

RESEARCH PAPERS

Wave mechanics in quantum phase space: hydrogen atom*

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Abstract The rigorous solutions of the stationary Schrödinger equation for hydrogen atom are solved with the wave-mechanics method within the framework of the quantum phase-space representation established by Torres-Vega and Frederick. The "Fourier-like" projection transformations of wave function from the phase space to position and momentum spaces are extended to three-dimensional systems. The eigenfunctions in general position and momentum spaces could be obtained through the transformations from eigenfunction in the phase space.

Keywords: quantum phase space, hydrogen atom, projection transformation.

Since the first quantum phase-space distribution function was introduced by Wigner^[1] in 1932, a variety of phase-space theories for quantum mechanics have been proposed^[2,3] and extensive uses have been found in many areas of physics and chemistry^[4-6]. The quantum phase-space theory can be used to describe the dynamical and statistical properties of physical system, and compare quantum mechanics for finite \hbar with classical mechanics for \hbar goes to zero^[7]. However, when persons want to consider position and momentum simultaneously in quantum mechanics, caution is required due to the Heisenberg uncertainty principle.

It is the most direct way for introducing phase-space representations of quantum mechanics to define quantum phase-space distribution functions. So far, the quantum phase-space distribution function used mostly in physics and chemistry is still the Wigner distribution function^[1,7], which is called quasi-probability distribution function. There have been many attempts to improve the inadequacy that the Wigner distribution function is not always positive in phase space^[2,8].

In addition, one can also define directly the quantum state functions and corresponding Schrödinger equations in phase space. Then, almost

all the mathematical properties in the general position or momentum representation of quantum mechanics are retained for quantum state functions in phase space, and a variety of useful methods and results can be replanted to phase-space representation. This idea is reflected in the quantum phase-space theory established by Torres-Vega and Frederick (T-F)^[9,10] in the 1990s. The principle operators of dynamic variables and the Schrödinger equations are defined directly in T-F phase-space representation, and the phase-space wavefunctions are determined by the Schrödinger equations are solved. The mean values of dynamic variables may be computed just as those in general position or momentum space^[11]. The foundation of theory was based on the assumption that there exists a set of complete base functions, $\Gamma(q, p)$, and any quantum state $|\Psi\rangle$ can be represented as

$$\langle \Gamma(q, p) | \Psi \rangle = \Psi(q, p), \quad (1)$$

while the principle operators \hat{Q} and \hat{P} may be directly represented in the phase space as

$$\hat{Q} = \frac{q}{2} + i \frac{\partial}{\partial p}, \quad (2)$$

$$\hat{P} = \frac{p}{2} - i \frac{\partial}{\partial q}. \quad (3)$$

Although this representation coincides with the totality of coherent state representations for the Heisenberg-Weyl group^[12], its advantage consists in the fact

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that there exist the similar formulas to those in general position or momentum representation of quantum mechanics. Especially the time-evolution equation of the wavefunction $\Psi(q, p)$ in the phase space is similar to the Schrödinger equation, i. e.,

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

Since the T-F phase-space representation of quantum mechanics was proposed, a variety of advances in the theory^[12,13] have motivated a new wave of interest in the applications to atomic and molecular systems^[14–16]. Torres-Vega and Frederick have treated the harmonic oscillator in the phase space^[9,10]. Møller et al. have considered a set of solutions to the stationary Schrödinger equation of the linear potential in the phase space, and discussed the possibilities and limitations of doing wave mechanics in the phase space^[12]. Hu et al. have obtained the rigorous solutions of Morse oscillator in the phase space^[14]. And then, we have also obtained the rigorous solutions of a particle in delta potential fields^[13] and one-dimensional hydrogen atom^[15], and discussed the vibration theory of diatomic molecules with an empirical potential function in the quantum phase-space representation^[16].

In quantum mechanics, the relatively few potential-energy functions $V(\mathbf{r})$ for which analytic solutions of the Schrödinger equation are possible are important beyond these immediate problems, since they offer serve as bases for approximate calculations on more complicated system^[17–19]. But in the phase space, the double number of variable for a physical system and the first derivative terms in either position or momentum operator makes the mathematical equations and the wave functions much more complicated in form than those in general position or momentum space. This is just the reason that, so far, we can only treat the one-dimensional systems in T-F phase-space representation.

It is generally impossible to obtain analytic solutions of the three-dimensional stationary Schrödinger equation (wave equation) unless it can be separated into total differential equations in each of the three space coordinates. If the potential energy is spherically symmetric, so that $V(\mathbf{r}) = V(r)$ is a function only of the magnitude r of \mathbf{r} measured from some ori-

gin, the wave equation can always be separated in spherical coordinates. Many problems of physical interest can be represented exactly or approximately in terms of spherically symmetric potentials of various shapes.

The hydrogen atom is the simplest atomic system. Its potential energy $V(r) = -\frac{1}{r}$, which represents the attractive coulomb interaction between an atomic nucleus and an electron, provides a wave equation that can be solved analytically. This problem is of direct physical interest, since apart from relativistic effects, the calculated energy eigenvalues are in agreement with the observed energy levels of the hydrogen atom^[17]. Hence, it is valuable to solve the stationary Schrödinger equation of hydrogen atomic system in phase space.

1 Analytic solution of hydrogen atom in phase space

In the hydrogen-atom problem, the potential energy $V(\mathbf{r})$ is spherically symmetric, and does not depend on the time. The corresponding stationary state Schrödinger equation for the system is

$$\left[\frac{\mathbf{p}^2}{2} + V(\mathbf{r}) \right] \Psi = E \Psi, \quad (5)$$

where $E < 0$ for a bound state. The position and momentum variables may be written in rectangular coordinates:

$$\begin{aligned} \mathbf{r} &= xi + yj + zk, \\ \mathbf{p} &= p_x i + p_y j + p_z k, \end{aligned}$$

then

$$\mathbf{p}^2 = p_x^2 + p_y^2 + p_z^2.$$

In T-F quantum phase-space representation, the position and momentum operators can be written as the canonical form^[9,10], i. e.,

$$\begin{aligned} x &\rightarrow X' = \frac{x}{2} + i \frac{\partial}{\partial p_x}, \\ y &\rightarrow Y' = \frac{y}{2} + i \frac{\partial}{\partial p_y}, \\ z &\rightarrow Z' = \frac{z}{2} + i \frac{\partial}{\partial p_z}, \end{aligned} \quad (6)$$

$$\begin{aligned} p_x &\rightarrow P_x = \frac{p_x}{2} - i \frac{\partial}{\partial x}, \\ p_y &\rightarrow P_y = \frac{p_y}{2} - i \frac{\partial}{\partial y}, \\ p_z &\rightarrow P_z = \frac{p_z}{2} - i \frac{\partial}{\partial z}, \end{aligned} \quad (7)$$

then Eq. (5) becomes

$$\left[\frac{1}{2}(P_x^2 + P_y^2 + P_z^2) + \hat{V}(X', Y', Z') \right] \Psi(\mathbf{r}, \mathbf{p}) = E\Psi(\mathbf{r}, \mathbf{p}). \quad (8)$$

If the following relations

$$\begin{aligned} \left(\frac{x}{2} + i \frac{\partial}{\partial p_x} \right)^n &= \exp\left(\frac{ixp_x}{2} \right) \left(i \frac{\partial}{\partial p_x} \right)^n \exp\left(-\frac{ixp_x}{2} \right), \\ \left(\frac{y}{2} + i \frac{\partial}{\partial p_y} \right)^n &= \exp\left(\frac{iyp_y}{2} \right) \left(i \frac{\partial}{\partial p_y} \right)^n \exp\left(-\frac{iyp_y}{2} \right), \\ \left(\frac{z}{2} + i \frac{\partial}{\partial p_z} \right)^n &= \exp\left(\frac{izp_z}{2} \right) \left(i \frac{\partial}{\partial p_z} \right)^n \exp\left(-\frac{izp_z}{2} \right), \end{aligned}$$

are used, it is easy to prove

$$\begin{aligned} \hat{V}(X', Y', Z') \\ = \exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2} \right) \hat{V}(X, Y, Z) \exp\left(\frac{i\mathbf{r} \cdot \mathbf{p}}{2} \right), \end{aligned} \quad (9)$$

here we define:

$$\begin{aligned} X &= x + i \frac{\partial}{\partial p_x}, \quad Y = y + i \frac{\partial}{\partial p_y}, \\ Z &= z + i \frac{\partial}{\partial p_z}. \end{aligned}$$

With the help of the relations

$$\begin{aligned} \left(\frac{p_x}{2} - i \frac{\partial}{\partial x} \right)^n &= \exp\left(-\frac{ixp_x}{2} \right) \left(-i \frac{\partial}{\partial x} \right)^n \exp\left(\frac{ixp_x}{2} \right), \\ \left(\frac{p_y}{2} - i \frac{\partial}{\partial y} \right)^n &= \exp\left(-\frac{iyp_y}{2} \right) \left(-i \frac{\partial}{\partial y} \right)^n \exp\left(\frac{iyp_y}{2} \right), \\ \left(\frac{p_z}{2} - i \frac{\partial}{\partial z} \right)^n &= \exp\left(-\frac{izp_z}{2} \right) \left(-i \frac{\partial}{\partial z} \right)^n \exp\left(\frac{izp_z}{2} \right), \end{aligned}$$

and Eq. (9), as well as the transformation of wave function

$$\Psi(\mathbf{r}, \mathbf{p}) = \exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2} \right) \Omega(X, Y, Z; \mathbf{p}), \quad (10)$$

Eq. (8) can be rewritten as follows:

$$\begin{aligned} \left[-\frac{1}{2} \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2} \right) + \hat{V}(X, Y, Z) \right] \\ \Omega(X, Y, Z; \mathbf{p}) = E\Omega(X, Y, Z; \mathbf{p}). \end{aligned} \quad (11)$$

It should be noted that X , Y , and Z are differential operators, and do not commute with \mathbf{p} . In the present paper, X , Y , and Z will be regarded as symbolic variables of wave function $\Omega(X, Y, Z; \mathbf{p})$, and always written in the front of \mathbf{p} . Then X , Y , and Z will be treated as differential operators after the solutions of Eq. (11) have been obtained. We define that $\frac{\partial}{\partial X}$, $\frac{\partial}{\partial Y}$, and $\frac{\partial}{\partial Z}$ represent evaluating the derivative only to "variables" X , Y , and Z respectively. It can be proved that

$$\frac{\partial}{\partial X} = \frac{\partial}{\partial x}, \quad \frac{\partial}{\partial Y} = \frac{\partial}{\partial y}, \quad \text{and} \quad \frac{\partial}{\partial Z} = \frac{\partial}{\partial z}.$$

It has been shown^[20] that there are 11 coordinates systems in which the free particle wave equation (with $V=0$) can be separated. One of the most important of these is the spherical polar coordinate system, in terms of which the rectangular coordinates are given by

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta.$$

In the phase space, the canonical coordinates can similarly be written as

$$\begin{aligned} X &= R\sin\Theta\cos\Phi, \quad Y = R\sin\Theta\sin\Phi, \\ Z &= R\cos\Theta. \end{aligned}$$

Then Eq. (11) can be written in spherical coordinates

$$\begin{aligned} \left\{ -\frac{1}{2} \left[\frac{1}{R^2} \frac{\partial}{\partial R} \left(R^2 \frac{\partial}{\partial R} \right) + \frac{1}{R^2 \sin^2\Theta} \frac{\partial}{\partial \Theta} \left(\sin\Theta \frac{\partial}{\partial \Theta} \right) \right. \right. \\ \left. \left. + \frac{1}{R^2 \sin^2\Theta} \frac{\partial^2}{\partial \Phi^2} \right] + \hat{V}(R) \right\} \Omega(R, \Theta, \Phi; \mathbf{p}) \\ = E\Omega(R, \Theta, \Phi; \mathbf{p}). \end{aligned} \quad (12)$$

Separating the radial and the angular parts by substituting

$$\begin{aligned} \Omega(R, \Theta, \Phi; \mathbf{p}) &= \frac{1}{R} u(R; \mathbf{p}) \chi_{lm}(\Theta, \Phi; \mathbf{p}), \\ (l &= 0, 1, 2, \dots, \text{and } m = l, l-1, \dots, -l) \end{aligned} \quad (13)$$

into Eq. (12), we obtain a radial equation

$$\frac{\partial^2 u(R; \mathbf{p})}{\partial R^2} + \left[2E + \frac{2}{R} - \frac{l(l+1)}{R^2} \right] u(R; \mathbf{p}) = 0 \quad (14)$$

and an angular equation

$$\begin{aligned} \left[\frac{1}{\sin\Theta} \frac{\partial}{\partial \Theta} \left(\sin\Theta \frac{\partial}{\partial \Theta} \right) + \frac{1}{\sin^2\Theta} \frac{\partial^2}{\partial \Phi^2} \right. \\ \left. + l(l+1) \right] \chi_{lm}(\Theta, \Phi; \mathbf{p}) = 0. \end{aligned} \quad (15)$$

The angular equation (15) can be further separated by substituting

$$\chi_{lm}(\Theta, \Phi; \mathbf{p}) = v(\Theta; \mathbf{p}) w(\Phi; \mathbf{p}) \quad (16)$$

into it and following the same procedure to obtain

$$\begin{aligned} \left\{ \frac{1}{\sin\Theta} \frac{\partial}{\partial \Theta} \left(\sin\Theta \frac{\partial}{\partial \Theta} \right) + \left[l(l+1) - \frac{m}{\sin^2\Theta} \right] \right\} v(\Theta; \mathbf{p}) \\ = 0, \end{aligned} \quad (17)$$

$$\left(\frac{\partial^2}{\partial \Phi^2} + m \right) w(\Phi; \mathbf{p}) = 0. \quad (18)$$

For Eqs. (14), (17) and (18), we should pay attention to that R , Θ , and Φ are differential operators and, therefore, do not commute with \mathbf{p} . We set that R , Θ , and Φ are always in the front of \mathbf{p} .

We first attempt to solve the radial equation

(14). Considering the property of the equation and the boundary condition of the wave functions, i. e., $u(R, \mathbf{p}) = u(r, \mathbf{p})$ should be finite when $r \rightarrow \infty$ or $p = |\mathbf{p}| \rightarrow \infty$, we select an attempted solution as

$$u(R; \mathbf{p}) = R^{l+1} \exp(-\beta R) \omega(R; \mathbf{p}), \quad (19)$$

where $\beta = \sqrt{-2E}$. Inserting it into Eq. (14) and putting $\xi = 2\beta R$, we obtain a confluent hypergeometric equation for variable ξ , i. e.,

$$\xi \frac{\partial^2 \omega(\xi, \mathbf{p})}{\partial \xi^2} + [2(l+1) - \xi] \frac{\partial \omega(\xi, \mathbf{p})}{\partial \xi} - \left[(l+1) - \frac{1}{\beta} \right] \omega(\xi, \mathbf{p}) = 0. \quad (20)$$

If $\omega(\xi, \mathbf{p})$ is expanded in a series about ξ , i. e.,

$$\omega(\xi, \mathbf{p}) = \sum_{i=0}^{\infty} \xi^i C_i(\mathbf{p}), \quad (21)$$

the solutions of Eq. (20) satisfying the boundary conditions that $\omega(\xi, \mathbf{p})$ should be finite when $r \rightarrow \infty$ or $p \rightarrow \infty$ should be

$$\omega(\xi, \mathbf{p}) = F(-n+l+1, 2l+2; \xi) C(\mathbf{p}) \quad (n = 1, 2, 3, \dots), \quad (22)$$

where $F(-n+l+1, 2l+2; \xi)$ is a confluent hypergeometric series, and $C(\mathbf{p})$ may be an arbitrary reasonable function satisfying the following condition:

$$\int_p d\mathbf{p} \left| \frac{d^j}{d\mathbf{p}^j} C(\mathbf{p}) \right| < \infty \quad (j = 0, 1, 2, \dots). \quad (23)$$

The energy eigenvalues are given by $\beta = \sqrt{-2E} = \frac{1}{n}$, i. e.,

$$E_n = -\frac{1}{2n^2}. \quad (24)$$

and the corresponding solutions of the radial equation (14) are

$$u_{nl}(R; \mathbf{p}) = \xi^{l+1} \exp\left(-\frac{1}{2}\xi\right) \cdot F(-n+l+1, 2l+2; \xi) C(\mathbf{p}). \quad (25)$$

In a similar way, we can obtain the solutions of two angular equations (17) and (18) respectively. The results are

$$v_{lm}(\Theta, \mathbf{p}) = P_l^m(\cos\Theta) C'(\mathbf{p}), \quad (26)$$

$$w_m(\Phi, \mathbf{p}) = \exp(im\Phi) C''(\mathbf{p}), \quad (27)$$

where $P_l^m(\cos\Theta)$ is the associated Legendre function, $C'(\mathbf{p})$ and $C''(\mathbf{p})$ the arbitrary reasonable functions satisfying the following conditions:

$$\int_p d\mathbf{p} \left| \frac{d^j}{d\mathbf{p}^j} C'(\mathbf{p}) \right| < \infty, \quad (28)$$

$$\int_p d\mathbf{p} \left| \frac{d^j}{d\mathbf{p}^j} C''(\mathbf{p}) \right| < \infty. \quad (29)$$

Therefore, we can write the eigenfunctions of hydrogen atom in the phase-space representation as follows:

$$\begin{aligned} \Psi_{nlm}(\mathbf{r}; \mathbf{p}) &= \exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2}\right) \left[N_{nl} \xi^l \exp\left(-\frac{1}{2}\xi\right) \right. \\ &\quad \cdot F(-n+l+1, 2l+2; \xi) C(\mathbf{p}) \left. \right] \\ &\quad \cdot [N_{lm} P_l^m(\cos\Theta) C'(\mathbf{p})] \\ &\quad \cdot [N_m \exp(im\Phi) C''(\mathbf{p})], \end{aligned} \quad (30)$$

where N_{nl} , N_{lm} and N_m are the normalization constants.

2 Discussion

The hydrogen-atom problem in the phase-space representation gives rise to an infinite number of discrete energy levels extending from $-\frac{1}{2}$ up to zero, and the energy eigenvalues in phase space [Eq. (24)] are also in agreement with those in the position space. This is easy to understand, because the values of dynamic variables are independent of mathematical representation for a physical system.

In position representation, the energy eigenvalues of hydrogen atom depend only on n and so are degenerate with respect to both l and m . The degeneracy of energy level is n^2 . However, in the phase space, there exist three arbitrary functions, $C(\mathbf{p})$, $C'(\mathbf{p})$ and $C''(\mathbf{p})$ of the momentum variable satisfying the condition Eqs. (23), (28) and (29) respectively. That is to say, there are at least as many solutions as $C(\mathbf{p}) C'(\mathbf{p}) C''(\mathbf{p})$, and if we use other methods to solve the wave equation (8), maybe we can find much more solutions. Hence the total degeneracy of energy level for the hydrogen atom system is more than n^2 in the phase space. The existence of degenerate energy eigenvalues means that linear combinations of the corresponding eigenfunctions are solutions of the wave equation with the same energy. In general, degeneracy will occur whenever the wave equation can be solved in more than one way^[17]. Therefore, it is reasonable to expect that other methods can be found to solve the wave equation (8).

Since position and momentum are now considered simultaneously in the phase space, the forms of eigenfunctions must be uncertain to incorporate the Heisenberg uncertainty principle. Although the wave equation (8) seems to be defined by the choice of op-

erators in equations (6) and (7), and there should be the corresponding unique eigenfunction in the phase space, as we know, the states of a physical system are determined by the eigenequation and the corresponding boundary conditions. For the wave equation (8), the boundary conditions of momentum (position) part in the eigenfunction cannot be specified, if those of position (momentum) parts are completely certain. The definite and unique solution will not be in agreement with the uncertainty principle.

In general, the eigenfunction (30) is a complicated function of variables \mathbf{r} and \mathbf{p} which cannot be separated from each other. However, a kind of particular simple solution can also be found out, in which the position and momentum parts can be separated. For example, we put

$$C(\mathbf{p}) = (2\pi)^{-\frac{3}{2}} \exp(i\mathbf{r}_0 \cdot \mathbf{p}), \quad (31)$$

$$C'(\mathbf{p}) = C''(\mathbf{p}) = 1, \quad (32)$$

where $\mathbf{r}_0 = x_0\mathbf{i} + y_0\mathbf{j} + z_0\mathbf{k}$ is the eigenvalue of position operator. Although the integral in Eq. (23) does not converge if taken over an infinite limit for Eq. (31), we may think of the region of space in which such a wave function is defined as being arbitrarily large but finite, while the integral in Eq. (23) is over the finite limit of this region and converges.

It is easy to prove

$$\begin{aligned} v_{lm}(\Theta, \mathbf{p}) &= N_{lm} P_l^m(\cos\Theta) C'(\mathbf{p}) \\ &= N_{lm} P_l^m(\cos\theta), \end{aligned}$$

$$\begin{aligned} w_m(\Phi, \mathbf{p}) &= \frac{1}{\sqrt{2\pi}} \exp(im\Phi) C''(\mathbf{p}) \\ &= \frac{1}{\sqrt{2\pi}} \exp(im\varphi), \end{aligned}$$

$$\begin{aligned} \left(x + i \frac{\partial}{\partial p_x}\right)^i \left(y + i \frac{\partial}{\partial p_y}\right)^j \left(z + i \frac{\partial}{\partial p_z}\right)^k C(\mathbf{p}) \\ = (x - x_0)^i (y - y_0)^j (z - z_0)^k C(\mathbf{p}) \end{aligned}$$

where $i, j, k = 0, 1, 2, \dots$, and

$$\langle C_{r'_0}(\mathbf{p}) | C_{r''_0}(\mathbf{p}) \rangle = \delta(\mathbf{r}'_0 - \mathbf{r}''_0),$$

if $C'(\mathbf{p})$ and $C''(\mathbf{p})$ are defined as Eq. (32), and $C(\mathbf{p})$ as Eq. (31). Therefore, the corresponding eigenfunction in the phase space is

$$\begin{aligned} \Psi_{nlm}(\mathbf{r}, \mathbf{p}) \\ = \exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2}\right) N_{nl} \left(\frac{2|\mathbf{r} - \mathbf{r}_0|}{n}\right)^l \\ \cdot \exp\left(-\frac{|\mathbf{r} - \mathbf{r}_0|}{n}\right) \\ \cdot F\left(-n + l + 1, 2l + 2; \frac{2|\mathbf{r} - \mathbf{r}_0|}{n}\right) \end{aligned}$$

$$\times Y_{lm}(\theta, \varphi) (2\pi)^{-\frac{3}{2}} \exp(i\mathbf{r}_0 \cdot \mathbf{p}), \quad (33)$$

where $Y_{lm}(\theta, \varphi) = N_{lm} P_l^m(\cos\theta) \frac{1}{\sqrt{2\pi}} \exp(im\varphi)$ is the spherical harmonic. Here the position and momentum parts have been separated completely except for the phase factor $\exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2}\right)$.

For the ground state, $n = 1$, there is only a single node at the point of $\mathbf{r} = \mathbf{r}_0$ in the radial wave function. We must have $l = 0$ and $m = 0$ for this state. Therefore, the eigenfunction in the phase space, Eq. (33), will become

$$\begin{aligned} \Psi_{100}(\mathbf{r}, \mathbf{p}) \\ = \frac{1}{2\sqrt{2}\pi^2} \exp\left[-|\mathbf{r} - \mathbf{r}_0| - \frac{i}{2}(\mathbf{r} - 2\mathbf{r}_0) \cdot \mathbf{p}\right]. \end{aligned} \quad (34)$$

By means of the ground-state eigenfunction, Eq. (34), we can obtain the distribution probability of radial position for the electron, i. e., the probability for finding the electron in the ball-shell $(|\mathbf{r} - \mathbf{r}_0|, |\mathbf{r} - \mathbf{r}_0| + d|\mathbf{r} - \mathbf{r}_0|)$, as follows:

$$\begin{aligned} \rho_{100}(\mathbf{r}, \mathbf{p}) d|\mathbf{r} - \mathbf{r}_0| \\ = (\mathbf{r} - \mathbf{r}_0)^2 d|\mathbf{r} - \mathbf{r}_0| \int d\omega |\Psi_{100}(\mathbf{r}, \mathbf{p})|^2 \\ = \frac{1}{8\pi^4} (\mathbf{r} - \mathbf{r}_0)^2 \exp(-2|\mathbf{r} - \mathbf{r}_0|) d|\mathbf{r} - \mathbf{r}_0|. \end{aligned} \quad (35)$$

Then, by solving the following equation

$$\frac{d}{d|\mathbf{r} - \mathbf{r}_0|} \rho_{100}(\mathbf{r}, \mathbf{p}) = 0, \quad (36)$$

we can also find the point where the probability density will be the maximum value in the phase space. The maximum-value point is

$$|\mathbf{r} - \mathbf{r}_0| = 1 \quad (\text{Bohr radius}). \quad (37)$$

This is exactly where the first Bohr orbit occurs in the early quantum theory. Clearly, these results are in agreement with those in position representation.

For position and momentum representations, a geometrical picture that is often used regards a wave function Ψ as a state vector in an infinite-dimensional Hilbert space. A particular state vector has different components when referred to as corresponding axes, and these constitute the corresponding representations of the state. Different choices for the orientation of the axes in the Hilbert space correspond to different choices for the representation, and a transformation from one representation to the other corresponds to a

rotation of axes in the Hilbert space. However, for the phase-space representation, there are two variables, q and p , in the wave function. The transformation of wave function between the phase-space representation and position or momentum representation is a kind of "Fourier-like" projection transformation^[9–11]. It is obvious that the inverse transformation of "Fourier-like" projection transformation is not unique. This exhibits that the phase-space eigenfunction is not unique.

The one-dimensional treatment is readily extended to three dimensions. It is natural to rewrite the "Fourier-like" projection equations as

$$\begin{aligned}\psi_{nlm}(\mathbf{r}) &= \int_{\mathbf{p}} d\mathbf{p} \exp\left(\frac{i\mathbf{r} \cdot \mathbf{p}}{2}\right) \Psi_{nlm}(\mathbf{r}, \mathbf{p}), \quad (38) \\ \phi_{nlm}(\mathbf{p}) &= \int_{\mathbf{r}} d\mathbf{r} \exp\left(-\frac{i\mathbf{r} \cdot \mathbf{p}}{2}\right) \Psi_{nlm}(\mathbf{r}, \mathbf{p}).\end{aligned}\quad (39)$$

If we project the phase-space eigenfunction (33) into position or momentum space through Eq. (38) or Eq. (39), we should obtain the unique eigenfunction in the corresponding space respectively, since the eigenfunction and the boundary conditions are completely certain in position or momentum space. The result for position space is

$$\begin{aligned}\psi_{nlm}(\mathbf{r}) &= N_{nl} \left(\frac{2r}{n}\right)^l \exp\left(-\frac{r}{n}\right) \\ &\cdot F\left(-n+l+1, 2l+2; \frac{2r}{n}\right) Y_{lm}(\theta, \varphi),\end{aligned}\quad (40)$$

and that for momentum space is

$$\begin{aligned}\phi_{nlm}(\mathbf{p}) &= \int d\mathbf{r} \exp(-i\mathbf{r} \cdot \mathbf{p}) N_{nl} \left(\frac{2r}{n}\right)^l \\ &\cdot \exp\left(-\frac{r}{n}\right) F\left(-n+l+1, 2l+2; \frac{2r}{n}\right) \\ &\cdot Y_{lm}(\theta, \varphi),\end{aligned}\quad (41)$$

in which the follow formula has been used:

$$\begin{aligned}&\int_{-\infty}^{\infty} dp_{\eta} \frac{1}{2\pi} \exp(i\eta_0 p_{\eta}) \\ &= \lim_{L \rightarrow \infty} \int_{-L/2}^{L/2} dp_{\eta} \frac{1}{L} \exp\left(\frac{i2\pi j p_{\eta}}{L}\right) = \delta_{j,0},\end{aligned}\quad (42)$$

where $\eta = x, y, z$ and $j = 0, \pm 1, \pm 2, \dots$. It is obvious that Eqs. (40) and (41) are the same as the eigenfunctions obtained in position and momentum space, respectively.

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