

$$E_n=-D\left[1-\frac{\hbar\beta}{\sqrt{2\mu D}}\left(n+\frac{1}{2}\right)\right]^2 \tag{10}$$

in which the quantum number n only takes on positive integers satisfying the inequality $n < \sqrt{2\mu D}/\hbar\beta - \frac{1}{2}$.

Up to now we have gained formally the complete solutions to the Schrödinger equation of a Morse oscillator in the phase-space representation,

$$\begin{aligned}
\psi_n(p,x) &= N_n \mathrm{e}^{-\mathrm{i}px/2\hbar} \xi^{s_n} \mathrm{e}^{-\xi\hat{T}/2} L_n^{2s_n}(\xi\hat{T}) C_0(p) \\
\xi &= 2\sqrt{2\mu D}/\hbar\beta \mathrm{e}^{-\beta x} \\
E_n &= -D\left[1 - \frac{\hbar\beta}{\sqrt{2\mu D}}\left(n + \frac{1}{2}\right)\right]^2
\end{aligned} \tag{11}$$

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 an arbitrary function $C_0(p)$. Considering the boundary conditions for p-coordinate, the $C_0(p)$ must be required to fulfil

$$\int_{-\infty}^{+\infty} \mathrm{d}p \left| \frac{d^k}{dp^k} C_0(p) \right| < \infty \qquad (k = 0, 1, 2, \ldots). \tag{12}$$

It is not surprising that the solutions to the Schrödinger equation are not unique in quantum phase-space, just as there are no unique distribution functions in the formulation of quantum mechanics in phase-space [2]. All these arise from the restriction of the uncertainty principle. Consequently, we cannot expect that one of the solutions is physically more meaningful than the others. As an illustration, we consider the following two simple classes of $C_0(p)$

$$\begin{aligned}
&(1) \qquad \hat{T}^m C_0^{(1)}(p) = C_0^{(1)}(p), \\
&(2) \qquad \hat{T}^m C_0^{(2)}(p) = C_0^{(2)}(p) B(p)^m \qquad B(p) > 0, \quad m = 0, 1, 2, \ldots \\
&C_0^{(2)}(p) = A(p) B(p)^{\mathrm{i}p/\hbar\beta} \qquad \hat{T}^m A(p) = A(p), \quad \hat{T}^m B(p) = B(p)
\end{aligned} \tag{13}$$

and thus the phase-space eigenfunctions $\psi_n(p,x)$ corresponding to them become

$$\begin{aligned}
\Psi_n^{(1)}(p,x) &= N_n^{(1)} \mathrm{e}^{-\mathrm{i}px/2\hbar} C_0^{(1)}(p) \xi^{s_n} \mathrm{e}^{-\xi/2} L_n^{2s_n}(\xi) \\
\Psi_n^{(2)}(p,x) &= N_n^{(2)} \mathrm{e}^{-\mathrm{i}px/2\hbar} C_0^{(2)}(p) \xi^{s_n} \mathrm{e}^{-\xi B(p)/2} L_n^{2s_n}(\xi B(p))
\end{aligned} \tag{14}$$

where indices (1) and (2) indicate the first and second class of $C_0(p)$, respectively.

The eigenfunctions in position and momentum space can be easily obtained through the Fourier projection transformation [3, 5]

$$\begin{aligned}
\psi_n(x) &= \int_{-\infty}^{+\infty} \mathrm{d}p\, \mathrm{e}^{\mathrm{i}px/2\hbar} \psi_n(p,x) \\
\phi_n(p) &= \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/2\hbar} \psi_n(p,x)
\end{aligned} \tag{15}$$

which do not change the eigenvalues of the $\psi_n(p,x)$. The results for the first class of $C_0(p)$ are

$$\Psi_n^{(1)}(x) = \left\{ N_n^{(1)} \int_{-\infty}^{+\infty} \mathrm{d}p\, C_0^{(1)}(p) \right\} \xi^{s_n} \mathrm{e}^{-\xi/2} L_n^{2s_n}(\xi) \tag{16a}$$

$$\phi_n^{(1)}(p) = N_n^{(1)} C_0^{(1)}(p) \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}px/\hbar} \xi^{s_n} \mathrm{e}^{-\xi/2} L_n^{2s_n}(\xi) \tag{16b}$$

and for the second

$$\begin{aligned}
\Psi_n^{(2)}(x) &= N_n^{(2)} \int_{-\infty}^{+\infty} \mathrm{d}p\, \xi^{s_n} \mathrm{e}^{-\xi\hat{T}/2} L_n^{2s_n}(\xi\hat{T}) C_0^{(2)}(p) \\
&= N_n^{(2)} \xi^{s_n} L_n^{2s_n}\left(-2\xi\frac{\partial}{\partial\xi}\right) \int_{-\infty}^{+\infty} \mathrm{d}p\, \mathrm{e}^{-\xi\hat{T}/2} C_0^{(2)}(p)
\end{aligned}$$

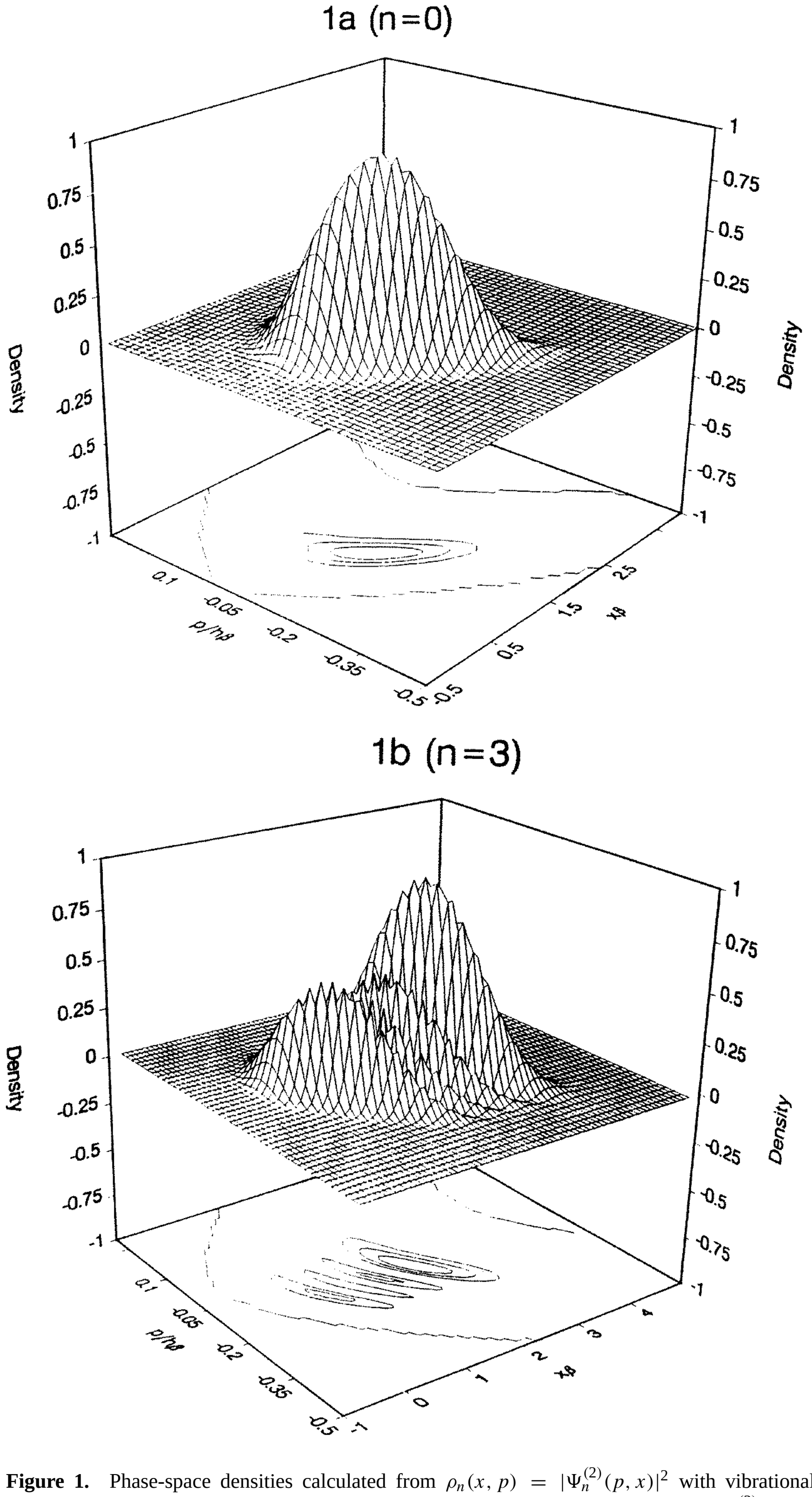
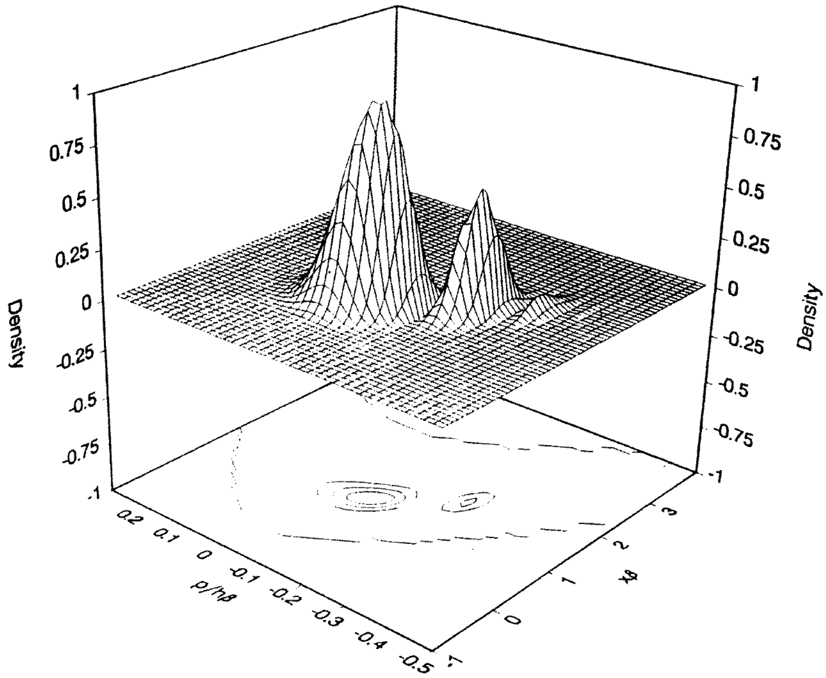


Figure 1. Phase-space densities calculated from $\rho_n(x, p) = |\Psi_n^{(2)}(p, x)|^2$ with vibrational quantum number $n = 0, 3$. Panels 1(a) and (b) correspond to choosing $(B^{(1)}, A^{(1)})$ for $\Psi_n^{(2)}(p, x)$; panels 2(a) and (b) to choosing $(B^{(1)}, A^{(2)})$; panels 3(a) and (b) to choosing $(B^{(2)}, A^{(1)})$. The contour of each phase-space density distribution is shown at the bottom of its own panel.

2a (n=0)



2b (n=3)

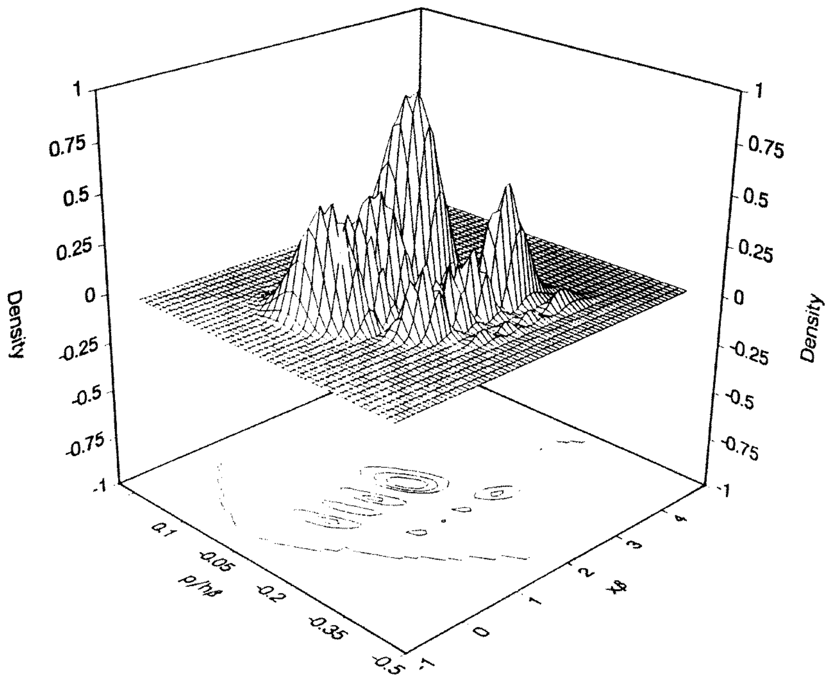


Figure 1. (Continued)

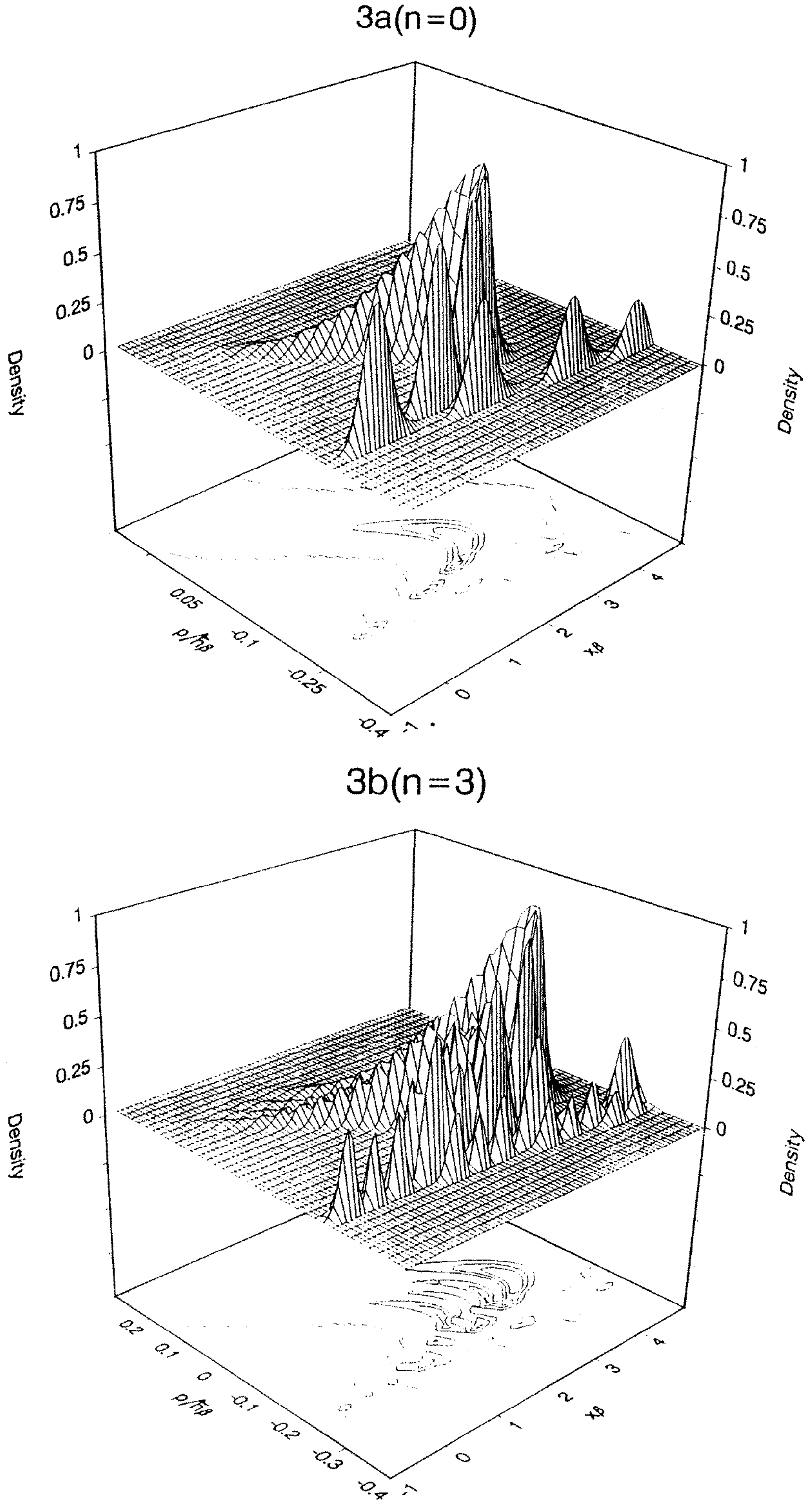


Figure 1. (Continued)

$$= \left\{ N_n^{(2)} \int_{-\infty}^{+\infty} \mathrm{d}p\, C_0^{(2)}(p) \right\} \xi^{s_n} \mathrm{e}^{-\xi/2} L_n^{2s_n}(\xi) \tag{17a}$$

$$\phi_n^{(2)}(p) = N_n^{(2)} \frac{A(p)}{B(p)^{s_n}} \int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar} \xi^{s_n} \mathrm{e}^{-\xi/2} L_n^{2s_n}(\xi). \tag{17b}$$

Note that the integral in the second equality of equation (17*a*) is evaluated by expanding $\mathrm{e}^{-\xi\hat{T}/2}$ in a series about the derivative $\frac{\partial}{\partial p}$ and integrating the obtained integrand by parts.

It is evident that these two sets of projected solutions fulfil the Schrödinger equations in their respective representations. From equations (16*a*) and (17*a*) we see that, no matter how the arbitrary functions $C_0(p)$ are chosen, the projected $\psi_n^{(1,2)}(x)$ are unique and at most differ by a constant from one another. However, the projected $\phi_n^{(1,2)}(p)$ are not unique, depending strongly on the choices of the function $C_0(p)$. It can be demonstrated that the Fourier transforms of the projected $\phi_n^{(1,2)}(p)$ into position space also satisfy the corresponding Schrödinger equation in position space, but there is only one of them whose Fourier transform corresponds to the unique L^2 solution of the Schrödinger equation in coordinate space. At this point we can say that other projected solutions in momentum space are physically meaningless.

An important feature common to the functions $A(p)$ and $B(p)$ is that they remain unchanged after successive actions of the momentum displacement operator $\hat{T}$. A possible way to generate this sort of function is first to select a fundamental characteristic function having invariance under successive actions of the $\hat{T}$ operator, of importance being the exponential function, i.e.

$$\hat{T}^n \mathrm{e}^{\pm 2\pi kp/\hbar\beta} = \mathrm{e}^{\pm 2\pi kp/\hbar\beta} \qquad (n, k = 1, 2, \ldots) \tag{18}$$

then to construct various elementary functions, polynomials, transcendental functions, and/or series using this characteristic function, and finally to produce the required functions $A(p)$ and $B(p)$ from reasonable combinations of the functions constructed above.

As an illustration, we merely choose such two simple groups of $A(p)$ and $B(p)$ for plotting as

$$\begin{cases} B^{(1)}(p) = \lambda_0(\zeta + \zeta^{-1})^{s_n+1} \\ B^{(2)}(p) = [\lambda_1 + (\zeta - \lambda_2)^2(\zeta - \lambda_3)^2]^{s_n+1} \\ A^{(1)}(p) = \zeta^2 \mathrm{e}^{-\lambda_4(\zeta+\zeta^{-1})} \\ A^{(2)}(p) = \zeta^2 \sin^2(\lambda_5\zeta)\mathrm{e}^{-\lambda_6(\zeta+\zeta^{-1})} \end{cases} \tag{19}$$

where $\zeta = \mathrm{e}^{-2\pi p/\hbar\beta}$ and λ_i, $(i = 0, 1, \ldots, 6)$ are any parameters larger than zero. For the convenience of computation we take $\lambda_2 = 0.4$, $\lambda_3 = 4$ and $\lambda_i = 1$ for $i = 0, 1, 4, 5, 6$. Figure 1 gives six three-dimensional grid diagrams of the phase-space densities calculated from $\rho_n(x, p) = |\psi_n^{(2)}(p, x)|^2$ with the combinations $(B^{(1)}, A^{(1)})$, $(B^{(1)}, A^{(2)})$, and $(B^{(2)}, A^{(1)})$ for vibrational quantum number $n = 0, 3$.

The panels in figure 1 exhibit the interesting point that different functions $A(p)$ and $B(p)$ can significantly affect the nodal behaviours of wavefunctions which reflect vibrational structures of a Morse oscillator in phase-space. Moreover, these panels are calculated and plotted only for the specific values of parameter λ_i, $(i = 0, 1, 2, \ldots, 6)$ and thus the pictures would get more and more complicated while changing the values of various parameters. It is likely that the special values of some parameters could give rise to singularities of the wavefunctions in phase-space.

Acknowledgment

This work was supported by the National Natural Science Foundation of China.

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