View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Online Research Database In Technology

Technical University of Denmark

# Comment on "Wigner phase-space distribution function for the hydrogen atom"

**Dahl, Jens Peder; Springborg, Michael**

*Published in:*
Physical Review A (Atomic, Molecular and Optical Physics)

*Link to article, DOI:*
10.1103/PhysRevA.59.4099

*Publication date:*
1999

*Document Version*
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

*Citation (APA):*
Dahl, J. P., & Springborg, M. (1999). Comment on "Wigner phase-space distribution function for the hydrogen atom". Physical Review A (Atomic, Molecular and Optical Physics), 59(5), 4099-4100. DOI: 10.1103/PhysRevA.59.4099

DTU Library
Technical Information Center of Denmark

**General rights**
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# COMMENTS

*Comments are short papers which criticize or correct papers of other authors previously published in the* **Physical Review.** *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

## Comment on ''Wigner phase-space distribution function for the hydrogen atom''

Jens Peder Dahl
*Chemical Physics, Department of Chemistry, Technical University of Denmark, DTU 207, DK-2800 Lyngby, Denmark*

Michael Springborg
*Department of Chemistry, University of Konstanz, D-78457 Konstanz, Germany*

(Received 10 August 1998)

We object to the proposal that the mapping of the three-dimensional hydrogen atom into a four-dimensional harmonic oscillator can be readily used to determine the Wigner phase-space distribution function for the hydrogen atom. [S1050-2947(99)07005-5]

PACS number(s): 03.65.Ca

In a recent paper [1], Nouri considers the mapping of the three-dimensional hydrogen atom into a four-dimensional harmonic oscillator, and proposes that the Wigner function for the hydrogen atom may be simply derived via this mapping. We contend that this is not a practicable procedure.

In the following, we deepen our contention by first giving a brief overview of the connection between the hydrogen atom and the four-dimensional oscillator. We then show that the procedure used by Nouri to derive his Wigner function is incomplete, and hence that the form of his function is incorrect. Finally, we make comparisons with the proper Wigner function for the ground state of the hydrogen atom, as previously determined by us [2].

As emphasized by Nouri, the connection between the Schrödinger equation for a hydrogenlike atom,

$$\left(-\frac{\hbar^2}{2m}\nabla_3^2-\frac{Ze^2}{r}-E\right)\psi=0, \tag{1}$$

and the equation for a four-dimensional harmonic oscillator,

$$\left(-\frac{\hbar^2}{2m}\nabla_4^2-4Eu^2-4Ze^2\right)\psi=0, \tag{2}$$

has been studied by several authors [3]. It is based on the Kustaanheimo-Stiefel (KS) transformation [4],

$$x=u_1^2-u_2^2-u_3^2+u_4^2,\quad y=2(u_1u_2-u_3u_4),$$
$$z=2(u_1u_3+u_2u_4), \tag{3}$$

with the property that

$$r=u^2,\quad r=\sqrt{x^2+y^2+z^2},\quad u^2=u_1^2+u_2^2+u_3^2+u_4^2. \tag{4}$$

The Laplacians in Eqs. (1) and (2) are defined by

$$\nabla_3^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2},\quad \nabla_4^2=\frac{\partial^2}{\partial u_1^2}+\frac{\partial^2}{\partial u_2^2}+\frac{\partial^2}{\partial u_3^2}+\frac{\partial^2}{\partial u_4^2}. \tag{5}$$

Direct evaluation of $\nabla_4^2$, under the assumption that $\psi$ only depends on $(u_1,u_2,u_3,u_4)$ through the bilinear combinations on the right-hand side of Eq. (3), gives that

$$\nabla_4^2=4r\nabla_3^2. \tag{6}$$

Hence, left multiplication of Eq. (1) by $4r$ yields Eq. (2).

The KS transformation has been classified as a diastrophical canonical transformation by Gracia-Bondía [5], that is, a canonical tranformation, which increases the number of coordinates. The transformation of the linear momenta is obtained from the differential mapping,

$$\begin{pmatrix} dx\\ dy\\ dz\\ dw\end{pmatrix}=2\begin{pmatrix} u_1 & -u_2 & -u_3 & u_4\\ u_2 & u_1 & -u_4 & -u_3\\ u_3 & u_4 & u_1 & u_2\\ u_4 & -u_3 & u_2 & -u_1\end{pmatrix}\begin{pmatrix} du_1\\ du_2\\ du_3\\ du_4\end{pmatrix}, \tag{7}$$

where $w$ is a ''dummy coordinate'' with the incomplete differential $dw$. We get

$$\begin{pmatrix} p_x\\ p_y\\ p_z\\ p_w\end{pmatrix}=\frac{1}{2u^2}\begin{pmatrix} u_1 & -u_2 & -u_3 & u_4\\ u_2 & u_1 & -u_4 & -u_3\\ u_3 & u_4 & u_1 & u_2\\ u_4 & -u_3 & u_2 & -u_1\end{pmatrix}\begin{pmatrix} p_1\\ p_2\\ p_3\\ p_4\end{pmatrix}. \tag{8}$$

For the relations (3) and (8) to define a caconical transformation, Poisson brackets must be independent of the phase-space coordinates in which they are evaluated. Using the coordinates $(u_1,u_2,u_3,u_4,p_1,p_2,p_3,p_4)$ gives

$$\{x_\alpha,x_\beta\}=0,\quad \{x_\alpha,p_\beta\}=\delta_{\alpha\beta},\quad \{x_\alpha,p_w\}=0,$$
$$\{p_\alpha,p_\beta\}=\sum_\gamma \epsilon_{\alpha\beta\gamma}\frac{x_\gamma}{r}p_w,\quad \{p_\alpha,p_w\}=\frac{x_\alpha}{r}p_w, \tag{9}$$

 ©1999 The American Physical Society

with $(\alpha,\beta,\gamma)$ referring to the $(x,y,z)$ directions, respectively. Hence, we get the well-known constraint

$$p_w = 0. \tag{10}$$

Returning now to Nouri's article, he writes the hydrogenic wave functions in four space as linear combinations of the harmonic-oscillator wave functions,

$$\psi_{n_1 n_2 n_3 n_4} = \prod_{j=1}^{4} \left( \frac{\alpha}{\sqrt{\pi} 2^{n_j} n_j!} \right)^{1/2} e^{-(\alpha^2/2)u_j^2} H_{n_j}(\alpha u_j). \tag{11}$$

This corresponds to Eq. (6) of Nouri's article. The appropriate linear combinations respect the condition that $\psi$ only depend on $(u_1,u_2,u_3,u_4)$ through the bilinear combinations on the right-hand side of Eq. (3). The ground-state wave function is, in particular,

$$\psi_{0000} = (\alpha^2/\pi)\, e^{-(\alpha^2/2)u^2}. \tag{12}$$

The standard definition of the Wigner function associated with a wave function $\psi(\boldsymbol{q})$, where $\boldsymbol{q}$ is a $D$-dimensional position vector, is

$$W(\boldsymbol{q},\boldsymbol{p}) = 1/(\pi\hbar)^D \int \psi(\boldsymbol{q}-\boldsymbol{q}')^* \psi(\boldsymbol{q}+\boldsymbol{q}') e^{-2i\boldsymbol{p}\cdot\boldsymbol{q}'/\hbar} d\boldsymbol{q}'. \tag{13}$$

Using this expression, with the coordinates $(u_1,u_2,u_3,u_4,p_1,p_2,p_3,p_4)$, and the expression (11) for the wave function, Nouri obtained explicit expressions for the hydrogenic Wigner functions. Here, it is sufficient to reproduce his result for the ground state, viz.,

$$W_{0,0,0,0}(u_1,u_2,u_3,u_4,p_1,p_2,p_3,p_4) = (\pi\hbar)^{-4} \exp[-(\alpha^2 u^2 + \tilde{p}^2/\alpha^2\hbar^2)], \tag{14}$$

where $\tilde{p}^2$ is given by

$$\tilde{p}^2 = p_1^2 + p_2^2 + p_3^2 + p_4^2. \tag{15}$$

But now it follows from Eq. (8) that we may also write

$$\tilde{p}^2 = 4r(p_x^2 + p_y^2 + p_z^2 + p_w^2). \tag{16}$$

Hence, the expression for $W_{0,0,0,0}$ does not obey the constraint (10). $W_{0,0,0,0}$ is consequently not a proper hydrogenic Wigner function.

We stress that it is not sufficient to simply neglect the contribution from $p_w$ in the expression for $W_{0,0,0,0}$. The fatal point is that the constraint $p_w = 0$ is absent in the expression (13), from which $W_{0,0,0,0}$ was evaluated.

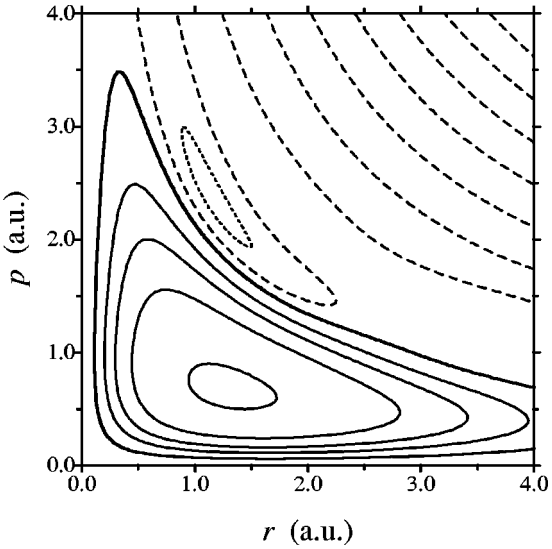


FIG. 1. Contour map of the function $F_{1s}(r,p)$. Starting from the nodal curves (dashed lines, contour value 0), contours have been drawn at 0.015, 0.05, 0.1, 0.2, and 0.5 a.u. (solid lines), and $-0.01$ a.u. (dotted lines). Adapted from Fig. 5 of Ref. [2].

To derive an expression for the Wigner function with the constraint (10) taken into account at every step is probably a very complicated matter. But even if it may be accomplished, the transformation of the result to three space is not at all simple. As clearly demonstrated in a recent article by Curtright *et al.* [6], the transformation of a Wigner function under a canonical transformation involves the generating function for the transformation in a very complicated manner.

The proper Wigner function for the hydrogen-atom ground state was determined by us several years ago [2]. It is a function of $r$, $p$, and $u$, where $r$ and $p$ are the magnitudes of the position and momentum vectors $\boldsymbol{r}$ and $\boldsymbol{p}$, respectively, and $u$ is the angle between them. The detailed characteristics of the Wigner function were described in [2]. Figure 1 shows the radial distribution function $F_{1s}(r,p)$, obtained by integrating over the angle $u$. It is normalized such that

$$\int_0^\infty \int_0^\infty F_{1s}(r,p)\, dr\, dp = 1. \tag{17}$$

We note that there are phase-space regions in which $F_{1s}(r,p)$ becomes negative. This is in contrast to the simple function (14), which is everywhere non-negative. We have presented similar figures for other atoms in [7].

This work was supported by the Danish Natural Science Research Council.

[1] S. Nouri, Phys. Rev. A **57**, 1526 (1998).
[2] J. P. Dahl and M. Springborg, Mol. Phys. **47**, 1001 (1982); see also J. P. Dahl, in *Dimensional Scaling in Chemical Physics*, edited by D. R. Herschbach, J. Avery, and O. Goscinski (Kluwer, Dordrecht, 1993), p. 165.
[3] See the references in [1].
[4] P. Kustaanheimo and E. Stiefel, J. Reine Angew. Math. **218**, 204 (1965).
[5] J. M. Gracia-Bondía, Phys. Rev. A **30**, 691 (1984).
[6] T. Curtright, D. Fairlie, and C. Zachos, Phys. Rev. D **58**, 025002 (1998).
[7] M. Springborg and J. P. Dahl, Phys. Rev. A **36**, 1050 (1987).