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Wigner function for the radial equation of the Coulomb problem in Langer space

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Abstract

In this paper a theoretical study of the Coulomb problem in quantum phase-space is reported. The Langer coordinate transformation is used to map the Coulomb problem into a one-dimensional Morse oscillator. As a result the Wigner distribution functions for the Morse oscillator are obtained. The form of these functions is presented for a few principal quantum number n and the angular momentum quantum number l. The results obtained correspond to the solution of the Coulomb problem in the spherical coordinate system.

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1. Introduction

Phase-space quantization is one of the three main autonomous and logically complete formulations of quantum mechanics (QM) [1]. The first is the standard one utilizing operators in Hilbert space, developed by Heisenberg, Schrödinger, Dirac and others. The second one relies on the path integrals, and was conceived by Dirac and constructed by Feynman. In the phase-space formulation of QM, the observables and matrix elements are computed through phase-space integrals of c-number functions weighted by a Wigner function [2],

$$f_{g,h}(y,k) = \frac{1}{\pi}\int w_g^*(y-y')w_h^*(y+y')\,\mathrm{e}^{-2\mathrm{i}y'p}\,\mathrm{d}y'. \tag{1}$$

This phase-space distribution function is a special representation of the density matrix in the Weyl correspondence [3, 4].

The Wigner distribution function (WDF) has been increasingly recognized as an important tool for the analysis of the quantum–classical connection, particularly in quantum optics [5, 6]. Based on the well-known concept of phase-space, it constitutes a natural language to study quantum chaos [7] and decoherence [8]. It can be used to calculate expectation values of any operator [9]. The WDF provides also easier interpretation and

thus the possibility of obtaining more comprehensive physical insights into the dynamics of any quantum systems. Therefore, it seems to be valuable to find as many as possible solvable quantum systems in the phase-space. The hydrogen atom is a system whose general properties are the foundation to understand the structure of other atoms or molecular systems. Its Schrödinger equation (SE), expressed in the position or momentum representation, can be solved rigorously [10], but in the phase-space the mathematical treatment is much more complicated [11–14]. In this paper we can show how to calculate WDF using a very simple mathematical trick that maps the radial Coulomb problem into the Morse oscillator. The advantage for treatment of the radial Coulomb problem as the Morse oscillator is a well-known representation of the WDF for the Morse oscillator problem [15]. Moreover, this approach permits a description of internal states in terms of Wigner trajectories without violating the Heisenberg uncertainty principle [16]. Next, the maxima of the marginal distribution of the WDF can be recovered as those of the radial distribution functions of the 1s, 2s, 2p, etc orbitals, obtained from the solution of the SE in spherical space.

The purpose of this paper is to determine the Wigner distribution function for the radial equation of the Coulomb problem using the scaled Langer transformation [17]. This transformation has previously been used in several branches of physics, including the WKB studies of the radial Schrödinger equation [18]. In a similar context the radial Wigner quasiprobability distribution function has been investigated by Twamley [19]. In his paper he showed how to construct the radial operator for a quantum state in a two-dimensional harmonic Fock representation satisfying the Heisenberg–Weyl algebra. However, all integrals have been calculated only numerically.

The outline of the paper is as follows: in section 2 the SE for the radial Coulomb problem is mapped into the one-dimension Morse oscillator by a coordinate transformation in Langer space and then in section 3 the relation between eigenfunctions of these two systems are obtained. In section 4 by using the above connection, the explicit Wigner phase-space distribution function for Coulomb problem is calculated. Finally, in section 5 we discuss the results, and present some conclusions.

2. Mapping of the Coulomb problem into the Morse oscillator

In this section we review the connection between the radial Schrödinger equation for a hydrogenic atom and the Morse potential. In spherical polar coordinates, the radial Schrödinger equation for the one-electron atom, after separation of the angular components, looks like

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R(r)}{\mathrm{d}r}\right)+V_{eff}(r)R(r)=E_nR(r), \tag{2}$$

with $V_{eff}(r)=\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}-\frac{Ze^2}{4\pi\varepsilon_0 r}$, where μ is the reduced mass of the nucleus–electron system, Ze is the nuclear charge, $-e$ is the electronic charge and ε_0 is the permittivity of vacuum. The effective potential $V_{eff}(r)$ contains, in addition to the contribution from Coulomb attraction, a repulsive term due to the angular motion of the electron. The magnitude of the angular momentum term depends on the quantum number l, which results from the solution of the angular part of SE. The common approach to the radial equation (2) is to transform it into the form of associated Laguerre equation with a well-known solution [9].

In this paper we use the mapping of the radial SE for the Coulomb problem into the Schrödinger problem for the one-dimension Morse oscillator. The relevant mapping which

shall lead to the Morse oscillator follows from the scaled Langer transformation. First, define a radial wave function $u(r)$ by $rR(r)$ which upon substitution into equation (2) yields

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2}+\left(\frac{\hbar l(l+1)}{2\mu r^2}-\frac{Ze^2}{4\pi\varepsilon_0 r}\right)u(r)=E_n u(r). \tag{3}$$

Changing the independent variable from r to $x=-\ln(r/r_0)$, where r_0 is the constant to be determined later, x is the dimensionless coordinate, and introducing the dependent variable as $u(r)=\mathrm{e}^{-x/2}w(x)$, we obtain the modified equation for $w(x)$

$$-\frac{\hbar^2}{2\mu r_0^2}\frac{\mathrm{d}^2w(x)}{\mathrm{d}x^2}+\left(-E_n\,\mathrm{e}^{-2x}-\frac{Ze^2}{4\pi\varepsilon_0 r_0}\,\mathrm{e}^{-x}\right)w(x)=-\frac{\hbar^2\left(l+\frac{1}{2}\right)^2}{2\mu r_0^2}w(x). \tag{4}$$

If we now define r_0 as

$$r_0=-\frac{Ze^2}{2(4\pi\varepsilon_0)E_n}, \tag{5}$$

SE (4) takes the form of SE for the Morse oscillator

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2w(x)}{\mathrm{d}x^2}+D(\mathrm{e}^{-2x}-2\mathrm{e}^{-x})w(x)=-\frac{\hbar^2\left(l+\frac{1}{2}\right)^2}{2\mu}w(x), \tag{6}$$

where D is defined as

$$D=-\frac{Z^2e^4}{4(4\pi\varepsilon_0)^2E_n}. \tag{7}$$

Note that the equation (6) is not the regular type of SE. The unknown eigenenergy E_n is a parameter, and determines the Morse well depth, whereas the eigenvalues $-\hbar^2\left(l+\frac{1}{2}\right)^2/2\mu$ are known and for each value of l determine an energy level in that well.

3. The Morse oscillator

The Morse potential $V_M(r)=D(\mathrm{e}^{-2\alpha x}-2\mathrm{e}^{-\alpha x})$ where D is related to the depth of the potential well, and α is the parameter controlling the width of this potential well, was proposed in 1929 for modelling internuclear potentials in diatomic molecules [20]. The SE for the vibrational levels of diatomic molecules can be expressed as

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2w(x)}{\mathrm{d}x^2}+D(\mathrm{e}^{-2\alpha x}-2\mathrm{e}^{-\alpha x})w(x)=\tilde{E}_\upsilon w(x). \tag{8}$$

The analytical solution of the SE associated with the Morse potential is given by

$$w_{\upsilon,\lambda}(y)=N_\upsilon\xi^\beta e^{-\xi/2}L_\upsilon^{2\beta}(\xi), \tag{9}$$

where $L_\upsilon^{2\beta}(\xi)$ are the associated Laguerre functions. The argument ξ is related to the displacement coordinate x by $\xi=2\lambda\,\mathrm{e}^{-y}$, where $y=\alpha x$. The variables λ and β are related to the potential and the energy, respectively, through

$$\lambda=\frac{\sqrt{2\mu D}}{\alpha\hbar} \tag{10a}$$

and

$$\beta=\frac{\sqrt{-2\mu\tilde{E}_\upsilon}}{\alpha\hbar}, \tag{10b}$$

with the constraint condition $\beta=\lambda-\upsilon-\frac{1}{2}$. The normalization constant is given by $N_\upsilon=\sqrt{\frac{(2\lambda-2\upsilon-1)\Gamma(\upsilon+1)}{\Gamma(2\lambda-\upsilon)}}$.

The corresponding eigenvalues can be written as

$$\tilde{E}_\upsilon = -D\left(1 - \frac{\alpha\hbar}{\sqrt{2\mu D}}(\upsilon + 1/2)\right)^2, \tag{11}$$

in which the quantum number υ only takes on positive integers satisfying the inequality

$$0 \leqslant \upsilon \leqslant \text{trunc}(\lambda - 1/2), \tag{12}$$

where trunc$(\lambda - 1/2)$ denotes the largest integer smaller than $\lambda - 1/2$, and gives a measure of the number of bound states. The formal similarity between the eigenequations (6) and (8) allows the use of the well-known representation of WDF of the Morse oscillator for the radial Coulomb problem. These two equations become identical if we put $\alpha = 1$. Comparing equation (6) with equation (8) and equaling (11) with the right-hand side of (6), we can obtain

$$D_{\alpha=1} = n^2\hbar^2/2\mu, \tag{13}$$

where n can take two possible values. The first one

$$n = \upsilon + l + 1 \tag{14a}$$

and the second one

$$n = \upsilon - l. \tag{14b}$$

Substituting the expression for D from (13) into (12) we can obtain restriction on l for fixed n: $0 \leqslant \upsilon \leqslant n - 1/2$. Because υ must be an integer correct expression for υ is $0 \leqslant \upsilon \leqslant n - 1$. Then, using the last inequality together with equation (14a), where $l = n - \upsilon - 1$, we obtain the well-known restriction on l to be $0 \leqslant l \leqslant n - 1$.

Equation (14b) can be rejected because it leads to negative integers for l, which are forbidden. Next, inserting (7) into equation (13) we can get the well-known result for discrete energies for the hydrogen atom

$$E_n = -\frac{Z^2 e^4 \mu}{(4\pi\varepsilon_0)^2 2n^2\hbar^2}. \tag{15}$$

Inserting once again (13) into (6), we can obtain for each principal quantum number n an individual SE for the Morse oscillator

$$-\hbar^2\frac{\mathrm{d}^2 w(x)}{\mathrm{d}x^2} + n^2\hbar^2(\mathrm{e}^{-2x} - 2\mathrm{e}^{-x})w(x) = -\hbar^2\left(l + \frac{1}{2}\right)^2 w(x) \tag{16}$$

with $-\hbar^2\left(l + \frac{1}{2}\right)^2/2\mu$ as the eigenvalue, and the effective potential $V(x) = n^2\hbar^2(\mathrm{e}^{-2x} - 2\mathrm{e}^{-x})$, depending on the quantum number n.

Equation (16) can be interpreted as SE for the centrifugal motion, because the effective potential in equation (16) includes the total energy minus the Coulomb potential. With the help of equation (5) we can find the minimum for the nth Morse potential. The new equilibrium coordinate $r_{0(n)}$ is given by the expression $r_{0(n)} = \frac{n^2\hbar^2(4\pi\varepsilon_0)}{Ze^2\mu} = n^2 a_0$, where a_0 is the Bohr radius.

The radius $r_{0(n)}$ is simply that of the nth Bohr orbit. Thus equation (16) describes just the oscillations about the Bohr orbit, subjected to the Morse potential, as a result of centrifugal motion. Using equation (13) for D and eigenvalues of equation (6) for $\tilde{E}_\upsilon$ and comparing these equations with (10a) and (10b), respectively, we can get

$$\lambda = n \text{ and } \beta = l + \tfrac{1}{2}. \tag{17}$$

Hence, the wave function $w(y)$ of the transformed radial equation (5) is given by

$$w_{n,l}(y) = N_{n,l}\xi^{l+\frac{1}{2}}e^{-\xi/2}L^{2l+1}_{n-l-1}(\xi), \tag{18}$$

where $N_{n,l} = \sqrt{\frac{(l+\frac{1}{2})\Gamma(n-l)}{\Gamma(n+l+1)}}$.

4. The Wigner function for the radial equation of the Coulomb problem

To find WDF for the radial equation of the Coulomb problem mapped into the Morse oscillator, we closely follow [14]. In the calculation of WDF we use a dimensionless coordinate y, and the dimensionless momentum k corresponding to y defined as $k_{\alpha=1} = p/(\alpha\hbar)$. Using equation (1), and introducing a new integration variable $\tau = \mathrm{e}^{-y'}$ we can get for the wave function given by equation (18) the expression for WDF

$$f_{g,p,h,q}(y,k) = \frac{1}{\pi}\int w^*_{g,p}\left(\frac{y}{\tau}\right) w_{h,q}(y\tau)\tau^{-2\mathrm{i}k}\frac{\mathrm{d}\tau}{\tau}. \tag{19}$$

Integration of equation (19) leads to the following results

$$f_{g,p,h,q}(y,k) = \frac{2}{\pi}N_{g,p}N_{h,q}\xi^{p+q+1}\sum_{r=0}^{g-p-1}\sum_{s=0}^{h-q-1} b_r(g,\,p)b_s(h,q)\xi^{r+s}K_v(\xi), \tag{20}$$

where $b_j(n,l) = \frac{(-1)^j}{j!}\frac{\Gamma(n+l+1)}{\Gamma(n-l-j)\Gamma(2l+j+2)}$ $(j = r, s\, n = g, h\, l = p, q)$, and

$$K_\eta(\xi) = \frac{1}{2}\int_0^\infty \tau^\kappa \exp\left[-\frac{y}{2}\left(\tau + \frac{1}{\tau}\right)\right]\frac{\mathrm{d}\tau}{\tau}. \tag{21}$$

The $K_\eta(\xi)$ are the modified Bessel functions of the third kind, also known as the MacDonald functions with $\eta = q - p + 2\mathrm{i}k + s - r$. The numerical integration of equation (21) is accompanied by a few difficulties, but several methods to circumvent these difficulties can be found in the literature (see for example [21]).

5. Results and conclusions

In this paper we present a detailed study of the WDF only for pure states, i.e., when $g = h = n$, and $p = q = l$.

In the two series of 3D plots and contour plots the results of the calculations performed are presented for n from $n = 0$ to $n = 5$ with $l = 0$, and for all angular momentum quantum number l allowed for the quantum number, $n = 5$, respectively.

In all figures of WDF we used the dimensionless coordinate $-\ln(r/a_0)$ defined as $y_{\alpha=1} \equiv x = -\ln(r/r_{0(n)}) = -\ln(r/n^2a_0) = -\ln(r/a_0) + 2\ln(n)$, and the dimensionless conjugate momentum k.

Our discussion is based upon the well-known observation that the whole phase-space region that supports the WDF can be separated into three subregions. The central part of the WDF is occupied by the highest maximum. This region borders on the inner region where the function oscillates between positive and negative values. The outer region is characterized by the fast oscillatory decay.

In figures 1(*a*)–(*d*) we present the results for the WDF when $l = 0$. For the ground state $(n = 0)$ the WDF is positive everywhere with one single maximum. The first excited state $(n = 1)$ is characterized by the highest peak localized at higher values of y, and negative minimum at the origin. Every succeeding excited state generates additional an even or odd number of extremums localized in the inner region, while the main maximum moves further to higher values of y.

In figures 1(*a*)–(*d*) we can also see the marginal distribution (MD) as the probability of finding an electron at a given radius from the nucleus. Note that these distributions correspond perfectly to the nodal behaviour of the radial distribution wave function in configuration space

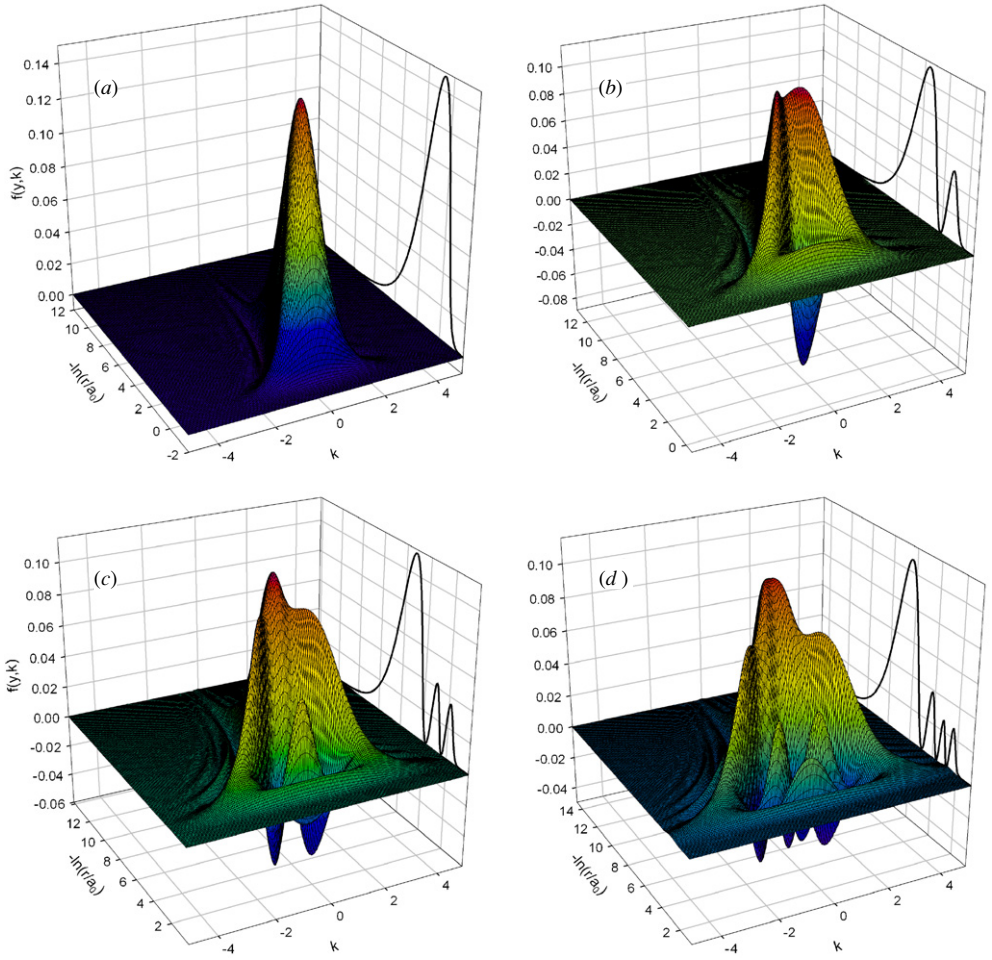

Figure 1. The Wigner distribution function $f_{n,l}(-\ln(x/a_0), k)$ for (a) $n = 1$, (b) $n = 2$, (c) $n = 3$ and (d) $n = 4$ with $l = 0$, and marginal distribution in the position representation.

representation. The highest maximum of MD is localized at the most probable and average distance equal to the Bohr radius which moves to the higher values of r as n increases. Also, the number of nodes $n - l - 1$ equals to that of the radial distribution function.

In the following figures 2(a)–(e) we show the contour plots of WDF of the excited state with $n = 5$, where $l = 0, 1, \ldots, 4$. These plots show clearly that the increase in l gives rise to a decrease in the number of singularities of WDF. This time the position of the main maximum gets closer to the origin of the WDF as l increases, which once again stresses the similarity between WDF and the radial distribution functions depicted in figure 3.

To conclude, we show that WDF is a very useful representation linking the quantum mechanics and classical description. Because this representation allows a description of a quantum system in terms of classical concepts, the Wigner approach seems to be very suitable for description of quantum chaos, collision dynamics, transport or radiation processes and many others from different branches of physics (see for example [22] and references therein). Hence, it is very significant to find every solvable quantum system in the phase-space.

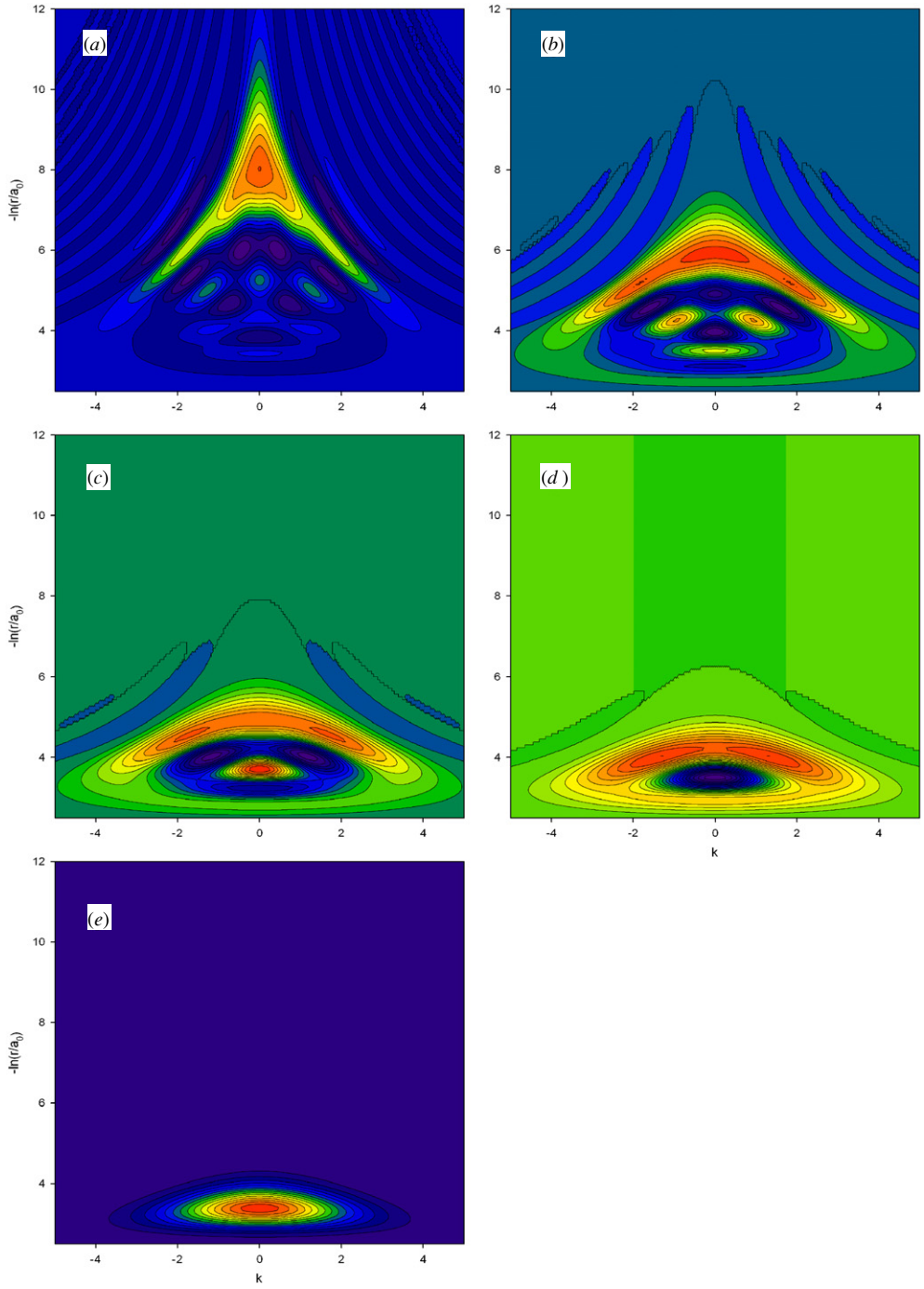

Figure 2. Contour plots of the WDF for $n = 5$ with (a) $l = 0$, (b) $l = 1$, (c) $l = 2$, (d) $l = 3$ and (e) $l = 4$.

The application of Langer transformation gives a complete equivalence of the radial Coulomb problem to the Morse oscillator. The knowledge of the solution of the WDF for

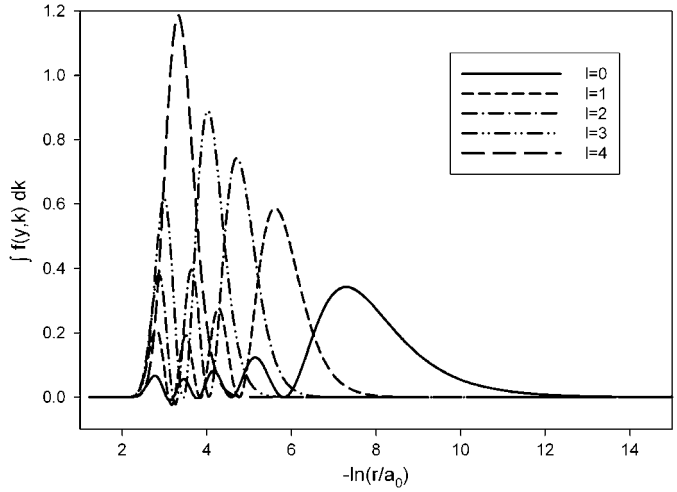

Figure 3. Curves of marginal distributions normalized to unity for the five quantum states corresponding to the contour plots in figures 2(*a*)–(*e*).

the Morse oscillator enables us to obtain in the same way the WDF for the radial Coulomb problem.

The power of this method lies in a very simple scheme leading to the correct radial WDF confirmed by the proper marginal probability distributions. In all calculations we obtained the appropriate characteristic of nodal points for the radial density of probability for the wave function in configuration space representation. Within the Langer transformation all integrals turned out to be particularly easy to solve analytically.

Another interesting result that should be mentioned is that the Langer transformation applied to the Coulomb problem with centrifugal force is changed into the Morse potential without the centrifugal term. It leads to a much easier solution of the problem discussed.

Finally, we demonstrate that the phase-space formulations provide different insights and 'easily understandable' visualization of the model studied and any other quantum system.

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