Hydrogen atom in phase space: The Wigner representation

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(Dated: November 7, 2018)

Abstract

We have found an effective method of calculating the Wigner function, being a quantum analogue of joint probability distribution of position and momentum, for bound states of nonrelativistic hydrogen atom. The formal similarity between the eigenfunctions of nonrelativistic hydrogen atom in the momentum representation and Klein-Gordon propagators has allowed the calculation of the Wigner function for an arbitrary bound state of the hydrogen atom. These Wigner functions for some low lying states are depicted and discussed.
There are many ways to visualize quantum states of a single particle. Wave functions in position representation are a natural tool to present probability distribution in the configuration space. On the other hand it is easier to visualize momentum distribution if the momentum representation of the wave function is used. Phase space description, namely Wigner function of a state, provides a natural generalization of joint position and momentum distribution. Wigner function corresponding to a state described by wave function $\psi(\vec{r})$ is defined as follows [1]:

$$ W_\psi(\vec{r}, \vec{k}) = \int \frac{d^3q}{(2\pi)^3} \psi^*(\vec{r} + \vec{q}/2) e^{i\vec{q}\cdot\vec{k}} \psi(\vec{r} - \vec{q}/2) $$

As it is well known the Wigner function for most quantum states is non-positive and bounded to an interval $\frac{1}{\pi}[-1, 1]$, with marginals in $\vec{r}$ and $\vec{k}$ corresponding to momentum (wave-vector) 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 [2].

It is well known that Wigner function given by Eq. (1) can be easily calculated, analytically or numerically, for most of one dimensional systems. In 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. Despite the existence of analytical expressions for the hydrogen atom wave functions in position and momentum representations [3], 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 [4, 5], and some of the published results have been achieved using some kind of approximate methods that have generated controversies [6]. In a different context, the hydrogen atom has been investigated recently using the Kirkwood-Rihaczek phase space representation, which is easy because it involves only products of the momentum and position wave functions with a proper phase [7].

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 [8]. 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 [9] or the phase sub-Planck structures of quantum interference [10]. Because of all these reasons an analytical formula for the phase space 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.

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 Letter 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.

Before we present the outline of the technical features of the general approach, we first summarize our main results, and illustrate the power of our methods 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:

$$W_{\psi_{nlm}}(\vec{r},\vec{k}) = D_{nlm} \left( \frac{\partial}{\partial \vec{k}}, \frac{\partial}{\partial b_1}, \frac{\partial}{\partial b_2} \right) I(r, k, \vec{r}\vec{k}, b_1, b_2) \bigg|_{b_1=b_2=1/na} .$$

(2)

In this formula $D_{nlm}$ is a linear differential operator reproducing the Wigner function for all hydrogen states from a simple hydrogen atom integral (HAI) defined below by Eq. (3). The HAI depends on three scalars only: $r = |\vec{r}|$, $k = |\vec{k}|$ and $r\vec{k} = rk \cos \theta$. 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. The form of this HAI is

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

(3)

where

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

(4)

The formula 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 $D_{nlm}$ 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 down the formula for the Wigner function of the ground state. For the 1s state this operator reads:

$$D_{100} = \frac{2e^{-2i\vec{k}\vec{r}}}{\pi^3a^3} \frac{\partial^2}{\partial(b_1^2)\partial(b_2^2)}$$

(5)

and the corresponding Wigner function (2) is

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

(6)

We can perform all the derivatives and write the Wigner function as a single integral, but this lengthy formula is rather useless for this letter, and we omit it. We note that the Wigner function for the ground state depends only on three scalars $r, k$ and $\theta$. 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 $4\pi r^2 k^2 W_{100}(r, k, \theta)$ for selected values of $\theta$. These figures should be compared with the only published numerical results obtained 22 years ago in reference [4]. In the following Figure (2) we have depicted the same function $W_{100}(r, k, \theta)$ multiplied by factor $r^2 k^2$ for $\theta = 0$ and $\theta = \pi/2$. We see explicitly regions of the phase space where the Wigner function is non-positive.
\( \theta = 0 \)
\( \theta = \pi/4 \)
\( \theta = \pi/2 \)

FIG. 1: 1s state: \( 4 \pi r^2 k^2 W_{1s}(\vec{r}, \vec{k}) \). Contour plots to be compared with those from reference \[4\]. Dashed lines denote a zero-level, dotted lines denote negative values, separate distance between the contours are chosen as in \[4\].

\( \theta = 0 \)
\( \theta = \pi/2 \)

FIG. 2: The Wigner function of 1s state multiplied by factor \( r^2 k^2 \). Only the cross-section for \( \theta = \pi/2 \) 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.

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:

\[
D_{200} = -\frac{e^{-2i\vec{r} \cdot \vec{k}}}{4\pi^2 a^3} \left[ \frac{\partial}{\partial b_1} - b_1 \frac{\partial^2}{\partial b_1^2} \right] \left[ \frac{\partial}{\partial b_2} - b_2 \frac{\partial^2}{\partial b_2^2} \right] \tag{7}
\]

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 Eq. \( \text{(2)} \) can be calculated and plotted. In Figure \( \text{(3)} \) we present contour plots of the 2s Wigner function for various values of \( \theta \). Again, the negative values of the Wigner function are clearly seen.

The next example that we want to present in this paper is the 2p\textsubscript{0} state. In this case

\[
D_{210} = \frac{2 \exp(2i\vec{r} \cdot \vec{k})}{(2\pi a)^5} \left( \frac{\partial}{\partial b_1} \frac{1}{2b_1} \frac{\partial}{\partial b_1} \right) \left( \frac{\partial}{\partial b_2} \frac{1}{2b_2} \frac{\partial}{\partial b_2} \right) \left( \frac{\partial^2}{\partial z^2} + 4i k z \frac{\partial}{\partial z} \right) e^{-4i\vec{r} \cdot \vec{k}}. \tag{8}
\]
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 \( 2p_0 \) state is no longer a function of scalars \( r^2, p^2 \) and \( r\vec{k} \) is a consequence of the fact that the wave function of this state distinguishes the \( z \) axis. As in all previous cases a close form expression for the Wigner function \( W_{\psi_{210}}(r, k) \) 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 \( r^2k^2W_{\psi_{210}}(r, k) \) plot.

Finally, in the Figure \( (5) \) the Wigner function of \( 2p \) state with \( m = 1 \) is shown. We have plotted the cross-sections of \( W_{\psi_{211}}(r, k) \) for \( \theta_1 = \theta_2 = \frac{\pi}{2}, \varphi_1 = 0 \) and selected values of \( k \) as a function of \( r \) and \( \varphi_2 \). These plots show clearly 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 \( n \).

In the remaining part of this Letter we illustrate the general calculational scheme showing explicitly 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 the Wigner function with arbitrary quantum numbers.
a) FIG. 4: The Wigner function of $2p_0$ state: Plot a) presents the Wigner function for $\theta_1 = \theta_2 = 0$; b) shows the same cross-section with the Wigner function is multiplied by $r^2k^2$.

b) FIG. 5: The Wigner function of $2p_1$ state (we have chosen $\theta_1 = \theta_2 = \frac{\pi}{2}$, $\varphi_1 = 0$). Red line denotes 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 $r^2k^2$ for $k = 0.5$. As we would expect maximum is obtained for $\varphi = \frac{\pi}{2}$ and $r \approx 4$.

We have found useful for our calculations to work with wave functions in momentum representation. For the wave function of the ground state we have:

$$\tilde{\psi}_{100}(\vec{k}) = \frac{8\sqrt{\pi}a^3}{(1+k^2a^2)^2}$$  \hspace{1cm} (9)

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, Eq. (1), we obtain:

$$W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2^9\pi a}{(2\pi a)^6} \int d^3q \frac{\exp(-2i\vec{r}(\vec{q} - \vec{k}))}{[(\frac{1}{a^2} + q^2)(\frac{1}{a^2} + (\vec{q} - 2\vec{k})^2)]^{3}}.$$  \hspace{1cm} (10)

The power of $q$ in the denominator can be reduced with the help of differentiation over
The Wigner function is given by:

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

(11)

where \(b_1\) and \(b_2\) are 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 of the phase factor, the structure of the integrand in Eq. (11) has a remarkable formal similarity to the product of two Klein-Gordon propagators of quantum field theory in momentum space [11]. 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

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

(12)

with \(A = b_1^2 + q^2\) and \(B = b_2^2 + (\vec{q} - 2\vec{k})^2\) to rearrange the integral in Eq. (11). The integral becomes:

\[
W_{\psi_{100}}(\vec{r}, \vec{k}) = \frac{2}{\pi^3 a^3} \frac{\partial^2}{\partial(b_1^2) \partial(b_2^2)} \int_0^1 du \times \int d^3q \frac{\exp[-2i(\vec{q} - \vec{k}) \vec{r}]}{[u(b_1^2 + q^2) + (1-u)(b_2^2 + (\vec{q} - 2\vec{k})^2)]^2}.
\]

(13)

After rearrangement of terms and substitution: \(s = \vec{q} - 2(1-u)\vec{k}\) we get

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

(14)

We recognize in this expression the function \(C(u)\) introduced in Eq. (12). This simplifies the notation and the integral (14) then becomes:

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

(15)

Fortunately, the integral over \(d^3s\) is elementary, we can use the following formula:

\[
\int d^3s \frac{\exp(-2i\vec{s}\vec{r})}{[s^2 + C(u)^2]^2} = \frac{\pi^2}{C(u)} \exp(-2rC(u)).
\]

(16)

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:

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

\[
W_{\psi_{100}}(\vec{r}, \vec{k}) = \bar{D}_{100} \left( \frac{\partial}{\partial k}, \frac{\partial}{\partial b_1}, \frac{\partial}{\partial b_2} \right) I(r, k, \vec{r}, \bar{k}, b_1, b_2) |_{b_1=b_2=1/a}.
\]

(17)
as it has been advertised in Eq. \[2\].

This method works for arbitrary state of the hydrogen atom. 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 in e.g. \[12\].

In conclusion, we have found and exploit formal similarity between the eigenfunctions of nonrelativistic hydrogen atom in the momentum representation and Klein-Gordon propagators. This allowed us to find and discussed the Wigner function for arbitrary bound state of hydrogen atom.

Acknowledgement
L. P. thanks prof. Schleich for his encouragement and an interesting discussion.

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