Hydrogen atom in phase space. The Kirkwood-Rihaczek representation

L. Praxmeyer,\textsuperscript{1} and K. Wódkiewicz\textsuperscript{1,2}

\textsuperscript{1}Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland
\textsuperscript{2}Department of Physics and Astronomy, University of New Mexico, 800 Yale Blvd. NE, Albuquerque, NM 87131 USA

(Dated: 16 December 2002)

We present a phase-space representation of the hydrogen atom using the Kirkwood-Rihaczek distribution function. This distribution allows us to obtain analytical results, which is quite unique because an exact analytical form of the Wigner functions corresponding to the atom states is not known. We show how the Kirkwood-Rihaczek distribution reflects properties of the hydrogen atom wave functions in position and momentum representations.

PACS numbers: 03.65.Ca

I. INTRODUCTION

The Wigner function \cite{1}, which was introduced in 1932, is up to now the most commonly used phase space quasi-distribution representation of physical systems in momentum and position representations. This function fully characterizes the quantum state and gives basic physical intuition about the investigated state. Moreover, there are some simple physical properties that make this function unique \cite{2}. Nevertheless, over the years many others quasi-distributions have been introduced and studied. Especially well-known are functions from the Glauber and Cahill s-parameterized class of distributions \cite{3} containing the Wigner function, the Glauber-Sudarshan $P$-representation \cite{4,5}, and the Husimi or the $Q$-representation \cite{6}.

For many systems the Wigner function is well known and has been carefully studied, but there are some elementary quantum mechanical states, for which this phase space representation is not known. An example of such system is the hydrogen atom. No exact analytical formula of the Wigner function is known even for the 1s state. In the literature one can find a limited number of papers devoted to this subject \cite{7,8,9,10}, and all the published results have been achieved using methods of approximation.

It is the purpose of this short communication to present an analytical phase space representation of the hydrogen atom using a lesser-known Kirkwood–Rihaczek (K-R) distribution function \cite{11}. Its form allows us to obtain analytical results, and as we have shown in \cite{12} this distribution, like the Wigner function, fully characterizes a quantum state.

II. DIFFERENT QUASI-DISTRIBUTION AND OPERATOR ORDERING

In general, the problem of defining a joint probability function in phase space lies in the operator ordering. Because different orderings of position $\hat{q}$ and momentum $\hat{p}$ operators are not equivalent, the association of the quantum operator with classical functions has no unique solution. The association of classical phase space functions $A(q, p)$ with quantum operators is shown by:

$$\{\hat{A}(\hat{q}, \hat{p})\}_{\text{ordering}} = \iint dqdp A(q, p) \{\delta(q - \hat{q})\delta(p - \hat{p})\}_{\text{ordering}},$$

The Fourier decomposition of the Dirac delta functions makes it possible to rewrite the above equation in the form

$$\{\delta(q - \hat{q})\delta(p - \hat{p})\}_{\text{ordering}} = \frac{1}{(2\pi\hbar)^2} \iint dq' dp' e^{i\frac{q'q}{\hbar}} e^{i\frac{p'p}{\hbar}} \{e^{i\frac{q'q}{\hbar}} e^{-i\frac{p'p}{\hbar}}\}_{\text{ordering}}.$$

For every operator ordering there exists a corresponding probability quasi-distribution in phase space.
The Wigner distribution function is obtained by taking a quantum average of the above formula with the respect to the Wigner-Weyl ordering:

\[
W(q, p) = \langle \Psi \mid \{ \delta(q - \hat{q}) \delta(p - \hat{p}) \} W \mid \Psi \rangle = \frac{1}{(2\pi\hbar)^2} \int dq' dp' e^{i\frac{(q'q - p'p)}{\hbar}} \langle \Psi \mid e^{i\frac{(\hat{q}'\hat{q} - \hat{p}'\hat{p})}{\hbar}} \mid \Psi \rangle.
\]

in which \( \hat{q} \) and \( \hat{p} \) operators are put in the same exponent.

The K–R distribution function corresponds to an ordering called the anti-standard ordering, that is obtained by putting all \( \hat{p} \) operators on the left of all \( \hat{q} \) operators:

\[
K(q, p) = \langle \Psi \mid \delta(p - \hat{p}) \delta(q - \hat{q}) \mid \Psi \rangle = \frac{1}{(2\pi\hbar)^2} \int dq' dp' e^{i\frac{(q'q - p'p)}{\hbar}} \langle \Psi \mid e^{i\frac{\hat{q}'\hat{p}}{\hbar}} e^{-i\frac{\hat{p}'\hat{q}}{\hbar}} \mid \Psi \rangle.
\]

The complex conjugation of the K–R function corresponds to the standard ordering (all operators \( \hat{q} \) are on the left followed by \( \hat{p} \) operators), and the real part of the K–R distribution function is obtained by a symmetric superposition of the anti-standard and the standard ordering: \( \frac{1}{2} (q^n \hat{p}^m + \hat{p}^m q^n) \).

Obviously, the Wigner-Weyl ordering and the anti-standard ordering are not equivalent, so they lead to different quasi-distributions. But both of these orderings are intuitive and simple ones, and appropriate phase space distribution functions have the same marginal properties.

## III. THE WIGNER AND THE KIRKWOOD-RIHACZEK DISTRIBUTION FUNCTIONS

The definition of the famous Wigner quasi-distribution function was firstly presented as:

\[
W_\Psi(q, p) = \frac{1}{2\pi\hbar} \int \Psi^*(q + \xi/2) e^{i\frac{\pi}{\hbar} q} \Psi(q - \xi/2) d\xi.
\]

Although for most one dimensional systems formula (4) allows to evaluate the Wigner function relatively easily, in three dimensions this problem is more complicated. Integrals become quite cumbersome and sometimes impossible to handle analytically. As we have mentioned before, an analytical formula for the Wigner function is not known even for 1s state of hydrogen atom.

That is why, in order to investigate the hydrogen atom in phase space we shall use the K–R distribution. This function was introduced by Kirkwood just one year after Wigner introduced his function. Then, in 1968, the same function was rediscovered by Rihaczek in the context of signal time-frequency distributions and is known by his name in signal transmitting theory. The definition of the K–R function in terms of anti-standard ordering has a simple form:

\[
K(q, p) = \frac{1}{2\pi\hbar} \int d\xi \Psi^*(\xi) e^{i\frac{\pi}{\hbar} q} \Psi(q) = \frac{1}{2\pi\hbar} \Psi(q) e^{-i\frac{\pi}{\hbar} q} \Psi^*(p).
\]

Elsewhere we have presented an extensive analysis of the K–R distribution and its comparison with the Wigner distribution function. Here we will only mention the main properties of the K–R function. Similar to the Wigner function, the K-R distribution has the correct marginal properties:

\[
\int K(q, p) \, dp = |\Psi(q)|^2, \quad \int K(q, p) \, dq = \frac{1}{2\pi\hbar} |\Psi(p)|^2,
\]

which is a fundamental requirement for a joint distribution in phase space. Unlike the Wigner distribution, the K-R function is a complex function, and its operator form is not hermitian. Nevertheless, for an arbitrary quantum state the knowledge of the K-R distribution at every point of the phase space allows a full reconstruction of this state (see).
IV. HYDROGEN ATOM IN PHASE SPACE

The definition of the K-R distribution \([3]\) allows one to evaluate analytical formulas of this distribution for many complicated quantum mechanical states, for which the analytical expression of the Wigner function is not accessible.

In the following we will present analytical results obtained for states of the hydrogen atom. The wave functions of a non-relativistic hydrogen atom are well known, both in position and momentum representation. The Schrödinger equation with Coulomb potential can be separated in the spherical polar coordinates (see, e.g. \([14]\)). The solutions of angular part of the equation are given by the spherical harmonics \(Y_{lm}(\theta, \varphi)\), and of the radial part can be expressed in terms of Laguerre functions \(L^k_m\) (in the position representation):

\[
R_{nl}(r) = -\left[\frac{(n-l-1)!}{(n+l)!}\frac{1}{2^{l+1}(2n)^{l+1}}\right]^{1/2} \left(\frac{2Z}{n}\right)^l e^{-\frac{Zr}{n}} \left(\frac{2Zr}{n}\right)^l F_{n+l}^{2l+1} \left(\frac{2Zr}{n}\right),
\]

or Gegenbauer functions \(C^m_n\) (in the momentum representation):

\[
F_{nl}(p) = \left[\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!}\right]^{1/2} \frac{n^2}{(n^2p^2+1)^{l+1}} \frac{n!p^l}{(n^2p^2+1)^{l+2}} C_{n-l-1}^{l+1} \left(\frac{n^2p^2-1}{n^2p^2+1}\right).
\]

As usual, \(n, l, m\) denote principal, orbital, and magnetic quantum numbers, respectively.

Substituting the expressions \((7, 8)\) into the definition of the K-R distribution Eq. \((6)\), and inserting the angular relation, we obtain the general formulas for K-R functions of the hydrogen atom states. In the next Section we shall present graphical results obtained for selected hydrogen quantum numbers. It is worth noting that the absolute square of the K-R function:

\[
|K(r, \theta, \varphi, p, \theta', \varphi')|^2 = \frac{1}{(2\pi)^3} |R_{nl}(r)Y_{lm}(\theta, \varphi)|^2 |F_{nl}(p)Y_{lm}(\theta', \varphi')|^2.
\]

is proportional to the product of probability densities in position and momentum representations \((\hbar = 1)\). Thus, one can treat it as the cornerstone of the phase space analysis of physical systems.

V. EXAMPLES

Figures 1 to 5 present phase space K-R representation of 1s, 2s, 2p, 10m, and 10l states of the hydrogen atom. Let us note that for a 3-dimensional systems the K–R distribution is a function of 6 variables \((r, \theta, \varphi, p, \theta', \varphi')\), so a graphical phase space representation can only present selected cross-sections. We have decided to use the following method to represent the hydrogen atom in phase space: all the Figures labelled by (a), (b) (later called Fig. X.a, X.b) are auxiliary ones – they present hydrogen atom wave functions in position and momentum representation and the arrows depicted on those figures show the directions chosen for the cross-sections. The corresponding cross-sections of the K-R phase space functions are plotted in Figures labelled by (c) and (d) (Fig. X.c, X.d).

All the Figures are organized as follows: Fig X.a shows cross-section \(\varphi = \text{const}\) of the absolute square of hydrogen atom wave function in the position representation, i.e. \(|R_{nl}(r)Y_{lm}(\theta, \varphi)|^2\) which is the probability density of finding an electron at point \((r, \theta, \varphi)\) (and which does not depend on the value of \(\varphi\)). Fig. X.b shows cross-section \(\varphi' = \text{const}\) of the absolute square of the same wave function in the momentum representation, i.e. \(|F_{nl}(p)Y_{lm}(\theta', \varphi')|^2\) which is the probability density of finding an electron with momentum \((p, \theta', \varphi')\) (and here again, a cross-section does not depend on the value of \(\varphi'\)). The arrows depicted on the Fig. X.a, X.b show the directions chosen for the cross-sections of the corresponding K-R phase space functions that are presented in Fig. X.c, where the real part of the K–R distribution and appropriate contour plot are shown, and in Fig X.d, where the absolute value of this K–R distribution and its contour plot are plotted.

Let us first study the K-R function of the 1s state. Well-known solutions of the radial part of the Schrödinger equation are given by, in atomic unit:

\[
R_{10}(r) = 2e^{-r} \quad \text{(in the position representation, and)}
\]

\[
F_{10}(p) = \sqrt{\frac{2}{\pi (1+p^2)^3}} \quad \text{(in the momentum representation)}.
\]
Fig. 1.a shows spatial probability density \(| R_{10}(r)/(4\pi) |^2\) of finding an electron at certain point, and Fig. 1.b shows momentum probability density \(| F_{10}(p)/(4\pi) |^2\) of finding an electron with definite momentum. Note, that those are not radial distributions and they have nonzero values at \(r = 0\) and \(p = 0\) as the wave functions were not multiplied by \(r^2\) or \(p^2\) factors. The K-R distribution of 1s state is given by:

\[
K_{10}(r, \theta, \varphi, p, \theta', \varphi') = (2\pi^3)^{-\frac{1}{2}} \frac{e^{-r}}{(1 + p^2)^2} \exp(-ipr \cos \Theta),
\]

where \(\Theta\) denotes the angle between \(r\) and \(p\):

\[
\cos \Theta = \cos(\theta - \theta') + (\cos(\varphi - \varphi') - 1) \sin \theta \sin \theta'.
\]

Fig. 1.c shows the real part of Eq. (9), \(K_{Re\,1s}\), multiplied by \((2\pi)^3\):

\[
K_{Re\,1s} = (2\pi)^3 \text{Re}\left[ K_{10}\left(r, \frac{\pi}{2}, 0, p, \frac{\pi}{2}, 0\right)\right].
\]

The cross-section is chosen in the directions depicted by arrows in Fig. 1.a, 1.b. Next we have displayed its contour plot. The absolute value of Eq. (9) multiplied by \((2\pi)^3\) is:

\[
K_{Abs\,1s} = (2\pi)^3 \text{Abs}\left[ K_{10}\left(r, \frac{\pi}{2}, 0, p, \frac{\pi}{2}, 0\right)\right]
\]

and its contour plot is presented in Fig. 1.d. In this case, \(K_{Re}\) and \(K_{Abs}\) look quite similar mainly because the wave function both in position and momentum representation decreases rapidly with the increase of \(r\) or \(p\), and the oscillating \(\cos(rp)\)-like structure characteristic for the real part of K-R distribution is not clearly seen on the scale used to make these figures. These oscillations are merely marked in the contour plot of \(K_{Re\,1s}\) by dashed lines which correspond to \(K_{Re} = 0\).

Next we shall examine the K-R distribution of 2s and 2p states. Solutions of the radial part of the Schrödinger equation in momentum representation are given by:

\[
F_{20}(p) = \frac{32}{\sqrt{3\pi}} \frac{4p^2 - 1}{(1 + 4p^2)^2},
\]

\[
F_{21}(p) = \frac{128}{\sqrt{3\pi}} \frac{p}{(1 + 4p^2)^2}.
\]

Thus, the corresponding K-R distribution are of the form:

\[
K_{20}(r, \theta, \varphi, p, \theta', \varphi') = \sqrt{(2\pi^3)^3} (2 - r) e^{-\frac{r}{2}} \frac{4p^2 - 1}{(1 + 4p^2)^2} \exp(-ipr \cos \Theta),
\]

\[
K_{21}(r, \theta, \varphi, p, \theta', \varphi') = \frac{\sqrt{(2\pi^3)^3}}{3} r e^{-\frac{r}{2}} \frac{p}{(1 + 4p^2)^2} \exp(-ipr \cos \Theta) \cos \theta \cos \theta',
\]

where \(\Theta\) is defined by Eq. (10). The real part of Eq. (13) and appropriate contour plot are shown in Fig. 2.c and the real part of Eq. (14) in Fig. 3.c. The absolute value of Eqs. (13,14) and their contour plots are presented in Fig. 2.d and Fig. 3.d, respectively. The plot presented in Fig. 3.d has one maximum at \((r, p) = (2, \sqrt{3}/6)\) the location of which does not depend on variables \(\theta, \varphi, \theta', \varphi'\) chosen for the cross section. This result is in perfect agreement with what we expect for the state which has quantum numbers \(n, l\) satisfying the condition \(n - l = 1\). In Fig. 3.c, where the real part of the K-R distribution is presented, we see the additional minimum. It is due to \(\cos(rp)\)-like oscillations of the real part of the K-R distribution. Actually, there is an infinite number of alternate maxima and minima but their amplitude decreases rapidly and only two are seen on this scale. Dashed lines depicted on this (and every other contour-plot) denote \(K_{Re} = 0\). According to the results of Fig. 2.d the absolute value of the K-R distribution for the 2s state also has quite a simple form: we notice one global and three local maxima on this cross section. Fig. 2.c, where the real part of the same function is presented, is much more complicated when we look at it close up (see contour plot): Extrema are localized on lines where \(\cos(rp)\) achieves its extremal value, but on this regular structure
is another one – the wave function dependence on $r$ and $p$ that is responsible for the appearance of additional zeros and sign–changes of the plotted figure.

Finally we shall present an instructive example of a Rydberg state. Figure 4 shows the K-R distribution for a state with $n = 10$ and $l = 9$. The real part of the K–R distribution is shown in Fig. 4.c, and the absolute value is shown in Fig. 4.d. Just as one would expect there is one peak in the absolute value plot and similar, but modified by $\cos(rp)$, structure in the real part of the plot. Comparing the figures with that shown in Fig. 3.c-d we notice similarities in their structure. Obviously, peaks are located at different values of $(r, p)$ but there is the property that for states with $n - l = 1$ we observe one maximum in the absolute value plot. Its location changes with the increase of $n$ (it moves towards larger $r$ and smaller $p$) and the maximum value gets much smaller, but it is apparent this class of states has much in common. Figure 5 shows the K–R distribution for state $n = 10$, $l = 8$. Analysis similar to that made above holds true when we compare Fig. 5 and 2. Without counting that all the scales have changed we find 4 extrema ($(n - l)^2$) in the absolute value plots and similar oscillating structures in the real part plots. It is a general and well known result that $n - l$ is equal to the number of extrema of hydrogen atom wave functions both in position and momentum representation. We only stress that the K-R distribution renders very well this property: its absolute value has $(n - l)^2$ extrema.

VI. SUMMARY REMARKS

We have presented a phase space representation of the hydrogen atom using the K-R distribution. An advantage of such a representation is that the system can be treated analytically. It is an attractive feature of the K-R distribution that as long as one knows the wave function of the system there is no need to perform any integrals to obtain this distribution value in every point of phase space.

We have described in detail the $1s$, $2s$, $2p$, $10m$, and $10l$ states of the hydrogen atom. Plots corresponding to the K–R functions of these states were presented and compared with the plots of probability densities in position and momentum representations.

Acknowledgments

We thank S. Daffer for comments about the final draft. This work was partially supported by a KBN grant 2P03 B 02123, and the European Commission through the Research Training Network QUEST.

[1] E. Wigner, Phys. Rev. 40, 749 (1932)
[2] R. F. O’Connell and E. P. Wigner, Phys. Lett. A vol 83 no 4 (1981), 145
[3] K.E. Cahill and R.J. Glauber, Phys. Rev. 177, 1857, 1882 (1969)
[4] R.J. Glauber, Phys. Rev. Lett. 10, 84 (1963)
[5] E.C.G Sudarshan, Phys. Rev. Lett. 10, 277 (1963)
[6] K. Husimi, Proc. Phys. Math. Soc. Japan, 22, 246 (1940)
  K. Takahashi, Suppl. Prog. Theor. Phys. 98, 109 (1989)
[7] J. P. Dahl and M. Springborg, Mol. Phys. 47 1001 (1982)
[8] M. Springborg and J. P. Dahl, Phys. Rev A 36 1050 (1987)
[9] J. P. Dahl and M. Springborg, Phys. Rev A 59 4099 (1999)
[10] S. Nouri Phys. Rev A 57 1526 (1998)
[11] J.G. Kirkwood, Phys. Rev. 44, 31 (1933)
[12] L. Praxmeyer, K. Wódkiewicz, Quantum Interference in the Kirkwood–Rihaczek representation, quant-ph/0207127
[13] A.N. Rihaczek, IEEE Trans. Inf. Theory 14, 369 (1968)
[14] H. A. Bethe, E. E. Salpeter Quantum Mechanics of One- and Two-Electron Atoms, Springer-Verlag (1957)
FIG. 1: The K-R phase space representation of 1s state (n = 1, l = 0):
(a) the cross section \( \varphi = \text{const} \) of spacial probability density \( |R_{10}(r)/(4\pi)|^2 \) of finding electron at point \((r, \theta, \varphi)\);
(b) the cross section \( \varphi' = \text{const} \) of momentum probability density \( |F_{10}(p)/(4\pi)|^2 \) of finding electron with momentum \((p, \theta', \varphi')\);
(c) the real part of the K-R distribution and its contour plot (the cross section is made in directions shown by arrows depicted on Fig. 1(a) and (b));
(d) the absolute value of the K-R distribution and its contour plot (the same cross section as above).

FIG. 2: The K-R phase space representation of 2s state (n = 2, l = 0):
(a) the cross section \( \varphi = \text{const} \) of spacial probability density \( |R_{20}(r)/(4\pi)|^2 \) of finding electron at point \((r, \theta, \varphi)\);
(b) the cross section \( \varphi' = \text{const} \) of momentum probability density \( |F_{20}(p)/(4\pi)|^2 \) of finding electron with momentum \((p, \theta', \varphi')\);
(c) the real part of the K-R distribution and its contour plot (the cross section is made in directions shown by arrows depicted on Fig. 1(a) and (b));
(d) the absolute value of the K-R distribution and its contour plot (the same cross section as above).

FIG. 3: The K-R phase space representation of 2p state (n = 2, l = 1)
(a) the cross section \( \varphi = \text{const} \) of spacial probability density \( |R_{21}(r)/(4\pi)|^2 \) of finding electron at point \((r, \theta, \varphi)\);
(b) the cross section \( \varphi' = \text{const} \) of momentum probability density \( |F_{21}(p)/(4\pi)|^2 \) of finding electron with momentum \((p, \theta', \varphi')\);
(c) the real part of the K-R distribution and its contour plot (the cross section is made in directions shown by arrows depicted on Fig. 1(a) and (b));
(d) the absolute value of the K-R distribution and its contour plot (the same cross section as above).
This figure "figure1.jpg" is available in "jpg" format from:

http://arxiv.org/ps/quant-ph/0212132v1
This figure "figure2.jpg" is available in "jpg" format from:

http://arxiv.org/ps/quant-ph/0212132v1
This figure "figure3.jpg" is available in "jpg" format from:

http://arxiv.org/ps/quant-ph/0212132v1
This figure "figure4.jpg" is available in "jpg" format from:

http://arxiv.org/ps/quant-ph/0212132v1
This figure "figure5.jpg" is available in "jpg" format from:

http://arxiv.org/ps/quant-ph/0212132v1