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Hydrogen atom in phase space: the Wigner representation

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Abstract

The hydrogen atom is a fundamental exactly soluble system for which the Wigner function, being a quantum analogue of the joint probability distribution of position and momentum, is unknown. In this paper, we present an effective method of calculating the Wigner function, for all bound states of the nonrelativistic hydrogen atom. The formal similarity between the eigenfunctions of the nonrelativistic hydrogen atom in the momentum representation and the Klein–Gordon propagator has allowed the calculation of the Wigner function for an arbitrary bound state of the hydrogen atom, using a simple atomic integral as a generator. These Wigner functions for some low-lying states are depicted and discussed.

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(Some figures in this article are in colour only in the electronic version)

Due to the discovery of quantum phase space tomography, Wigner functions have been experimentally reconstructed for quantum states of light, vibrational modes of molecules and superpositions of diffracted cold atoms by a double slit [1]. It has been discovered recently that the phase space plots of the Wigner function provide a unique visualization of the quantum state that can unravel such unique quantum properties like entanglement of correlated systems [2] or the phase space sub-Planck structures of quantum interference [3]. Because of all these reasons an analytical formula for the Wigner function, of such a fundamental system like the hydrogen atom, can be useful for quantum tomography, quantum state diagnostic and phase space visualization of negative structures of quantum interference.

However, despite the existence of analytical expressions for the hydrogen atom wavefunctions in position and momentum representations [4], the form of the phase space Wigner function is unknown. Analytical formula for the Wigner function is not even known

for the 1s state of the hydrogen atom. In the literature one can find only a limited number of papers devoted to this subject that are based on approximate methods [5, 6], and the only other published result has generated controversies [7]. In a different context, the hydrogen atom has been investigated recently using the Kirkwood–Rihaczek phase space representation, which is easier because it involves only products of the momentum and position wavefunctions with a proper phase [8]. This rather vexing situation regarding the analytical form of Wigner functions for the hydrogen atom indicates that the calculation of the phase space representation for the hydrogen requires a new approach based on a new method or a calculational trick to overcome the old difficulties.

It is the purpose of this paper to present an analytical computational scheme for the calculation of the phase space Wigner function for arbitrary bound-energy eigenfunction of the hydrogen atoms in terms of a set of generating differential operators acting on a simple single integral. This general ‘hydrogen atom integral’ (HAI), dependent on the Bohr radius and other geometrical parameters of the hydrogen eigenfunction, can be easily calculated numerically.

It happens that the methods of investigating integrals, similar to the one defining the Wigner function for the bound states of hydrogen atom, are known, but have been used in an entirely different physical context. Surprisingly, the integrals defining the Wigner function for the states of the hydrogen atom are formally nearly the same as ‘two-centre integrals’ investigated in the theory of charge exchange during hydrogen–proton collisions. Such integrals have been studied for collisions of other heavy particles. In [9], a very general and effective method of reducing ‘two-centre integrals’ to a single integral has been introduced. In the papers that followed, this method has been developed further [10–12]. Methods introduced in the theory of charge exchange in the hydrogen–proton collisions, especially numerical methods of calculations of ‘two-centre integrals’, can be used for obtaining the Wigner function. However, our method of reducing the calculation of the Wigner function to a single integral does not use these results and has a more direct character. The technical tricks in our method are closer in spirit to the techniques used in [13]. It is also worth noting that we calculate slightly different integrals, as in our case there are no $\frac{1}{r}$ factors coming from the interaction term of hydrogen–proton scattering Hamiltonian essential in the integrals investigated in [9–13]. Moreover, despite formal similarities, we solve an entirely different physical problem. We believe that the results presented in this paper after some modifications may be adapted for investigations of hydrogen–proton collisions with more complicated configurations (hyperbolic trajectory of motion, etc)

The paper is constructed in the following way: first we present a general formula that reduces the Wigner function of the bound states of the hydrogen atom to a single integral. Using this formula we calculate the Wigner function for the following bound states: 1s, 2s, 2p₀, 2p₁. Then we present more details of the calculation leading to the formula for the Wigner function of bound hydrogen atom states as a single integral. We derive the hydrogen atom integral (HAI) and describe a method allowing the calculation of the Wigner function for an arbitrary hydrogen atom bound states Ψ_{nlm} from this integral.

Phase space description, namely the Wigner function of a state, provides a natural generalization of joint position and momentum distribution. The Wigner function corresponding to a state vector $|\psi\rangle$ (for $\hbar = 1$) is defined as follows [14]:

$$\begin{aligned} W_{\psi}(\vec{r}, \vec{k}) &= \int \frac{d^3q}{(2\pi)^3} \psi^*(\vec{r} + \vec{q}/2) e^{i\vec{q}\vec{k}} \psi(\vec{r} - \vec{q}/2) \\ &= \int \frac{d^3q}{(2\pi)^6} \tilde{\psi}^*(\vec{k} + \vec{q}/2) e^{-i\vec{q}\vec{r}} \tilde{\psi}(\vec{k} - \vec{q}/2). \end{aligned} \quad (1)$$

In this formula we have exhibited the symmetry of the Wigner function with respect to position $\psi(\vec{r})$ and momentum $\tilde{\psi}(\vec{k})$ representations of the state vector. As it is well known the Wigner function for most quantum states can take negative values and is bounded to the interval $\frac{1}{\pi^3}[-1, 1]$, with marginals in \vec{r} and \vec{k} corresponding to momentum (wave vector with $\hbar = 1$) and position quantum probability distributions. In the classical limit the Wigner function becomes a classical phase space distribution. These and other properties of the Wigner function with its applications in various branches of physics have been reviewed in a number of articles and books [15–17]. It is well known that Wigner function given by equation (1) can be easily calculated, analytically or numerically, for most one-dimensional systems. In the case of three-dimensional problems, especially the ones with spherical symmetry, calculations are usually much more difficult. Integrals become quite cumbersome and in most cases impossible to handle analytically.

Before we present the outline of the technical features of our general approach, we first summarize the main results and illustrate the power of our method showing for the first time exact phase space plots of the hydrogen in the Wigner representation. The main result of our paper can be written in the form of the following formula for the phase space Wigner function for the hydrogen energy eigenvectors of bound states:

$$W_{\psi_{nlm}}(\vec{r}, \vec{k}) = \mathbb{D}_{nlm} \left(\frac{\partial}{\partial \vec{r}}, \frac{\partial}{\partial b_1}, \frac{\partial}{\partial b_2} \right) I(r, k, \vec{r}\vec{k}, b_1, b_2) \Big|_{b_1=b_2=1/na}. \quad (2)$$

The form of this HAI is

$$I(r, k, \vec{r}\vec{k}, b_1, b_2) = \int_0^1 du \exp(4iu\vec{r}\vec{k}) \frac{1}{C(u)} \exp(-2rC(u)) \quad (3)$$

where

$$C(u) = \sqrt{ub_1^2 + (1-u)b_2^2 + 4u(1-u)k^2}. \quad (4)$$

The HAI depends on three scalars only: $r = |\vec{r}|$, $k = |\vec{k}|$ and $\vec{r}\vec{k} = rk \cos \theta$. The two arbitrary running parameters b_1 and b_2 are determined at the end of the calculations only by $1/na$, where n is the principal quantum number and a is the Bohr radius. Formula (3) is the central result of our paper. It can be used to generate the Wigner function for an arbitrary hydrogen energy eigenfunction. The HAI plays a role of a generating function for all Wigner functions of the hydrogen atom. Differential operators \mathbb{D}_{nlm} acting on HAI give Wigner functions for all bound states of hydrogen atom.

Before we explain how this central result has been obtained, we write the formula for the Wigner function of the ground state:

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2e^{-2i\vec{k}\vec{r}}}{\pi^3 a^3} \frac{\partial^2}{\partial(b_1^2)\partial(b_2^2)} I(r, k, \vec{r}\vec{k}, b_1, b_2) \Big|_{b_1=b_2=1/a}. \quad (5)$$

One can perform all the derivatives and write the Wigner function as a single integral, but this lengthy formula is rather useless for this paper, thus we omit it. We note that the Wigner function for the ground state depends only on three scalars r , k and θ . A very simple numerical calculations of the HAI leads to the Wigner function for the ground state.

In figure 1, we have depicted contours of $4\pi r^2 k^2 W_{\psi_{100}}(r, k, \theta)$ for selected values of θ . In all figures, we have fixed the scale setting the Bohr radius $a = 1$. These figures should be compared with the only published numerical results obtained 22 years ago in [5]. In figure 2, we have depicted the same function $W_{\psi_{100}}(r, k, \theta)$ multiplied by factor $r^2 k^2$ for $\theta = 0$ and $\theta = \frac{\pi}{2}$. We see explicitly regions of the phase space where the Wigner function is non-positive. In the case of $\vec{r} \perp \vec{k}$, corresponding to $\theta = \frac{\pi}{2}$, the motion corresponds to a classical orbit,

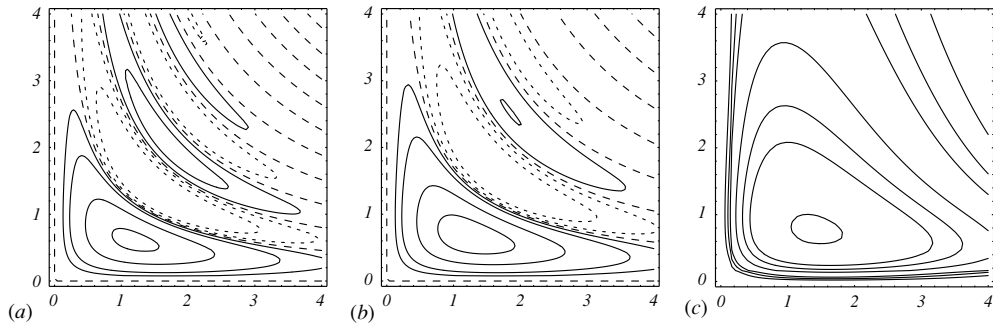


Figure 1. The Wigner function of 1s state multiplied by a factor $4\pi r^2 k^2$. Contour plots to be compared with those from [5]. Cross sections made for: (a) $\theta = 0$; (b) $\theta = \frac{\pi}{4}$; (c) $\theta = \frac{\pi}{2}$. Dashed lines denote a zero level, dotted lines denote negative values, separate distance between the contours is chosen as in [5].

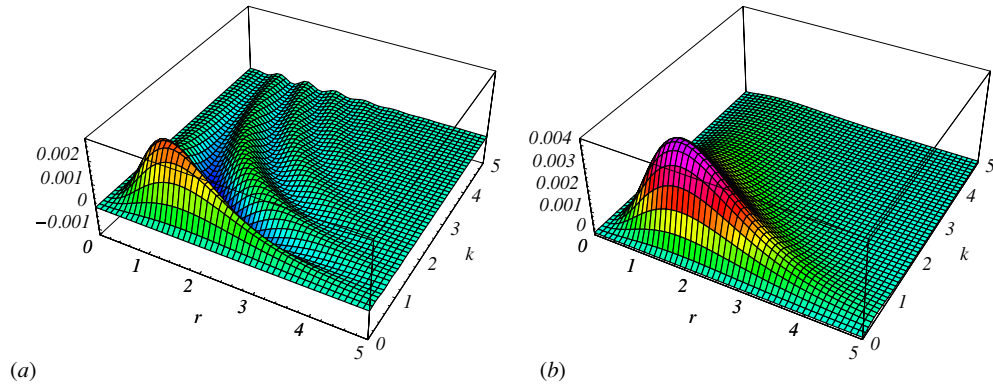


Figure 2. The Wigner function of 1s state multiplied by a factor $r^2 k^2$: (a) $\theta = 0$; (b) $\theta = \pi/2$. Only the cross section obtained for $\theta = \frac{\pi}{2}$ is a positive function, for all others values of the angle between position and momentum vectors cross sections have negative values. For $\theta = 0$, we see explicitly an oscillating structure.

and as a result of this the Wigner function is positive everywhere. For $\vec{r} \parallel \vec{k}$, corresponding to $\theta = 0$, the Wigner function exhibits non-classical features at distances of several Bohr radii.

The power of our method can be exhibited further if higher states of the hydrogen atom are considered. Below we just quote the corresponding differential operators for the 2s state:

$$\mathbb{D}_{200} = -\frac{e^{-2i\vec{k}\vec{r}}}{4\pi^3 a^3} \left[\frac{\partial}{\partial b_1} - b_1 \frac{\partial^2}{\partial b_1^2} \right] \left[\frac{\partial}{\partial b_2} - b_2 \frac{\partial^2}{\partial b_2^2} \right], \quad (6)$$

where after all the calculations we put $b_1 = b_2 = 1/2a$. With a little patience or help from a symbolic software all the differentiations of the HAI can be performed, and a close form expression for the Wigner function $W_{\psi_{200}}(r, k, \theta)$ from equation (2) can be calculated and plotted.

In figure 3, contour plots of the 2s Wigner function for various values of θ are presented. Again, the oscillations of the Wigner function and its negative values are clearly seen.

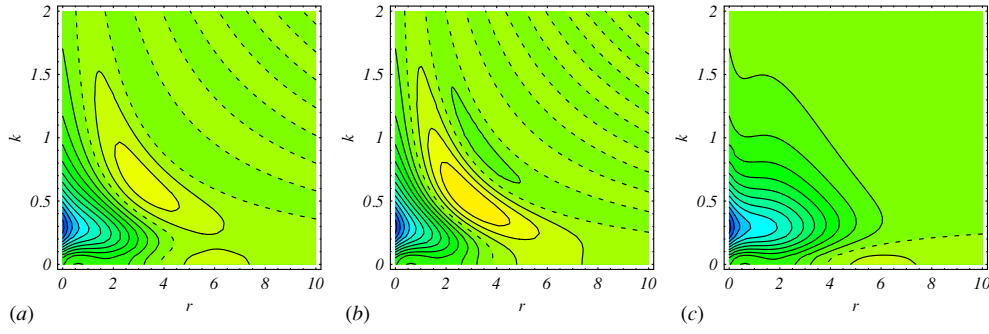


Figure 3. The Wigner function of the 2s state. Cross sections made for: (a) $\theta = 0$; (b) $\theta = \frac{\pi}{4}$; (c) $\theta = \frac{\pi}{2}$. Dashed lines denote a zero level. Other contours are separated by 0.01.

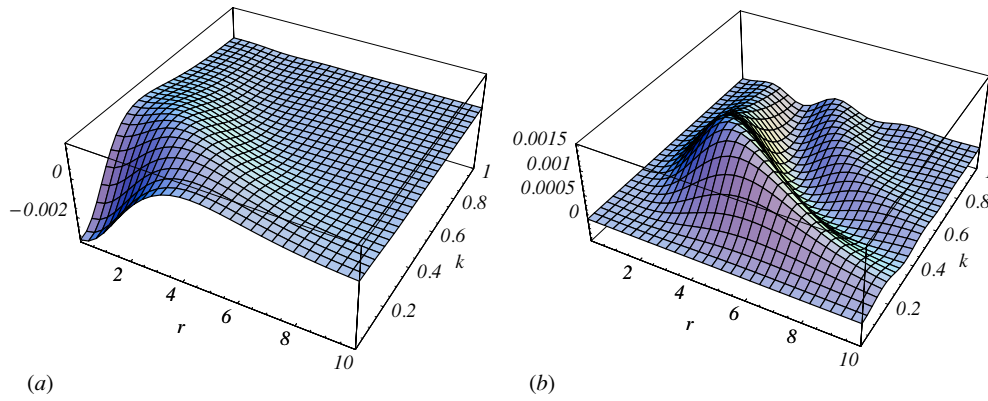


Figure 4. The Wigner function of 2p₀ state: Plot (a) presents the Wigner function for $\theta_1 = \theta_2 = 0$; plot (b) shows the same cross section of the Wigner function multiplied by $r^2 k^2$.

The next example that we want to present in this paper is the 2p₀ state. In this case,

$$\mathbb{D}_{210} = \frac{2 \exp(2i\vec{r}\vec{k})}{(2\pi)^3 a^5} \left(\frac{\partial}{\partial b_1} \frac{1}{2b_1} \frac{\partial}{\partial b_1} \right) \left(\frac{\partial}{\partial b_2} \frac{1}{2b_2} \frac{\partial}{\partial b_2} \right) \left(\frac{\partial^2}{\partial z^2} + 4ik_z \frac{\partial}{\partial z} \right) e^{-4i\vec{r}\vec{k}}. \quad (7)$$

The form of this differential operator indicates that the corresponding Wigner function will depend on the scalars (r, k) and two solid angles describing the orientations of \vec{r} and \vec{k} . The Wigner function of the 2p₀ state is no longer a function of scalars r, k and $\vec{r}\vec{k}$, which is a consequence of the fact that the wavefunction of this state distinguishes the z axis. As in all previous cases, a closed-form expression for the Wigner function $W_{\psi_{210}}(\vec{r}, \vec{k})$ can be calculated and plotted. In figure 4, we show cross section of $W_{\psi_{210}}(r, k)$ for $\theta_1 = \theta_2 = 0$ and the corresponding $r^2 k^2 W_{\psi_{210}}(r, k)$ plot.

Finally, in figure 5 the Wigner function of 2p₁ state ($m = 1$) is shown. We have plotted the cross sections of $W_{\psi_{211}}(\vec{r}, \vec{k})$ for $\theta_1 = \theta_2 = \frac{\pi}{2}$, $\varphi_1 = 0$ and selected values of k as a function of r and φ_2 . These plots clearly show that the maxima of the Wigner function are reached for \vec{k} perpendicular to \vec{r} , which entirely agrees with classical intuition that angular momentum has the maximum value for such geometry. Thus, the semiclassical features begin to be visible already in the 2p state. Of course, the classical features are much more pronounced for larger n .

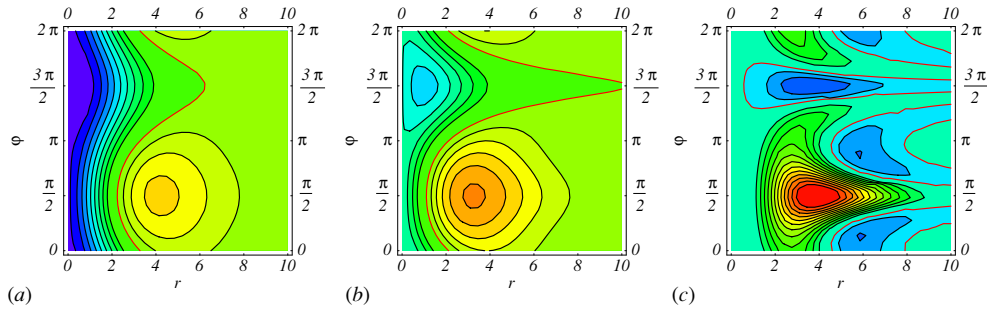


Figure 5. The Wigner function of $2p_1$ state (we have chosen $\theta_1 = \theta_2 = \frac{\pi}{2}$, $\varphi_1 = 0$). Red lines (light grey in black and white pictures) denote a zero level. Plots (a) and (b) show cross section of the Wigner function for fixed values of momentum $k = 0.1$ and $k = 0.2$, respectively. On the axes are r and the angle between \vec{r} and \vec{k} . It is seen that maximum is obtained when position and momentum vectors are perpendicular, which agrees with classical intuition that angular momentum has the maximum value for such geometry. Plot (c) presents similar cross section of the Wigner function multiplied by $r^2 k^2$ for $k = 0.5$. As we would expect maximum is obtained for $\varphi_2 = \frac{\pi}{2}$ and $r \simeq 4$.

In the remaining part of this paper, we illustrate the general calculational scheme explicitly showing how one can calculate the Wigner function for the ground state of the hydrogen atom. From our derivation it will be clear that the method is general and can be applied to all bound states of the hydrogen atoms. Although most of the calculations for higher excited states look tedious, simple symbolic differentiation of the fundamental HAI formula leads to explicit expression for the Wigner function with arbitrary quantum numbers.

We have found useful for our calculations to work with wavefunctions in momentum representation [4]. For the wavefunction of the ground state, we have

$$\tilde{\psi}_{100}(\vec{k}) = \frac{8\sqrt{\pi}a^3}{(1+k^2a^2)^2}. \quad (8)$$

It is a regular function that for large k decreases as $(ka)^{-4}$. Inserting this expression into the definition of the Wigner function in the momentum representation, equation (1), we obtain

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2^9 \pi a}{(2\pi a)^6} \int d^3 q \frac{\exp(-2i\vec{r}(\vec{q} - \vec{k}))}{\left[\left(\frac{1}{a^2} + q^2\right)\left(\frac{1}{a^2} + (\vec{q} - 2\vec{k})^2\right)\right]^2}. \quad (9)$$

The power of q in the denominator can be reduced with the help of differentiation over parameters. The following expression for the Wigner function is obtained:

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2}{\pi^5 a^3} \frac{\partial^2}{\partial(b_1^2) \partial(b_2^2)} \int d^3 q \frac{\exp(-2i(\vec{q} - \vec{k})\vec{r})}{(b_1^2 + q^2)(b_2^2 + (\vec{q} - 2\vec{k})^2)}, \quad (10)$$

where b_1 and b_2 are the running parameters to be fixed by the Bohr radius at the end of all calculations. Now comes the key element of the calculation. We recognize that apart from the phase factor the structure of the integrand in equation (10) has a remarkable formal similarity to the product of two Klein–Gordon propagators of quantum field theory in momentum space [18]. Due to this analogy, we shall proceed with our calculations using the standard propagator disentanglement techniques introduced by Feynman and represented by the following identity:

$$\frac{1}{AB} = \int_0^1 du \frac{1}{[uA + (1-u)B]^2} \quad (11)$$

with $A = b_1^2 + q^2$ and $B = b_2^2 + (\vec{q} - 2\vec{k})^2$ to rearrange the integral in equation (10). After the rearrangement of terms and substitution $\vec{s} = \vec{q} - 2(1-u)\vec{k}$ we get

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2e^{2i\vec{k}\vec{r}}}{\pi^5 a^3} \frac{\partial^2}{\partial(b_1^2)\partial(b_2^2)} \int_0^1 du \int d^3s \frac{\exp[-2i(\vec{s} + 2(1-u)\vec{k})\vec{r}]}{[s^2 + ub_1^2 + (1-u)b_2^2 + 4(1-u)uk^2]^2}. \quad (12)$$

We recognize in this expression the function $C(u)$ introduced in equation (4). This simplifies the notation and the integral (12) then becomes

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2e^{2i\vec{k}\vec{r}}}{\pi^5 a^3} \frac{\partial^2}{\partial(b_1^2)\partial(b_2^2)} \int_0^1 du \exp(-4i(1-u)\vec{k}\vec{r}) \int d^3s \frac{\exp(-2i\vec{s}\vec{r})}{[s^2 + C(u)]^2}. \quad (13)$$

Fortunately, the integral over d^3s is elementary and as a result of all these steps the only remaining integral is over u . The final formula for the Wigner function is, thus, given by

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2e^{-2i\vec{k}\vec{r}}}{\pi^3 a^2} \frac{\partial^2}{\partial(b_1^2)\partial(b_2^2)} \int_0^1 du \exp(i4u\vec{k}\vec{r}) \frac{1}{C(u)} \exp(-2rC(u)) \quad (14)$$

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \mathbb{D}_{100} \left(\frac{\partial}{\partial \vec{r}}, \frac{\partial}{\partial b_1}, \frac{\partial}{\partial b_2} \right) I(r, k, \vec{r}\vec{k}, b_1, b_2) \Big|_{b_1=b_2=1/a},$$

as it has been advertized in equation (2).

This method works for arbitrary state of the hydrogen atom (for details see the appendix). The key concept in such calculations is to express a given state with quantum numbers (nlm) in momentum representation as a differential operator acting on the ground state followed by a change of scale. It is worth noting that these differential operators form an elegant group theoretical structure, explained for example in [19].

In conclusion, we have noted and exploited the formal similarity between the eigenfunctions of the nonrelativistic hydrogen atom in the momentum representation and the Klein–Gordon propagator. This allowed us to find and discuss the Wigner function for arbitrary bound state of hydrogen atom.

Acknowledgments

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Appendix

An arbitrary state of hydrogen atom in the momentum representation can be expressed as

$$\tilde{\psi}_{nlm}(\vec{k}) = \tilde{\psi}_{nlm} \left(\vec{k}, \frac{1}{na} \right)$$

where

$$\tilde{\psi}_{nlm}(\vec{k}, b) = A_{nlm} \mathbb{P}_m(\vec{k}) \mathbb{Z}_{lm}(\vec{k}) \mathbb{B}_{nl}(b) \left[\frac{1}{b^2 + \vec{k}^2} \right], \quad (A1)$$

operators $\mathbb{B}_{nl}(b)$, $\mathbb{P}_m(\vec{k})$ and $\mathbb{Z}_{lm}(\vec{k})$ are defined as

$$\mathbb{B}_{nl}(b) := \sum_{\alpha=0}^{n-l-1} \frac{1}{\alpha!} \left(\frac{2Z}{na} \right)^\alpha \binom{n+l}{\alpha+2l+1} \left(\frac{\partial}{\partial b} \right)^{\alpha+1}, \quad (A2)$$

$$\mathbb{P}_m(\vec{k}) := \left(\frac{\partial}{\partial k_x} + i \operatorname{sgn}(m) \frac{\partial}{\partial k_y} \right)^{|m|}, \quad (\text{A3})$$

$$\mathbb{Z}_{lm}(\vec{k}) := \sum_{\beta=g(l+|m|)}^l \frac{(-1)^\beta (2\beta)!}{(2\beta-l-|m|)!} \binom{l}{\beta} \left(\frac{\partial^2}{\partial k_1^2} + \frac{\partial^2}{\partial k_2^2} + \frac{\partial^2}{\partial k_3^2} \right)^{(l-\beta)} \left(\frac{\partial}{\partial k_z} \right)^{2\beta-l-|m|}, \quad (\text{A4})$$

$$g^{(m+l)} = \begin{cases} \frac{l+|m|}{2} & \text{for } (l+|m|) \in 2\mathbb{N} \\ \frac{l+|m|+1}{2} & \text{for } (l+|m|) \in (2\mathbb{N}+1), \end{cases} \quad (\text{A5})$$

and the normalization constant A_{nlm} is given by

$$A_{nlm} = -4\pi \left(\frac{i}{a} \right)^l \frac{(-1)^{\frac{3|m|-m+2l}{2}} \left(\frac{2Z}{an} \right)^{3/2} \left(\frac{2Z}{n} \right)^l}{2^l l! (2l+1)! \binom{n+l}{2l+1}} \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!} \left[\frac{(n+l)!}{2n(n-l-1)!} \right]^{1/2}}. \quad (\text{A6})$$

Following the method of calculation described in the main text of the paper and making use of formula (A1) the Wigner function of hydrogen atom state ψ_{nlm} can be written as

$$W_{\psi_{nlm}}(\vec{r}, \vec{k}) = \frac{e^{2i\vec{r}\vec{k}}}{8\pi^4} \left[A_{nlm} \mathbb{B}_{nl}(b_1) \mathbb{O}_{lm} \left(-\frac{i}{2} \frac{\partial}{\partial \vec{r}}, b_1 \right) \right]^* \left[A_{nlm} \mathbb{B}_{nl}(b_2) \mathbb{O}_{lm} \left(-\frac{i}{2} \frac{\partial}{\partial \vec{r}}, b_2 \right) \right] \\ \times \left[e^{-4i\vec{r}\vec{k}} \int_0^1 du \frac{e^{-2rC(u)+4iu\vec{r}\vec{k}}}{C(u)} \right]_{b_1=b_2=1/na}, \quad (\text{A7})$$

where operator \mathbb{O}_{lm} is defined as

$$\mathbb{O}_{lm} \left(-\frac{i}{2} \frac{\partial}{\partial \vec{r}}, b \right) = \sum_{\gamma=0}^{|m|} \binom{|m|}{\gamma} (i \operatorname{sgn}(m))^\gamma \sum_{\beta=g_{lm}}^l \frac{(-1)^\beta (2\beta)!}{(2\beta-l-|m|)!} \binom{l}{\beta} \\ \times \sum_{\eta=0}^{l-\beta} \binom{l-\beta}{\eta} \sum_{\rho=0}^{\eta} \binom{\eta}{\rho} \mathbb{U}_{l-2\eta-|m|} \left(-\frac{i}{2} \frac{\partial}{\partial r_3}, \frac{1}{b} \frac{\partial}{\partial b} \right) \mathbb{U}_{2\rho+\gamma} \\ \times \left(-\frac{i}{2} \frac{\partial}{\partial r_2}, \frac{1}{b} \frac{\partial}{\partial b} \right) \mathbb{U}_{2(\eta-\rho)+|m|-\gamma} \left(-\frac{i}{2} \frac{\partial}{\partial r_1}, \frac{1}{b} \frac{\partial}{\partial b} \right), \quad (\text{A8})$$

and operator \mathbb{U}_N is given by

$$\mathbb{U}_N \left(-\frac{i}{2} \frac{\partial}{\partial r_j}, \frac{1}{b} \frac{\partial}{\partial b} \right) = \sum_{\alpha=0}^{\lfloor N/2 \rfloor} \frac{N!}{\alpha! (N-2\alpha)! 2^\alpha} \left(-\frac{i}{2} \frac{\partial}{\partial r_j} \right)^{N-2\alpha} \left(\frac{1}{b} \frac{\partial}{\partial b} \right)^{N-\alpha}. \quad (\text{A9})$$

Similarly, the following formula can be introduced:

$$W_{(nlm|n'l'm')}(\vec{r}, \vec{k}; b_1, b_2) = \int \frac{d^3q}{(2\pi)^6} \tilde{\psi}_{nlm}^*(\vec{k} + \vec{q}/2, b_1) e^{-i\vec{q}\vec{r}} \tilde{\psi}_{n'l'm'}(\vec{k} - \vec{q}/2, b_2) \\ = \frac{e^{2i\vec{r}\vec{k}}}{8\pi^4} \left[A_{nlm} \mathbb{B}_{nl}(b_1) \mathbb{O}_{lm} \left(-\frac{i}{2} \frac{\partial}{\partial \vec{r}}, b_1 \right) \right]^* \left[A_{n'l'm'} \mathbb{B}_{n'l'}(b_2) \mathbb{O}_{l'm'} \left(-\frac{i}{2} \frac{\partial}{\partial \vec{r}}, b_2 \right) \right] \\ \times \left[e^{-4i\vec{r}\vec{k}} \int_0^1 du \frac{e^{-2rC(u)+4iu\vec{r}\vec{k}}}{C(u)} \right]$$

for the calculation of the Wigner function for linear superpositions of hydrogen atom states.

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