

## State reconstruction and irregular wavefunctions for the hydrogen atom

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1997 J. Phys. A: Math. Gen. 30 4783

(<http://iopscience.iop.org/0305-4470/30/13/026>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.72

The article was downloaded on 02/06/2010 at 04:25

Please note that [terms and conditions apply](#).

# State reconstruction and irregular wavefunctions for the hydrogen atom

D S Krähler and U Leonhardt

Abteilung für Quantenphysik, Universität Ulm, 89069 Ulm, Germany

Received 24 March 1997

**Abstract.** Inspired by a recently proposed procedure by Leonhardt and Raymer for wavepacket reconstruction, we calculate the irregular wavefunctions for the bound states of the Coulomb potential. We select the irregular solutions which have the simplest semiclassical limit.

## 1. State reconstruction

There are deeply rooted reasons why the state of a quantum system cannot be seen directly. For instance, quantum states may comprise complementary features (such as position and momentum information) which cannot be observed simultaneously. There are experimental techniques to infer the state of a quantum system from observations [1–6]. In particular the observation of moving one-dimensional wavepackets reveals the quantum state [7–9]. The measured quantity is the position probability distribution evolving in time. Since the position operators at different times do not commute with each other, in general, these measurements probe different complementary features of the wavepacket, to the extent that the complete state can be inferred from observations.

This state-reconstruction procedure is summarized in a couple of lines [10, 11]: The density matrix  $\rho_{mn}$  in energy representation<sup>†</sup> is the classical average

$$\rho_{mn} = \left\langle \left\langle \frac{\partial}{\partial x} [\psi_m^*(x, t) \varphi_n(x, t)] \right\rangle \right\rangle_{x, t} \quad (1)$$

with respect to the observed position  $x$  and time  $t$  denoted by double brackets. The quantity  $\partial[\psi_m^*(x, t)\varphi_n(x, t)]/\partial x$  that is averaged consists of the regular wavefunction  $\psi_m(x, t)$  and of the *irregular wavefunction*  $\varphi_n(x, t)$ . They are defined as

$$\psi_n(x, t) = \psi_n(x) \exp(-i\omega_n t) \quad (2)$$

$$\varphi_n(x, t) = \varphi_n(x) \exp(-i\omega_n t) \quad (3)$$

where  $\psi_n(x)$  and  $\varphi_n(x)$  are both solutions of the time-independent Schrödinger equation

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + U(x) \right] \phi_n(x) = \omega_n \phi_n(x) \quad (4)$$

with the eigenfrequency  $\omega_n$ . (The mass  $m$  and  $\hbar$  are set to unity.) However, only  $\psi_n(x)$  is normalizable and can be regarded as a proper quantum-mechanical wavefunction. The irregular wavefunction should obey the Wronskian condition [7, 8]

$$\psi_n(x) \frac{d\varphi_n(x)}{dx} - \frac{d\psi_n(x)}{dx} \varphi_n(x) = 2. \quad (5)$$

<sup>†</sup> We assume that only the discrete part of the spectrum is excited.

This condition implies that  $\varphi_n$  is not normalizable since none of the discrete levels are degenerate [14, section 21]. Nevertheless, the regular wavefunctions decay rapidly enough so that the average (1) converges [10, 11]. The Wronskian condition (5) plays the role of a ‘normalization’ for the irregular wavefunctions. However, these functions are not uniquely determined because we could always add a multiple of a regular wavefunction  $\psi_n$  to  $\varphi_n$  without changing the Wronskian. We note that we can also reverse the order of the regular and irregular part in equation (1) without changing the result

$$\rho_{mn} = \left\langle \left\langle \frac{\partial}{\partial x} [\varphi_m^*(x, t) \psi_n(x, t)] \right\rangle \right\rangle_{x,t}. \quad (6)$$

The mutual relation of the regular and the irregular wavefunctions is especially transparent in the semiclassical representation [10,12]

$$\psi_n(x) = \frac{c_n}{\sqrt{p_n(x)}} \cos \left[ S_n(x) - \frac{\pi}{4} \right] \quad (7)$$

$$\varphi_n(x) = \frac{2c_n^{-1}}{\sqrt{p_n(x)}} \sin \left[ S_n(x) - \frac{\pi}{4} \right] \quad (8)$$

with

$$p_n(x) = \frac{dS_n}{dx}. \quad (9)$$

They appear as standing position-probability waves which are out of phase with respect to each other. In the semiclassical approximation and in the classically allowed region, the quantity  $p_n(x)$  is the classical momentum

$$p_n(x) = \sqrt{2\omega_n - 2U(x)} \quad (10)$$

and  $S_n(x)$  is the time-independent part of the classical action

$$S_n(x) = \int_{a_n}^x p_n(x) dx. \quad (11)$$

Here  $a_n$  denotes the left turning point where  $p_n(a_n)$  vanishes. As we have already mentioned we could always add a multiple of the regular solution (7) to the irregular one (8) and the Wronskian condition (5) would not be affected. However, formula (8) appears as the most natural and aesthetical choice. In particular, this irregular solution leads to a very simple expression for the diagonal case [12]

$$f_{nn}(x) \equiv \frac{\partial}{\partial x} [\psi_n^* \varphi_n] \sim 2 \sin[2S_n(x)]. \quad (12)$$

Here we have neglected the slow variation of the semiclassical momentum  $p_n(x)$  compared with the action  $S_n(x)$ .

## 2. Hydrogen atom

One of the most beautiful exactly solvable problems in quantum mechanics is the hydrogen atom. Throughout the history of quantum physics it has been used as the classic benchmark for the state of theory and experiment. So it seems quite natural to consider the hydrogen atom as an example of the state reconstruction of anharmonic wavepackets<sup>†</sup>. This requires the calculation of the irregular wavefunctions.

<sup>†</sup> The other classic example, the harmonic oscillator, was extensively treated in [12] and references therein.

We consider only the radial motion of the bound states and we assume the angular-momentum quantum numbers  $l$  and  $m$  as being fixed and given. There is not much difference between this quasi-one-dimensional motion and the true one-dimensional case. The radius  $r$  must not be negative and there may be a singularity at the origin  $r = 0$ . Let us write the stationary Schrödinger equation for the (regular or irregular) radial wavefunction  $\phi_n(r) = rR_n(r)$  in atomic units

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} + \frac{l(l+1)}{2r^2} \right] \phi_n(r) = -\frac{1}{2n^2} \phi_n(r). \tag{13}$$

This equation has two linearly independent solutions which are conveniently expressed in terms of the Whittaker functions [13]  $W_{n,l+1/2}(2r/n)$  and  $W_{-n,l+1/2}(e^{i\pi} 2r/n)$ . Because  $W_{-n,l+1/2}$  is a multiple-valued function we prefer to write  $e^{i\pi}$  instead of  $-1$  in the argument. Since [13, section 2, equation (28)]

$$W_{n,l+1/2}(2r/n) = (-1)^{n_r} n_r! \left( \frac{2r}{n} \right)^{l+1} e^{-\rho/n} L_{n_r}^{2l+1}(2\rho/n) \tag{14}$$

with the radial quantum number

$$n_r = n - l - 1 \tag{15}$$

we may write the familiar normalized wavefunctions [14, equation (36.13)] (in the modern notation of the Laguerre polynomials  $L_n^a$  (cf [15, p 439])) in terms of the Whittaker function

$$\psi_n(r) = \frac{(-1)^{n_r}}{n} (n_r!(n+l)!)^{-1/2} W_{n,l+1/2}(2r/n). \tag{16}$$

We wish to find the real irregular wavefunctions with the asymptotic limit (8) for high quantum numbers. However, the second linearly independent solution  $W_{-n,l+1/2}(e^{i\pi} 2r/n)$  is complex valued for  $r > 0$ . Therefore we must compensate the imaginary part of  $W_{-n,l+1/2}(e^{i\pi} 2r/n)$  by a proper multiple of the regular solution. For this purpose we make the general ansatz

$$\varphi_n(r) = A W_{n,l+1/2}(2r/n) + B W_{-n,l+1/2}(e^{i\pi} 2r/n). \tag{17}$$

We seek the constants  $A$  and  $B$  such that  $\varphi_n(r)$  is real and obeys the Wronskian condition (5). Since the Wronskian of  $W_{n,l+1/2}(z)$  and  $W_{-n,l+1/2}(e^{i\pi} z)$  equals  $(-1)^n$ , see [13, section 2, equation (34b)], we obtain immediately from representation (16) and ansatz (17)

$$B = (-1)^{l+1} n^2 \sqrt{n_r!(n+l)!}. \tag{18}$$

To compensate the imaginary part of ansatz (17) we employ the logarithmic expansion [16, equation (9.237.1)]

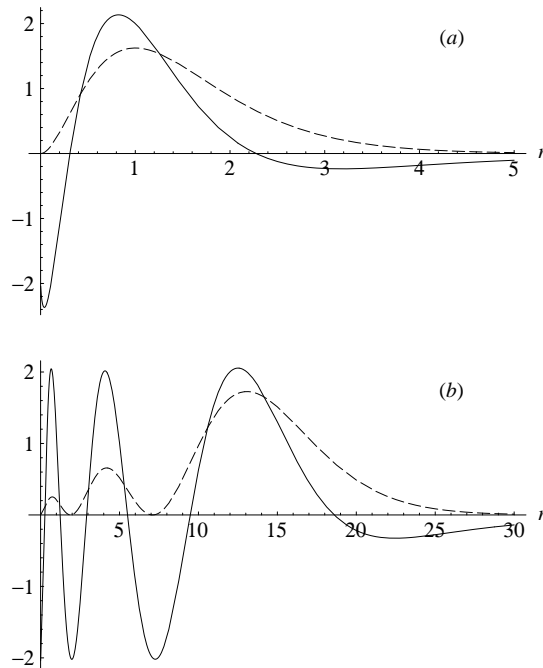
$$W_{-n,l+1/2}(e^{i\pi} 2r/n) = \frac{1}{(n+l)!} \left( -\frac{2r}{n} \right)^{l+1} e^{-r/n} L_{n_r}^{2l+1}(2r/n) [\ln(2r/n) + i\pi] + f(2r/n). \tag{19}$$

Here  $f(z)$  is an analytic function of  $z$  which is real on the real axis. We see that the only imaginary term in equation (19) is proportional to the regular solution. We utilize relation (16) and find

$$A = -\frac{i\pi n^2 (-1)^{n_r}}{\sqrt{n_r!(n+l)!}}. \tag{20}$$

Consequently, the irregular wavefunction  $\varphi_n(r)$  is given as

$$\varphi_n(r) = -\frac{i\pi n^2 (-1)^{n_r}}{\sqrt{n_r!(n+l)!}} W_{n,l+1/2}(2r/n) + (-1)^{l+1} n^2 \sqrt{n_r!(n+l)!} W_{-n,l+1/2}(e^{i\pi} 2r/n). \tag{21}$$



**Figure 1.** Plot of some diagonal sampling functions for the state reconstruction (1), defined as  $f_{nn}(r) = \partial(\psi_n^* \varphi_n) / \partial r$  (full curves), versus the squared regular wavefunctions  $\psi_n^2(r)$  (broken curves). In (a) we have set  $n = 1$  (ground state) whereas in (b)  $n = 3$  (second excited state). For both figures the  $l$  quantum number equals zero. We see that the sampling functions resemble the typical features of the squared wavefunctions  $\psi_n^2(r)$ . They detect these typical patterns in the measured probability distribution. Therefore the  $f_{nn}(r)$  are also called *pattern functions*. The pattern functions oscillate between  $-2$  and  $+2$ , as can be seen from the semiclassical approximation equation (12). Only the ground state shows a departure from this typical behaviour. On the other hand, we would not expect that a semiclassical theory is justified for the ground state.

Although this expression ‘looks complex’ we have seen that  $\varphi_n(r)$  is indeed real valued for  $r > 0$ . In figure 1 we have plotted for two different values of  $n$ , the diagonal pattern functions  $f_{nn}(r)$  and have compared them with the probability distributions  $\psi_n^2(r)$ .

### 3. Semiclassical limit

We have found some irregular wavefunctions for the hydrogen atom. Are they the desired sine-like oscillations (8) in the semiclassical limit? Let us recall the semiclassical approximation for the Coulomb problem. As is well known, we must replace the centrifugal term  $l(l+1)/2r^2$  by  $(l + \frac{1}{2})^2/2r^2$  because of the singularity of the  $r^{-1}$  potential (*Langer modification*, see for instance [17]). In this way we obtain the semiclassical momentum

$$p_n(r) = \left( -\frac{1}{n^2} + \frac{2}{r} - \frac{(l + \frac{1}{2})^2}{r^2} \right)^{1/2} \quad (22)$$

with the left turning point

$$a_n = n^2 - n \sqrt{n^2 - (l + \frac{1}{2})^2} \quad (23)$$

and by integration (11) the time-independent part of the action

$$S_n(r) = rp_n(r) + n \operatorname{arccot} \frac{n^2 - r}{nrp_n(r)} - \left(l + \frac{1}{2}\right) \left[ \frac{\pi}{2} + \arctan \frac{r - (l + \frac{1}{2})^2}{(l + \frac{1}{2})rp_n(r)} \right]. \quad (24)$$

To see whether our choice of  $\varphi_n(r)$  leads indeed to the sine-like behaviour (8) we consider the product  $\psi_n(r)\varphi_n(r)$ . First, we find an asymptotic expression using the exact formulae and then we compare it with the semiclassical approximation.

We utilize the known asymptotical behaviour of the Whittaker functions

$$W_{n,l+1/2}(z) \sim - \left(\frac{4z}{n}\right)^{1/4} e^{-n} n^n \sin\left(2\sqrt{nz} - n\pi - \frac{\pi}{4}\right) \quad (25)$$

$$W_{-n,l+1/2}(z) \sim \left(\frac{z}{4n}\right)^{1/4} e^n n^{-n} \exp(-2\sqrt{nz}) \quad (26)$$

for  $n \gg 1$ ,  $n \gg |z|$ ,  $n \gg l$  and  $\arg\sqrt{z} < 3\pi/4$ , see [13, section 7, equation (19)], and obtain from equations (16) and (21)

$$\psi_n(r)\varphi_n(r) \sim \sqrt{\frac{r}{2}} \cos(4\sqrt{2r}). \quad (27)$$

To find the asymptotics of the semiclassical approximation in the limit  $(l + \frac{1}{2})^2 \ll r \ll n^2$  we approximate

$$p_n(r) \sim \sqrt{\frac{2}{r}} \quad (28)$$

in expression (24) and note that

$$\frac{n^2 - r}{nrp_n(r)} \sim \frac{n}{\sqrt{2r}} - \frac{1}{2} \frac{\sqrt{2r}}{n} \quad (29)$$

$$\frac{r - (l + \frac{1}{2})^2}{(l + \frac{1}{2})rp_n(r)} \sim -\frac{l + \frac{1}{2}}{\sqrt{2r}} + \frac{\sqrt{2r}}{2l + 1}. \quad (30)$$

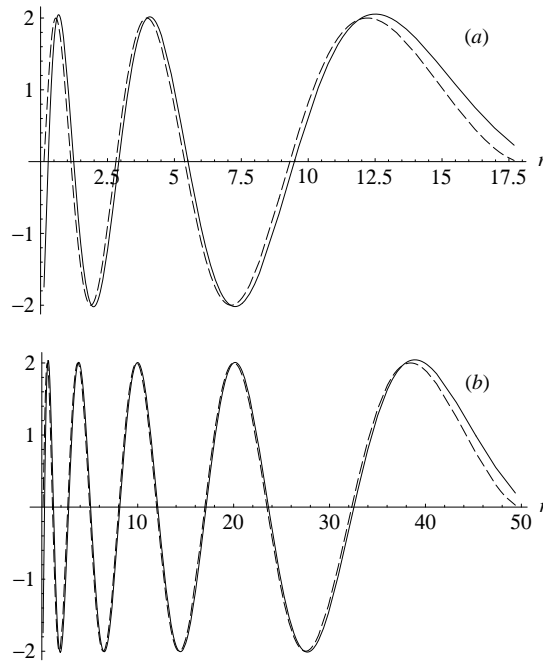
We utilize that  $\operatorname{arccot} z \rightarrow z^{-1}$  and  $\arctan z \rightarrow \pi/2$  for large  $z$  and obtain from equation (24)

$$\begin{aligned} S_n(r) &\sim \sqrt{2r} + n \left( \frac{n}{\sqrt{2r}} - \frac{1}{2} \frac{\sqrt{2r}}{n} \right)^{-1} - \left(l + \frac{1}{2}\right) \pi \\ &\sim 2\sqrt{2r} - (l + \frac{1}{2})\pi. \end{aligned} \quad (31)$$

Consequently, the product of  $c_n p_n^{-1/2} \cos(S_n - \pi/4)$  and  $2c_n^{-1} p_n^{-1/2} \sin(S_n - \pi/4)$  tends to the same expression (27) as the product  $\psi_n(r)\varphi_n(r)$  of the exact wavefunctions. This proves that our choice of the irregular wavefunction  $\varphi_n(r)$  leads indeed to the sine-like behaviour (8). In figure 2 we compare the exact pattern functions  $f_{nn}(r)$  with their semiclassical approximation (12) and find a good agreement.

#### 4. Summary

We have found the irregular wavefunctions of the hydrogen atom that satisfy the Wronskian condition (5) and correspond to the simple semiclassical representation (8). In this way we have performed the first explicit calculations to illustrate a recent proposal [7] for the state reconstruction of anharmonic wavepackets. Although we were primarily guided by the beauty of exactly solvable problems in quantum mechanics, our analysis may



**Figure 2.** Comparison of the exact,  $f_{nn}(r) = \partial(\psi_n^* \varphi_n) / \partial r$  (full curve), with the semiclassical formula  $f_{nn}(r) \sim 2 \sin[2S_n(r)]$  for the sampling functions. In (a) we have set  $n = 3$  (second excited state) whereas in (b)  $n = 5$  (fourth excited state). For both figures the  $l$  quantum number equals zero. The agreement between the curves is remarkably good.

be experimentally relevant for state determinations of hydrogenic wavepackets. These wavepackets occur in various areas of physics (they describe hydrogen-like atoms or excitons, for instance). An experiment of this kind would require the determination of the position probability distribution of the evolving wavepacket using a pump-probe technique. To our knowledge these measurements have not been performed yet for hydrogenic wavepackets. (On the other hand, wavepacket collapses and revivals have been measured [18].) One reason is probably the experimental difficulty involved. However, the reconstruction of the quantum state is an aim which is worth the effort of finding experimental ways to measure hydrogenic wavepackets. Therefore we have reasons to believe that our analysis will stimulate new experiments.

### Acknowledgment

The work presented in this paper was supported by the Deutsche Forschungsgemeinschaft.

### References

- [1] Smithey D T, Beck M, Raymer M G and Faridani A 1993 *Phys. Rev. Lett.* **70** 1244
- [2] Dunn T J, Walmsley I A and Mukamel S 1995 *Phys. Rev. Lett.* **74** 884
- [3] Munroe M, Boggavarapu D, Anderson M E and Raymer M G 1995 *Phys. Rev. A* **52** R924
- [4] Breitenbach G, Müller T, Pereira S F, Poizat J-Ph, Schiller S and Mlynek J 1995 *J. Opt. Soc. Am. B* **12** 2304
- [5] Schiller S, Breitenbach G, Pereira S F, Müller T and Mlynek J 1996 *Phys. Rev. Lett.* **77** 2933
- [6] Kurtsiefer Ch, Pfau T and Mlynek J 1997 *Nature* **386** 150

- [7] Leonhardt U and Raymer M G 1996 *Phys. Rev. Lett.* **76** 1985
- [8] Richter Th and Wünsche A 1996 *Phys. Rev. A* **53** R1974
- [9] Richter Th and Wünsche A 1996 *Acta Phys. Slov.* **46** 487
- [10] Leonhardt U 1996 *Acta Phys. Slov.* **46** 309
- [11] Leonhardt U 1997 *Measuring the Quantum State of Light* (Cambridge: Cambridge University Press)
- [12] Leonhardt U, Munroe M, Kiss T, Richter Th and Raymer M G 1996 *Opt. Commun.* **127** 144
- [13] Buchholz H 1953 *Die Konfluente Hypergeometrische Funktion* (Berlin: Springer)
- [14] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon) ch VII
- [15] Liboff R L 1992 *Introductory Quantum Mechanics* (Reading, MA: Addison-Wesley)
- [16] Gradshteyn I S and Ryzhik I M 1980 *Table of Integrals, Series, and Products* (San Diego, CA: Academic)
- [17] Fröman N and Fröman P O 1965 *JWKB Approximation* (Amsterdam: North-Holland)
- [18] Yeazell J A, Mallalieu M and Stroud C R Jr 1990 *Phys. Rev. Lett.* **64** 2007