

## Charged anisotropic harmonic oscillator and the hydrogen atom in crossed fields

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(Received 22 November 1993)

We perform a gauge-independent pseudoseparation of the center-of-mass motion for neutral two-body systems in crossed fields. The resulting Hamiltonian is investigated for two different cases of the interaction. First, we reduce the Hamiltonian for a two-particle system with anisotropic harmonic interaction in a magnetic field to the Hamiltonian of a charged anisotropic harmonic oscillator in a magnetic field. For the latter we derive closed-form analytical expressions of its eigenenergies and wave functions. Second, we investigate the hydrogen atom in crossed fields. The potential for the relative motion of electron and proton exhibits an outer potential well at large distances. We perform extensive numerical calculations of a large number of eigenvalues and wave functions and compare these to the analytical results of a harmonic approximation of the potential well.

PACS number(s): 32.60.+i, 03.65.-w, 31.50.+w, 32.30.-r

### I. INTRODUCTION

The hydrogen atom in strong external fields has been the subject of intensive study during the past two decades. The existence of huge magnetic fields in the vicinity of neutron stars (confirmed by observations in the late 1970s) has led to an increasing interest in phenomena in strong magnetic fields. Theoretical [1–3] and experimental [4,5] investigations have improved our knowledge about the spectrum of the hydrogen atom in magnetic fields enormously. In particular, the hydrogen atom in a magnetic field is also one of the simplest physical systems that shows both classically as well as quantum mechanically a transition from regularity to chaos [6].

The subject of the present paper are the two-body effects for the hydrogen atom in external fields that arise due to the finite nuclear mass and the fact that the collective and internal motion of the atom cannot be separated in the presence of a field. The first rigorous treatment of the true two-particle nature of the problem has been published by Avron, Herbst, and Simon [7]. They introduced a new operator connected with the center-of-mass motion, the so-called pseudomomentum, and showed that it represents a conserved quantity for the system. It was also shown that the center-of-mass motion cannot be separated completely from the internal motion as in the absence of external fields. For neutral systems, however, it is possible to perform a so-called pseudoseparation of the center-of-mass motion. This pseudoseparation leads to a Hamiltonian that is connected to the center-of-mass motion via the eigenvalue of the pseudomomentum. Herold, Ruder, and Wunner [8] used the results of Avron, Herbst, and Simon in order to calculate the energies of a neutral two-particle system with isotropic harmonic interaction in a magnetic field. In a number of publications [9–15] the pseudoseparation has been performed using specific choices for the gauge of the vector potential. Recently, Schmelcher and Cederbaum [16] used Newton's equations of motion to show that the kinetic

energy of the center-of-mass motion can be interpreted as part of the effective potential for the internal motion of the neutral two-particle system. In particular, in this classical investigation it has been argued that this effective potential is gauge independent thus offering a potential picture for the internal motion. In the present work we provide a rigorous proof of the claim made in [16].

The paper is organized as follows. In the first part (Sec. II) we present a complete analytical solution for both the energies and eigenfunctions of a charged particle in a magnetic field and an *anisotropic* harmonic potential. In Sec. III we present a gauge-independent quantum-mechanical pseudoseparation of the center-of-mass motion for neutral two-body systems with translation-invariant interaction. It is shown that the only gauge-dependent term in the resulting Hamiltonian of the internal motion is that of the kinetic energy of the internal motion. The remaining terms of this Hamiltonian are gauge independent and represent a potential for the relative motion of the atom.

In Sec. IV we first discuss the effective potential of the internal motion of the hydrogen atom in crossed fields. An additional potential well exists for large separations of the electron and the proton. We present and discuss our exact numerical results obtained for two different values of the pseudomomentum and compare them to the analytical results obtained for the harmonic approximation of the well. This will allow us to point out the effects that are due to the anharmonicity of the potential.

### II. A CHARGED PARTICLE IN A MAGNETIC FIELD AND AN ANISOTROPIC HARMONIC POTENTIAL

#### A. Formulation of the problem

Let us consider a charged particle with charge  $q$  in a static homogeneous magnetic field  $\mathbf{B} = B\mathbf{e}_z$  and an aniso-

tropic harmonic potential  $V(\mathbf{r})$ . One of the principal axes of the harmonic potential is assumed to point along the direction of the magnetic field. For the vector potential we choose the symmetric gauge  $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ . The Hamiltonian of the system is given by

$$\begin{aligned} H &= \frac{1}{2\mu}(\mathbf{p} - q\mathbf{A})^2 + V(\mathbf{r}) \\ &= \frac{\mathbf{p}^2}{2\mu} - \frac{qB}{2\mu}(xp_y - yp_x) + \frac{q^2 B^2}{8\mu}(x^2 + y^2) \\ &\quad + \frac{\mu}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \end{aligned} \quad (1)$$

Obviously, the  $z$  direction can be separated from the  $x$  and  $y$  directions, i.e., the Hamiltonian  $H$  is a sum of the Hamiltonian  $H_{xy}$  of the two-dimensional system in the plane perpendicular to the magnetic field and the Hamiltonian  $H_z$  of the one-dimensional harmonic oscillator in the  $z$  direction. The eigenvalues of  $H$  are given by

$$E_{n_1 n_2 n_z} = E_{n_1 n_2} + E_{n_z},$$

where  $E_{n_z} = (n_z + 1/2)\omega_z$  and  $E_{n_1 n_2}$  are the eigenvalues of  $H_{xy}$ .

Accordingly, the eigenfunction of  $H$  are given by the product of the eigenfunction of the one-dimensional harmonic oscillator  $\phi_{n_z}(z)$  and the eigenfunctions  $\Psi_{n_1 n_2}(x, y)$  of  $H_{xy}$ . Both the eigenvalues and eigenfunctions of  $H_{xy}$  will be calculated in the following.

### B. Transformation of $H_{xy}$

Due to the existence of the angular momentum term  $qB/2\mu(xp_y - yp_x)$  in  $H_{xy}$  the solution of the corresponding Schrödinger equation is a nontrivial task. Because of the loss of symmetry caused by the anisotropic harmonic potential the angular momentum is not a conserved quantity. Therefore, its quantum number cannot be used to reduce the two-dimensional problem to a one-dimensional differential equation as in the case of an isotropic potential [8]. We have to find a unitary transformation of the Hamiltonian that eliminates the angular momentum term and the explicit dependence on the magnetic field in  $H_{xy}$ . We will end up with a Hamiltonian that has the usual form of the kinetic energy in the ab-

sence of a magnetic field, i.e.,  $p^2/2m$ , and potential terms that do not contain momentum operators. In fact, the final Hamiltonian will describe two independent particles in their individual one-dimensional harmonic potentials. The corresponding eigenvalues and eigenfunction are well known.

Let us begin our considerations by introducing the operators

$$\begin{aligned} J &= xp_y + yp_x, \quad V = \frac{1}{2}(x^2 + y^2), \quad T = \frac{1}{2}(p_x^2 + p_y^2), \\ L &= xp_y - yp_x, \quad W = \frac{1}{2}(x^2 - y^2), \quad S = \frac{1}{2}(p_x^2 - p_y^2) \end{aligned}$$

and the abbreviations

$$\begin{aligned} a &= \frac{\omega_c}{2}, \quad b = \frac{\mu}{2} \left[ \omega_x^2 + \omega_y^2 + \frac{\omega_c^2}{2} \right], \\ c &= \frac{\mu}{2}(\omega_x^2 - \omega_y^2), \quad d = \frac{1}{\mu}, \end{aligned}$$

where  $\omega_c = -qB/\mu$  is the cyclotron frequency. Then the Hamiltonian  $H_{xy}$  is given by

$$H_{xy} = aL + bV + cW + dT.$$

The time-independent Schrödinger equation for the Hamiltonian  $H_{xy}$

$$H_{xy} \Psi_{n_1 n_2}(x, y) = E_{n_1 n_2} \Psi_{n_1 n_2}(x, y) \quad (2)$$

can be rewritten in the form

$$H_3 \psi_{n_1 n_2} = E_{n_1 n_2} \psi_{n_1 n_2} \quad (3)$$

where we have introduced the eigenfunction  $\psi_{n_1 n_2}$  of the Hamiltonian  $H_3 = U^{-1}H_{xy}U$  defined by

$$\Psi_{n_1 n_2}(x, y) = (U \psi_{n_1 n_2})(x, y). \quad (4)$$

Let us consider the unitary operator

$$U = \exp(i\alpha xy) \exp(i\beta p_x p_y). \quad (5)$$

The transforms of the operators  $J, L, V, W, T$ , and  $S$  with respect to the operators  $\exp(i\alpha xy)$  and  $\exp(i\beta p_x p_y)$  are given in the paper of Meyer, Kucar, and Cederbaum [17]. Transforming  $H_{xy}$  by the operator  $U$  we obtain the new Hamiltonian

$$\begin{aligned} H_3 &= U^{-1}H_{xy}U \\ &= (\alpha d - \beta(b + \alpha^2 d))J + (a - \beta(c + 2\alpha a))L \\ &\quad + (b + \alpha^2 d)V + (c - 2\alpha a)W + (d - 2\alpha\beta d + \beta^2(b + \alpha^2 d))T + (2\beta a - \beta^2(c + 2\alpha a))S. \end{aligned}$$

For this operator to become a Hamiltonian of two independent particles in one-dimensional harmonic potentials it is necessary that the coefficients of  $J$  and  $L$  vanish. For  $B \neq 0$  we find

$$\alpha = -\frac{\mu}{2} \left[ \frac{\omega_x^2 - \omega_y^2}{\omega_c} \right] \pm \frac{\mu}{2\omega_c} \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2 \omega_y^2} \quad (6)$$

and

$$\beta = \pm \frac{\omega_c}{\mu \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2 \omega_y^2}}. \quad (7)$$

For  $B \rightarrow 0$ , we require  $\alpha$  to vanish or at least to be finite. Therefore, we have to choose the positive sign in  $\alpha$  and  $\beta$  for  $\omega_x^2 \geq \omega_y^2$  and the negative sign for  $\omega_x^2 < \omega_y^2$ .

Now  $H_3$  is given in terms of squares of coordinate and momentum operators only,

$$H_3 = \frac{p_x^2}{2M_1} + \frac{p_y^2}{2M_2} + \frac{M_1}{2}\omega_1^2 x^2 + \frac{M_2}{2}\omega_2^2 y^2. \quad (8)$$

From the terms containing the momentum operators the masses  $M_1$  and  $M_2$  can be obtained in terms of the variables  $a$ ,  $b$ ,  $c$ , and  $d$  and the parameters  $\alpha$  and  $\beta$ . After some algebra we arrive at

$$M_{1,2} = \frac{2\mu\sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}}{\text{sgn}[\omega_x^2 - \omega_y^2](\omega_x^2 - \omega_y^2 \pm \omega_c^2) + \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}},$$

where

$$\text{sgn}[\omega_x^2 - \omega_y^2] = \begin{cases} +1 & \text{for } \omega_x^2 \geq \omega_y^2 \\ -1 & \text{otherwise.} \end{cases}$$

With these masses we can calculate the frequencies  $\omega_1$  and  $\omega_2$  using those terms of Eq. (8) that contain the squares of the coordinates. The result is

$$\omega_{1,2} = \frac{1}{\sqrt{2}}[\omega_x^2 + \omega_y^2 + \omega_c^2 \pm \text{sgn}[\omega_x^2 - \omega_y^2]\sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}]^{1/2}. \quad (9)$$

Now, the original two-dimensional one-particle Hamiltonian  $H_{xy}$  which mixes the  $x$  and  $y$  directions via the angular momentum term has been transformed into the sum of two Hamiltonians of independent particles with masses  $M_1$  and  $M_2$  in one-dimensional harmonic potentials with frequencies  $\omega_1$  and  $\omega_2$ , respectively. The new masses and frequencies are given in terms of the original frequencies  $\omega_x$ ,  $\omega_y$ , and  $\omega_c$ . Via  $\omega_c$ , there is an implicit dependence of the Hamiltonian  $H_3$  on the magnetic field strength  $B$ .

The eigenvalues of  $H_3$ , which are also those of  $H_{xy}$ , are given by

$$E_{n_1, n_2} = (n_1 + \frac{1}{2})\omega_1 + (n_2 + \frac{1}{2})\omega_2. \quad (10)$$

The eigenfunctions of  $H_3$  are products

$$\psi_{n_1 n_2}(x, y) = \phi_{n_1}(x)\phi_{n_2}(y)$$

of the one-dimensional eigenfunctions  $\phi_{n_i}$  of the harmonic oscillators with frequencies  $\omega_i$  and masses  $M_i$ .

### C. Calculation of the wave functions

In order to obtain the eigenfunctions of  $H_{xy}$  we have to apply the transformation operator  $U$  [Eq. (5)] to  $\psi_{n_1 n_2}$  according to Eq. (4). This is a nontrivial task. If the operator  $\exp(i\beta p_x p_y)$  acts on a function of the coordinates  $x$  and  $y$ , the result cannot be derived directly. It is very simple, though, to get the result if the operator acts on a function in momentum space.

Therefore, let us begin the transformation by taking the Fourier transform  $\mathcal{F}(\psi)$  of the eigenfunction  $\psi_{n_1 n_2}$  of  $H_3$ .  $\mathcal{F}(\psi)$  is a function in momentum space. Then we apply the operator  $\exp(i\beta p_x p_y)$  to  $\mathcal{F}(\psi)$  which means multiplying  $\mathcal{F}(\psi)$  by  $e^{i\beta p_x p_y}$ , where  $p_x$  and  $p_y$  are now the corresponding eigenvalues. Next we take the inverse Fourier transform of the result in order to obtain the function  $f_{n_1 n_2}(x, y)$  in the coordinate space of  $H_{xy}$ . In this step we use the convolution theorem [18] for Fourier transforms. The first steps of the transformation read

$$\begin{aligned} f_{n_1 n_2}(x, y) &= (e^{i\beta p_x p_y} \psi_{n_1 n_2})(x, y) \\ &= \mathcal{F}^{-1}(e^{i\beta p_x p_y} \mathcal{F}(\psi_{n_1 n_2}))(x, y) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\beta} e^{-i/\beta(x-x')(y-y')} \psi_{n_1 n_2}(x', y') dx' dy' \\ &= \frac{(-i)^{n_2}}{\beta\sqrt{2\pi M_2 \omega_2}} e^{-i/\beta(xy)} \int_{-\infty}^{\infty} e^{i/\beta(x'y')} \phi_{n_1}(x') \phi_{n_2} \left[ \frac{x-x'}{\beta M_2 \omega_2} \right] dx' \\ &= \tilde{N} \int_{-\infty}^{\infty} e^{-z^2} H_{n_1}(Dz + F) H_{n_2}(Gz + H) dz, \end{aligned} \quad (11)$$

where

$$\begin{aligned}\bar{N} &= \frac{(-i)^{n_2}}{\pi \sqrt{2^{n_1+n_2+1} n_1! n_2!}} \left[ \frac{\sqrt{M_1 \omega_1 M_2 \omega_2}}{\beta^2 M_1 \omega_1 M_2 \omega_2 + 1} \right]^{1/2} \\ &\times \exp \left[ \frac{-M_1 \omega_1 x^2 - 2i\beta M_1 \omega_1 M_2 \omega_2 xy - M_2 \omega_2 y^2}{2(\beta^2 M_1 \omega_1 M_2 \omega_2 + 1)} \right], \\ D &= \left[ \frac{2\beta^2 M_1 \omega_1 M_2 \omega_2}{\beta^2 M_1 \omega_1 M_2 \omega_2 + 1} \right]^{1/2}, \\ F &= \frac{\sqrt{M_1 \omega_1} (x + i\beta M_2 \omega_2 y)}{\beta^2 M_1 \omega_1 M_2 \omega_2 + 1}, \\ G &= -\operatorname{sgn}[\omega_x^2 - \omega_y^2] \left[ \frac{2}{\beta^2 M_1 \omega_1 M_2 \omega_2 + 1} \right]^{1/2}, \\ H &= \frac{\sqrt{M_2 \omega_2} (\beta M_1 \omega_1 x - iy)}{\beta^2 M_1 \omega_1 M_2 \omega_2 + 1}.\end{aligned}$$

$$c_{kl}(n_1, n_2) = \begin{cases} 0 & \text{for } k+l \text{ odd} \\ 2^{2l+k} \binom{n_1}{k} \binom{n_2}{l} \Gamma \left[ \frac{k+l+1}{2} \right] D^l G^l (2D^2 - 1)^{[(k-l)/2]} \\ \times {}_2F_1 \left[ -\frac{l}{2}, \frac{1-l}{2}; \frac{1-k-l}{2}; \frac{1}{2D^2} + \frac{1}{2G^2} - \frac{1}{4D^2 G^2} \right] & \text{otherwise.} \end{cases}$$

Here  ${}_2F_1$  denotes the hypergeometric function [18].

Finally, in order to obtain the eigenfunction  $\Psi_{n_1 n_2}(x, y)$  of  $H_{xy}$  we apply the operator  $\exp(i\alpha xy)$  to  $f_{n_1 n_2}(x, y)$  which means multiplying  $f_{n_1 n_2}(x, y)$  by  $e^{i\alpha xy}$ . The result is

$$\begin{aligned}\Psi_{n_1 n_2}(x, y) &= N e^{g(x, y)} \sum_{k=0}^{n_1} \sum_{l=0}^{n_2} c_{kl}(n_1, n_2) H_{n_1-k}(\sqrt{2}F) \\ &\quad \times H_{n_2-l}(\sqrt{2}H),\end{aligned}\tag{13}$$

where

$$N = \frac{(-i)^{n_2}}{2^{n_1+n_2} \pi} \left[ \frac{\sqrt{M_1 \omega_1 M_2 \omega_2}}{n_1! n_2! (\beta^2 M_1 \omega_1 M_2 \omega_2 + 1)} \right]^{1/2}$$

and

$$g(x, y) = i\alpha xy - \frac{M_1 \omega_1 x^2 + 2i\beta M_1 \omega_1 M_2 \omega_2 xy + M_2 \omega_2 y^2}{2(\beta^2 M_1 \omega_1 M_2 \omega_2 + 1)}.$$

$\Psi_{n_1 n_2}(x, y)$  are the eigenfunctions of  $H_{xy}$  given in coordinate space. They are finite sums of products of two Hermite polynomials with different complex arguments.

#### D. Trajectories of the classical motion

Before we discuss the form of the wave function  $\Psi_{n_1 n_2}(x, y)$  let us derive the trajectories of the classical

The Hermite polynomials  $H_n(az + b)$  in Eq. (11) can be written as [19]

$$H_n(az + b) = \frac{1}{\sqrt{2}^n} \sum_{k=0}^n H_{n-k}(\sqrt{2}az) H_k(\sqrt{2}b).$$

Using this formula, we are left with integrals of the form

$$\int_{-\infty}^{\infty} e^{-z^2} H_k(\sqrt{2}Dz) H_l(\sqrt{2}Gz) dz$$

which can be found in the table of Apelblat [20]. We arrive at

$$\begin{aligned}f_{n_1 n_2}(x, y) &= \frac{\bar{N}}{\sqrt{2}^{n_1+n_2}} \sum_{k=0}^{n_1} \sum_{l=0}^{n_2} c_{kl}(n_1, n_2) H_{n_1-k}(\sqrt{2}F) \\ &\quad \times H_{n_2-l}(\sqrt{2}H),\end{aligned}\tag{12}$$

where the coefficients are given by

motion of a charged particle in a magnetic field and an anisotropic potential. This will help us to understand the appearance of the quantum-mechanical wave function. In the following we denote the greater of the two frequencies  $\omega_1$  and  $\omega_2$  by  $\omega_+$  and the corresponding quantum number  $n_+$  and in analogy the smaller frequency  $\omega_-$  with the quantum number  $n_-$ .

The classical equations of motion have been solved by Schmelcher and Cederbaum [16]. The coordinates as functions of time read as follows:

$$x(t) = a_+ \cos \omega_+ t + a_- \cos \omega_- t,\tag{14}$$

$$y(t) = b_+ \sin \omega_+ t + b_- \sin \omega_- t,\tag{15}$$

where

$$b_+ = -a_+ \frac{\omega_+ \omega_c}{\omega_y^2 - \omega_+^2}$$

and

$$b_- = -a_- \frac{\omega_- \omega_c}{\omega_y^2 - \omega_-^2}.$$

We see that the classical motion is given as a superposition of two elliptical motions with different frequencies  $\omega_+$  and  $\omega_-$ . To find the values of  $a_+$  and  $a_-$  we set the quantum-mechanical energy  $E_{n_+, n_-} = (n_+ + \frac{1}{2})\omega_+ + (n_- + \frac{1}{2})\omega_-$  equal to the classical energy  $E = \mu/2(\dot{x}^2 + \dot{y}^2) + \mu/2(\omega_x^2 x^2 + \omega_y^2 y^2)$ . Note that in clas-

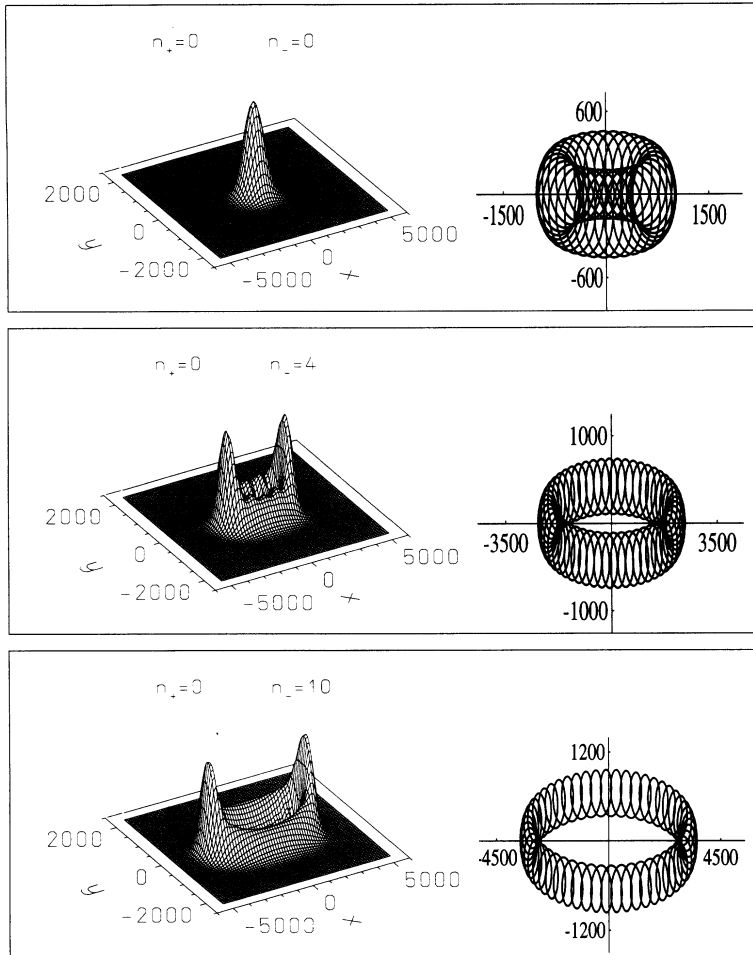


FIG. 1. Square of the absolute values of the wave functions of  $H_{xy}$  and corresponding classical trajectories. Quantum numbers are indicated in the plots. Parameters:  $B=10^{-5}$ ,  $\omega_x=10^{-7}$ , and  $\omega_y=5\times 10^{-7}$ . All values are given in atomic units.

sical mechanics the kinetic energy  $\mu/2(\dot{x}^2 + \dot{y}^2)$  contains all the contributions from the magnetic field like the paramagnetic and diamagnetic terms of the Hamiltonian. That is why in the total energy the potential has the original form with frequencies  $\omega_x$  and  $\omega_y$ . Using Eqs. (14) and (15) in the classical energy expression the energy equation can be transformed into

$$(n_+ + \frac{1}{2})\omega_+ + (n_- + \frac{1}{2})\omega_- = a_+^2 \frac{M_+}{2}\omega_+^2 + a_-^2 \frac{M_-}{2}\omega_-^2,$$

with the masses

$$M_+ = \frac{2\mu\sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}}{\omega_x^2 - \omega_y^2 + \omega_c^2 + \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}}$$

and

$$M_- = \frac{2\mu\sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}}{\omega_y^2 - \omega_x^2 - \omega_c^2 + \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2\omega_y^2}}.$$

Since the two frequencies  $\omega_+$  and  $\omega_-$  are independent we can split this equation into two and solve them for  $a_+$  and  $a_-$ . We finally arrive at

$$a_+ = \left( \frac{2n_+ + 1}{M_+\omega_+} \right)^{1/2}$$

and

$$a_- = \left( \frac{2n_- + 1}{M_-\omega_-} \right)^{1/2}$$

Having obtained the coefficients of the trajectories given in Eqs. (14) and (15) we can plot the classical trajectories and compare them to the quantum-mechanical wave function.

#### E. Comparison of classical trajectories and quantum-mechanical wave functions

We have plotted numerous quantum-mechanical wave functions (13) and compared them to the classical trajectories. As an example, let us choose the mass<sup>1</sup>  $\mu=1$ , the charge  $q=-1$ , the frequencies  $\omega_x=10^{-7}$  and  $\omega_y=5\times 10^{-7}$ , and the magnetic field  $B=10^{-5}$ . These parameters lead to the frequencies  $\omega_+=1.00\times 10^{-5}$  and  $\omega_-=5.00\times 10^{-9}$ . In Figs. 1 and 2 we have plotted the

<sup>1</sup>Throughout the paper we will use atomic units.

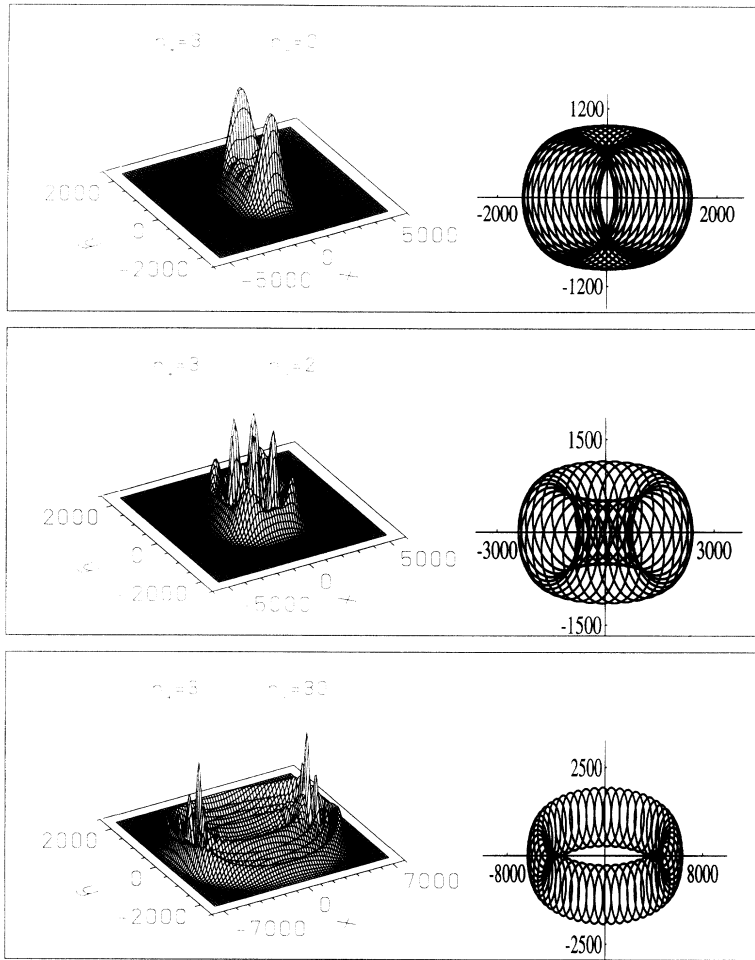


FIG. 2. Square of the absolute values of the wave functions of  $H_{xy}$  and corresponding classical trajectories. Quantum numbers are indicated in the plots. Parameters:  $B = 10^{-5}$ ,  $\omega_x = 10^{-7}$ , and  $\omega_y = 5 \times 10^{-7}$ .

square of the absolute value of the wave functions and their corresponding classical trajectories for different combinations of quantum numbers  $n_+$  and  $n_-$ . For the plots of the trajectories the frequencies  $\omega_+$  and  $\omega_-$  have been scaled independently for reasons of illustration.

The form of the ground-state wave function is that of a Gaussian function. The other states shown in Fig. 1 exhibit an elliptic ring of high probability density that encloses a region of low intensity. These features can be explained by the form of the classical motion that consists of an elliptical motion with high frequency  $\omega_+$  that itself is moving on an elliptical path with smaller frequency. Depending on the sizes of the semiaxes which are determined by the quantum numbers the classical motion either completely fills the corresponding area of coordinate space around the origin or leaves an inner ellipse uncovered leading to an elliptical ring in space that is covered by the motion. In general, we observe the tendency that the quantum-mechanical probability density is enhanced in regions of coordinate space that are frequently visited by the classical trajectories. However, this correspondence should not be overemphasized. For example, as we see in Fig. 2 for the state  $n_+ = 3$ ,  $n_- = 2$  the quantum-mechanical peak structures cannot be explained in detail by the classical path.

### III. A NEUTRAL TWO-PARTICLE SYSTEM IN EXTERNAL FIELDS

#### A. Gauge-independent pseudoseparation of the center-of-mass motion

For many-body systems with translation invariant interaction without external fields it is possible completely separate the motion of the center of mass from the internal degrees of freedom. In general, if there is an external field this separation is no longer possible. For neutral systems in static homogeneous magnetic and electric fields, however, one can perform a so-called “pseudoseparation,” which results in an effective Hamiltonian for the relative motion. This Hamiltonian depends parametrically on the eigenvalue of the so-called “pseudomomentum” which is a conserved quantity connected to the center-of-mass motion of the system.

In the literature [7–12,16,21,22] this pseudoseparation has always been performed using specific choices of the gauge for the vector potential. We shall perform the pseudoseparation for a neutral two-body system in a magnetic and electric field without restricting ourselves to a specific gauge. As a consequence in the resulting effective Hamiltonian we will obtain terms that depend

on a vector potential and terms that are gauge independent. We will be able to identify the terms representing the kinetic energy of the relative motion. The remaining terms will be gauge independent and can therefore be assigned to an effective potential of the relative motion.

The Hamiltonian of a neutral two-body system in homogeneous static magnetic and electric fields reads

$$\mathcal{H} = \frac{1}{2m_1}(\mathbf{p}_1 - e \mathbf{A}_1)^2 + \frac{1}{2m_2}(\mathbf{p}_2 + e \mathbf{A}_2)^2 - e \mathbf{E} \cdot \mathbf{r}_1 + e \mathbf{E} \cdot \mathbf{r}_2 + V(\mathbf{r}_1 - \mathbf{r}_2), \quad (16)$$

where  $m_i$  are the masses,  $\pm e$  the charges, and  $\mathbf{r}_i$  and  $\mathbf{p}_i$  ( $i=1,2$ ) the operators of the coordinates and momenta of

the two particles.  $\mathbf{A}_i = \mathbf{A}(\mathbf{r}_i)$  is the operator of the vector potential and  $V(\mathbf{r}_1 - \mathbf{r}_2)$  the operator of the translation invariant interaction potential. The magnetic field is given by  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ . Therefore, the vector potential is not uniquely defined but can be gauged using the gradient of a scalar field  $\Lambda$ :  $\mathbf{A}'_i = \mathbf{A}_i + \nabla_i \Lambda(\mathbf{r}_i)$ . As a result, the vector potential in an arbitrary gauge is given by, for example,

$$\mathbf{A}_i = \frac{1}{2} \mathbf{B} \times \mathbf{r}_i + \nabla_i \Lambda(\mathbf{r}_i). \quad (17)$$

Let us now introduce the center-of-mass vector  $\mathbf{R}$  and the relative coordinate vector  $\mathbf{r}$ . In these coordinates the Hamiltonian in Eq. (16) with the vector potential given in Eq. (17) reads

$$\mathcal{H} = \frac{1}{2m_1} \left[ \frac{m_1}{M} \mathbf{P} + \mathbf{p} - \frac{e}{2} \mathbf{B} \times \left[ \mathbf{R} + \frac{m_2}{M} \mathbf{r} \right] - e \left[ \frac{m_1}{M} \nabla_R + \nabla_r \right] \Lambda_2 \right]^2 + \frac{1}{2m_2} \left[ \frac{m_2}{M} \mathbf{P} - \mathbf{p} + \frac{e}{2} \mathbf{B} \times \left[ \mathbf{R} - \frac{m_1}{M} \mathbf{r} \right] + e \left[ \frac{m_2}{M} \nabla_R - \nabla_r \right] \Lambda_1 \right]^2 + V(\mathbf{r}) - e \mathbf{E} \cdot \mathbf{r}, \quad (18)$$

where  $\Lambda_1 = \Lambda(\mathbf{R} - (m_1/M)\mathbf{r})$  and  $\Lambda_2 = \Lambda(\mathbf{R} + (m_2/M)\mathbf{r})$ .

The Hamiltonian  $\mathcal{H}$  possesses a constant of motion, the so-called pseudomomentum, which is given by [10,21,23,24],

$$\hat{\mathbf{K}}' = \mathbf{p}_1 - e \mathbf{A}_1 + e \mathbf{B} \times \mathbf{r}_1 + \mathbf{p}_2 + e \mathbf{A}_2 - e \mathbf{B} \times \mathbf{r}_2 - M \mathbf{v}_D = \hat{\mathbf{K}} - M \mathbf{v}_D = \mathbf{P} + \frac{e}{2} \mathbf{B} \times \mathbf{r} + e \left[ \frac{m_2}{M} \nabla_R - \nabla_r \right] \Lambda_1 - e \left[ \frac{m_1}{M} \nabla_R + \nabla_r \right] \Lambda_2 - M \mathbf{v}_D,$$

where  $\hat{\mathbf{K}}'$  and  $\hat{\mathbf{K}}$  denote the operator of the pseudomomentum with and without the electric field, respectively.  $M = m_1 + m_2$  is the total mass and  $\mathbf{v}_D = (\mathbf{E} \times \mathbf{B})/B^2$  the drift velocity of charged particles in crossed fields. The latter is independent of the charge and mass of the particle [25]. For a physical interpretation of the pseudomomentum we refer the reader to Avron, Herbst, and Simon [7], Johnson, Hirschfelder, and Yang [10], or Schmelcher, Cederbaum, and Kappes [23,24]. In static magnetic fields the components of the pseudomomentum commute with the Hamiltonian. For neutral systems the components of the pseudomomentum commute with each other. Therefore, the eigenfunctions of the corresponding Schrödinger equation can be chosen as simultaneous eigenfunctions to the pseudomomentum. As a consequence of the discussed properties of  $\mathcal{H}$  it is possible to decompose the total wave function  $\Psi$  in the following way:

$$\Psi(\mathbf{r}, \mathbf{R}) = U(\mathbf{r}, \mathbf{R}) \Psi_0(\mathbf{r}). \quad (19)$$

The center-of-mass coordinate dependency is, therefore, solely given by the unitarian  $U$ , which will in the following be determined by the condition that  $\Psi$  must be an eigenfunction to the operator  $\hat{\mathbf{K}}'$ , i.e.,  $\hat{\mathbf{K}}' \Psi = \mathbf{K}' \Psi$ , where  $\mathbf{K}'$  and  $\mathbf{K}$  denote the corresponding eigenvalues. Together with the ansatz

$$U = \exp \left[ i \mathbf{K} \cdot \mathbf{R} - i \frac{e}{2} (\mathbf{B} \times \mathbf{r}) \cdot \mathbf{R} + i \chi(\mathbf{r}, \mathbf{R}) \right] \quad (20)$$

we arrive at the following differential equation for the unknown function  $\chi$ :

$$\nabla_R \chi(\mathbf{r}, \mathbf{R}) = e \left[ \frac{m_2}{M} \nabla_R - \nabla_r \right] \Lambda_1 + e \left[ \frac{m_1}{M} \nabla_R + \nabla_r \right] \Lambda_2.$$

Noticing that  $\nabla_r \Lambda_1 = -(m_1/M) \nabla_R \Lambda_1$  and  $\nabla_r \Lambda_2 = (m_2/M) \nabla_R \Lambda_2$ , we rewrite this equation as

$$\nabla_R \chi(\mathbf{r}, \mathbf{R}) = -e \nabla_R (\Lambda_1 - \Lambda_2).$$

This equation has the solution

$$\chi(\mathbf{r}, \mathbf{R}) = -e (\Lambda_1 - \Lambda_2) + f(\mathbf{r}). \quad (21)$$

Note that the integration constant  $f(\mathbf{r})$  is a function of the internal coordinate  $\mathbf{r}$  only. Now, knowing  $\chi$  we use the unitary operator  $U$  in order to transform  $\mathcal{H}$  and finally arrive at the following effective Hamiltonian for the system:

$$H = \frac{1}{2\mu} \left[ \mathbf{p} - \frac{e}{2} \frac{\mu}{\tilde{\mu}} \mathbf{B} \times \mathbf{r} + \nabla_r f(\mathbf{r}) \right]^2 + \frac{1}{2M} (\mathbf{K} - e \mathbf{B} \times \mathbf{r})^2 + V(\mathbf{r}) - e \mathbf{E} \cdot \mathbf{r}. \quad (22)$$

Here, we have introduced the reduced masses  $\mu = m_1 m_2 / M$  and  $\tilde{\mu} = m_1 m_2 / (m_2 - m_1)$  with  $m_1 < m_2$ . The only gauge-dependent term of the Hamiltonian (22) is the first term on its rhs. Schmelcher and Cederbaum [16] used Newton's equations of motion to show that this

term can be associated with the kinetic energy of the internal motion. With the charge  $q = e\mu/\bar{\mu}$  and the vector potential  $\mathbf{A}(\mathbf{r}) = \frac{1}{2}(\mathbf{B} \times \mathbf{r}) + 1/q \nabla_r f(\mathbf{r})$ , the operator of the kinetic energy of the internal relative motion can be written as

$$T = \frac{1}{2\mu}(\mathbf{p} - q \mathbf{A}(\mathbf{r}))^2. \quad (23)$$

The term  $1/2M(\mathbf{K} - e\mathbf{B} \times \mathbf{r})^2$  represents the kinetic energy of the center-of-mass motion. It depends only parametrically on the eigenvalue  $\mathbf{K}$  of the pseudomomentum. This kinetic energy and the remaining terms of  $H$  are according to Eq. (22) gauge independent. Therefore, they represent an effective potential for the internal motion,

$$\mathcal{V} = \frac{1}{2M}(\mathbf{K} - e\mathbf{B} \times \mathbf{r})^2 + V(\mathbf{r}) - e\mathbf{E} \cdot \mathbf{r}. \quad (24)$$

If  $\mathbf{E}$  is perpendicular to  $\mathbf{B}$  we get with  $\mathbf{K}' = \mathbf{K} - M\mathbf{v}_D$

$$\mathcal{V} = \frac{1}{2M}(\mathbf{K}' - e\mathbf{B} \times \mathbf{r})^2 + V(\mathbf{r}) + \frac{M}{2}\mathbf{v}_D^2 + \mathbf{K}' \cdot \mathbf{v}_D. \quad (25)$$

Here, the electric field appears only in  $\mathbf{K}'$  and the constant  $(M/2)\mathbf{v}_D^2 + \mathbf{K}' \cdot \mathbf{v}_D$ . The Hamiltonian now reads

$$H = T + \mathcal{V}. \quad (26)$$

This is an effective one-particle Hamiltonian for the internal motion of the two-particle system. It depends only on operators of the relative coordinates and momenta but it is linked to the center-of-mass motion via the eigenvalue  $\mathbf{K}'$  of the total pseudomomentum.

We were able to identify an effective potential for the internal motion containing the interaction potential, the potential due to the electric field, and the kinetic energy of the center-of-mass motion. In order to identify the latter term as a part of the effective potential we performed a gauge-independent pseudoseparation to make sure that it does not depend on the initial choice of the gauge.

### B. Elimination of the pseudomomentum for anisotropic harmonic interaction

We shall now apply another unitary transformation to the Hamiltonian (26) with an anisotropic harmonic interaction potential  $V(\mathbf{r}) = \mu/2(\tilde{\omega}_x^2 x^2 + \tilde{\omega}_y^2 y^2 + \omega_z^2 z^2)$ . The goal of this unitary transformation will be to eliminate the pseudomomentum dependent terms from the Hamiltonian by using shifted relative coordinates. We choose the magnetic field  $\mathbf{B} = (0, 0, B)$  and the symmetric gauge  $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ . It is sufficient to consider the case of a vanishing electric field. To transfer the results of the following to cases with nonvanishing electric field we only need to replace  $\mathbf{K}$  by  $\mathbf{K}' = \mathbf{K} - M\mathbf{v}_D$  and to add the constant  $(M/2)\mathbf{v}_D^2 + \mathbf{K}' \cdot \mathbf{v}_D$  to the energy [see Eqs. (24) and (25)].

Starting with the time-independent Schrödinger equation

$$H\Psi_0(\mathbf{r}) = E\Psi_0(\mathbf{r})$$

we follow an idea of Herold, Ruder, and Wunner [8] us-

ing the ansatz

$$\Psi_0(\mathbf{r}) = \exp\left[i\frac{\mu}{2\bar{\mu}}(\alpha_y K_x x + \alpha_x K_y y)\right] \Phi(\mathbf{r}') \quad (27)$$

for the eigenfunction where

$$\alpha_n = \left[1 + \frac{\mu M \tilde{\omega}_n^2}{e^2 B^2}\right]^{-1} \quad \text{for } n = x, y$$

and  $\mathbf{r}' = \mathbf{r} - \alpha \mathbf{r}_0$  with  $\mathbf{r}_0 = (\mathbf{K} \times \mathbf{B}) / (eB^2) = (1/eB)(K_y, -K_x, 0)$  and  $\alpha = (\alpha_x, \alpha_y, 0)$ . In the following we omit the primes on the coordinates. For the wave function  $\Phi(\mathbf{r})$  we get the Schrödinger equation in the form

$$\begin{aligned} H_1 \Phi(\mathbf{r}) &= \left[ \frac{\mathbf{p}^2}{2\mu} - \frac{eB}{2\bar{\mu}}(xp_y - yp_x) + \frac{\mu}{2} \left( \omega_x^2 + \frac{\omega_c^2}{4} \right) x^2 \right. \\ &\quad \left. + \frac{\mu}{2} \left( \omega_y^2 + \frac{\omega_c^2}{4} \right) y^2 + \frac{\mu}{2} \omega_c^2 z^2 + C \right] \Phi(\mathbf{r}) \\ &= E \Phi(\mathbf{r}). \end{aligned} \quad (28)$$

Here we used the abbreviations

$$\omega_c = \frac{-eB}{\bar{\mu}} \quad \text{and} \quad \omega_n = \left[ \frac{e^2 B^2}{M\mu} + \tilde{\omega}_n^2 \right]^{1/2} \quad (n = x, y) \quad (29)$$

and the constant

$$C = \frac{\mathbf{K}^2}{2M} - \frac{1}{2M}(K_x \alpha_y + K_y \alpha_x).$$

Introducing the charge  $q = e\mu/\bar{\mu}$  the Hamiltonian  $H_1$  is apart from the constant  $C$  identical to the Hamiltonian  $H$  of one particle in a magnetic field and an anisotropic harmonic potential given in Eq. (1). Therefore, all results obtained in Sec. II can be applied to the case of a neutral two-body system with anisotropic harmonic interaction in a magnetic field.

## IV. THE HYDROGEN ATOM IN CROSSED FIELDS

Having determined the eigenvalues and eigenfunctions of a two-particle system with anisotropic harmonic interaction in a magnetic field we now proceed considering a real physical system, the hydrogen atom. We will see that for the relative motion of electrons and protons in a magnetic field there is a potential well besides the Coulomb singularity. This well is approximately an anisotropic harmonic potential in the vicinity of its minimum. Accordingly, we can use the results of the preceding sections and compare them to the numerically calculated eigenstates of the hydrogen atom in the well.

### A. The potential of the internal motion

The interaction potential of the hydrogen atom is given by  $V(\mathbf{r}) = -e^2/|\mathbf{r}|$ . We choose  $e = -1$ ,  $\mathbf{B} = (0, 0, B)$ , and  $\mathbf{K} = (0, K, 0)$  orthogonal to  $\mathbf{B}$  since all components of  $\mathbf{K}$  parallel to the magnetic field result in an energy shift only



as can be seen from the potential operator in Eq. (25). The electric field is again assumed to vanish. To transfer the results of the following to the case of a nonvanishing electric field orthogonal to the magnetic field we only have to redefine  $\mathbf{K}$  as  $\mathbf{K}' = \mathbf{K} - M\mathbf{v}_D$  and add the constant  $(M/2)\mathbf{v}_D^2 + \mathbf{K}' \cdot \mathbf{v}_D$  to the energy. The operator of the potential of the relative motion [16] now reads [see Eq. (25)]

$$\mathcal{V} = \frac{B^2}{2M}(x^2 + y^2) + \frac{BK}{M}x - \frac{1}{|r|} + \frac{K^2}{2M}. \quad (30)$$

In Fig. 3 we have plotted this potential for  $B = 10^{-5}$  a.u. = 2.35 T with  $K = 1$  and 0.6. From the condition for a potential minimum ( $\partial V / \partial r_i = 0$ ) we calculate the  $y$  and  $z$  coordinates of the minimum,  $y_0 = z_0 = 0$ , and get an equation for the  $x$  coordinate,

$$x_0^3 + \frac{K'}{B}x_0^2 - \frac{M}{B^2} = 0,$$

where

$$x_0 < 0. \quad (31)$$

In order to get both a minimum and a saddle point the cubic equation must have three real zeros. From the form of the discriminant follows

$$K^3 > \frac{27}{4}BM \quad (32)$$

as a necessary condition for the existence of a minimum. Schmelcher and Cederbaum [16] have given an explicit

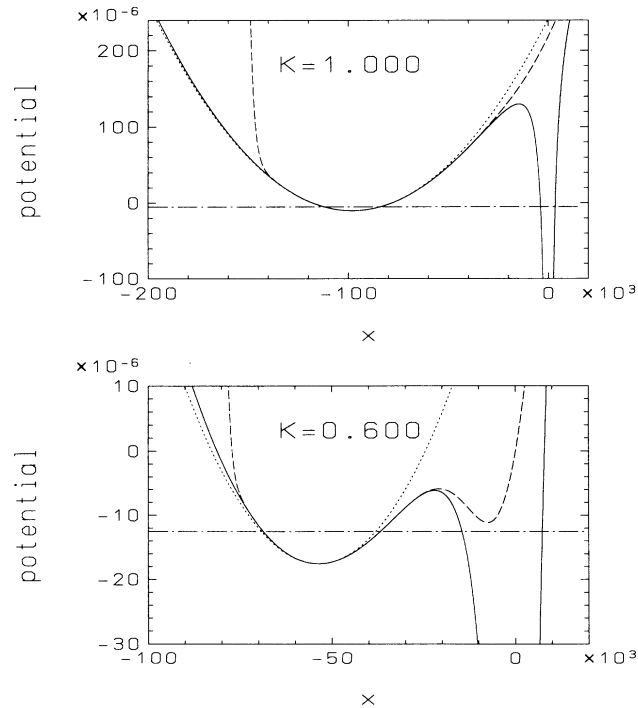


FIG. 3. Potentials of the internal motion of a hydrogen atom in a magnetic field. Solid line, exact potential; dashed line, expanded potential used in the numerical calculations; dotted line, harmonically approximated potential; horizontal line, ground-state energy. Parameters: (a)  $B = 10^{-5}$ ,  $K = 1.0$ ; (b)  $B = 10^{-5}$ ,  $K = 0.6$ .

approximation formula for the minimum coordinate:  $x_0 \approx -K/B + KM/(K^3 - 2MB)$ . Hence, for laboratory field strengths ( $B \sim 10^{-5}$  a.u.) and pseudomomenta of the order of 1 a.u. the minimum is located at a distance of about  $10^5$  a.u. from the Coulomb singularity. Therefore, for states in the well the electron and proton are separated about 100 000 times as much as they are in the ground state of the hydrogen atom without external fields, i.e., we encounter a strongly delocalized atom of almost macroscopic size. Since the well exists only for negative values of  $x$  the separation is fixed in a certain direction of space resulting in a large permanent dipol moment of the atom in contrast to the well-known Rydberg states with vanishing pseudomomentum in a magnetic field that do not exhibit a permanent dipol moment.

In the following we will investigate the quantum-mechanical states in the outer potential well. In the literature there are investigations on strongly delocalized states of the hydrogen atom by Baye, Clerbaux, and Vincke [26], Dzyaloshinskii [27], Schmelcher and Cederbaum [16], and Vincke, LeDourneuf, and Baye [28]. In Refs. [26], [27], and [16] the spectrum of the low-lying states in the potential well has been derived in a harmonic approximation using different methods. In Ref. [28] the spectrum and wave functions for states with energies above the saddle-point energy, i.e., above our potential well, have been calculated. The techniques used in Ref. [28] are only applicable for astrophysical field strengths  $B \gtrsim 10$  a.u. which corresponds roughly to  $2 \times 10^6$  T.

In [16] the potential picture has been given. Here, we present the results of exact numerical calculations of the spectrum and the corresponding wave functions in the well for laboratory field strengths. Many states up to a very high degree of excitation will be considered. We will compare both the numerically obtained eigenvalues and eigenfunctions of the atom to those of the harmonic oscillator approximation for which we presented the closed analytical form of the wave functions in Sec. II C.

### B. Approximation of the potential well

In order to interpret the full numerical results for the energies and wave functions of the hydrogen atom in a magnetic field to be presented in Sec. IV D we use an expansion of the Coulomb potential  $1/|r|$  around the minimum of the potential well. Including only terms up to  $x_0^{-3}$  we get the approximated potential [16]

$$V_h = \frac{\mu}{2}\omega_x^2 x^2 + \frac{\mu}{2}\omega_y^2 y^2 + \frac{\mu}{2}\omega_z^2 z^2 + C_3, \quad (33)$$

where we used new coordinates with the origin at the minimum of the well. The frequencies are given by

$$\begin{aligned} \omega_x &= \left[ \frac{2}{\mu} \left( \frac{B^2}{2M} + \frac{1}{x_0^3} \right) \right]^{1/2}, \\ \omega_y &= \left[ \frac{1}{\mu} \left( \frac{B^2}{M} - \frac{1}{x_0^3} \right) \right]^{1/2}, \\ \omega_z &= \left[ \frac{1}{\mu} \left( -\frac{1}{x_0^3} \right) \right]^{1/2}, \end{aligned} \quad (34)$$

and the constant reads  $C_3 = 2/x_0 - (B^2 x_0^2)/2M + K^2/2M + ME^2/2B^2 + KE/B$ . With this potential the Hamiltonian of the hydrogen atom takes on the form of the Hamiltonian of a charged particle in a magnetic field with anisotropic interaction [see Eq. (1)]. Therefore, we can use the analytical results of Sec. II as an approximation for the low-lying energies and wave functions of the hydrogen atom in the well. The approximate energies are given by

$$E_{n_+ n_- n_z} = (n_+ + \frac{1}{2})\omega_+ + (n_- + \frac{1}{2})\omega_- + (n_z + \frac{1}{2})\omega_z + C_3 \quad (35)$$

with the frequencies

$$\omega_{+,-} = \frac{1}{\sqrt{2}} [\omega_x^2 + \omega_y^2 + \omega_c^2 \pm \sqrt{(\omega_x^2 + \omega_y^2 + \omega_c^2)^2 - 4\omega_x^2 \omega_y^2}]^{1/2}.$$

The quantum numbers  $n_+$ ,  $n_-$ , and  $n_z$  apply to the eigenstates of the Hamiltonian with the harmonic potential  $V_h$  only. However, we will also use them as labels for the states of the hydrogen atom. For all calculated cases  $\omega_+$  will be much larger than  $\omega_-$ , therefore  $n_+$  will always be zero. An increase of the value of the label  $n_-$  will correspond to an increase of the extension of the wave function in the  $x$  and  $y$  directions, and an increase of the value of the label  $n_z$  will correspond to an increase of the extension of the wave function in the  $z$  direction.

In a second step, in order to determine the influence of the anharmonicity in the exact potential, we will expand the  $1/|\mathbf{r}|$  term up to higher powers of the components of  $\mathbf{r}$  and treat them as small perturbations to the harmonic approximation of the Hamiltonian by means of first-order perturbation theory. These perturbative calculations offer insight into the effects of the anharmonic parts of the potential onto the energies and the form of the wave functions.

### C. Numerical calculation of the exact eigenenergies and eigenfunctions in the outer potential well

In the following section we introduce the basis set and the computational techniques used for the numerical calculation of the eigenenergies and eigenfunctions in the outer potential well. Since the frequencies  $\omega_x$  and  $\omega_y$  in Eq. (33) differ only by a few percent for the values of the magnetic field strengths and pseudomomenta considered here the potential well of the atom has approximately cylindrical symmetry in the vicinity of its minimum. That is why we will express the Hamiltonian in cylindric coordinates and use the eigenfunctions of a charged particle in a magnetic field in cylindric coordinates [29] as basis functions in the plane perpendicular to the magnetic field.

Using the constant  $C_4 = ((B^2 x_0)/2M + BK/M + E)x_0 + K^2/2M$  and again taking the minimum of the well as the origin of the new coordinate system the Hamiltonian is now given as

$$H = H_0 + \frac{B^2}{2M} \rho^2 + \left[ \frac{B^2 x_0}{M} + \frac{BK}{M} + E \right] \rho \cos \phi - \frac{1}{\sqrt{\rho^2 + z^2 + x_0^2 + 2x_0 \rho \cos \phi}} + C_4, \quad (36)$$

where  $H_0$  is the Hamiltonian of a free charged particle with charge  $q = -\mu/\bar{\mu}$  in the magnetic field:

$$H_0 = -\frac{1}{2\mu} \left[ \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right] - i \frac{\omega_c}{2} \frac{\partial}{\partial \phi} + \frac{B^2 \mu}{8\bar{\mu}^2} \rho^2.$$

For our calculations we used the basis functions

$$\Psi_{nm}(\rho, \phi, z) = R_{nm}(\rho) \frac{e^{im\phi}}{\sqrt{2\pi}} \phi_{n_z}(z), \quad (37)$$

where  $\phi_{n_z}(z)$  are the eigenfunctions of the harmonic oscillator in  $z$  with the frequency  $\omega_z$  defined in Eq. (34) and the radial functions  $R_{nm}(\rho)$  are given by

$$R_{nm}(\rho) = \frac{1}{a_B^{|m|+1}} \left[ \frac{(|m|+n)!}{2^{|m|} n! (|m|)!} \right]^{1/2} \exp \left[ -\frac{\rho^2}{4a_B^2} \right] \times \rho^{|m|} F \left[ -n, |m|+1, \frac{\rho^2}{2a_B^2} \right]. \quad (38)$$

Here  $a_B = (1/\mu\omega_c)^{1/2}$  is the cyclotron radius and  $F(\alpha, \beta, \gamma)$  denotes the confluent hypergeometric function which for negative integers  $\alpha = -n$  and positive integers  $\beta = |m|+1$ , apart from a factor, equals the generalized Laguerre polynomial  $L_n^{(|m|)}(\gamma)$ . The  $\rho$  and  $\phi$  parts of the basis functions are eigenfunctions of  $H_0$  [29] with the eigenvalues

$$E_{nm} = \left[ n + \frac{|m|+m+1}{2} \right] \omega_c, \quad (39)$$

where  $n = 0, 1, 2, \dots$  and  $m = 0, \pm 1, \pm 2, \dots$ . In order to calculate the matrix elements of the Hamiltonian  $H$  given in Eq. (36) we expand the Coulomb term and use the discrete variable representation [30–34] for the  $z$  direction. The expansion is performed up to terms of very high powers ( $\approx 20$ ) of the components of  $\mathbf{r}$ . Neglecting higher terms of the Coulomb potential does not result in any significant deviation of the approximated potential from the exact potential in the relevant regions of the well where the calculated wave functions are localized. The remaining integrals over powers of  $\rho$  and  $\cos \phi$  can be calculated analytically. The free parameters of the calculation are the upper bound  $N$  of the quantum number  $n$ , the lower ( $M_{\min}$ ) and upper ( $M_{\max}$ ) bound of  $m$ , and the upper bound  $N_z$  of  $n_z$ . For our calculations we used IBM RS/6000 model 580 workstations. On these machines the diagonalization of a real  $10\,000 \times 10\,000$  matrix needs about 10 h of CPU time.

### D. Results

In the following we discuss the results of our calculations of eigenenergies and wave functions of the hydrogen atom in a magnetic field  $B = 10^{-5}$  for the values  $K = 1.0$  and  $0.6$ . One-dimensional intersections along the  $x$  axis of the exact potential for these two cases are plotted in Fig. 3 together with the harmonic approximated potential and the expanded potential we used in our calculations. In these plots we have also drawn a dashed horizontal line corresponding to the ground-state energy.

#### 1. $K = 1$

Let us first discuss the case  $B = 10^{-5}$  and  $K = 1.0$ . The results have been calculated using the parameters  $N = 3$ ,  $M_{\min} = -126$ ,  $M_{\max} = 10$ , and  $N_z = 25$  for the basis set. By comparison with calculations using smaller basis sets we can safely assume that about 700 eigenvalues and eigenfunction are converged. The accuracy of the energies is at least 10 digits.

The energy of the ground state in the potential well is  $E_0 = -5.0765 \times 10^{-6}$  a.u. =  $-0.138$  meV; the energy gap between the ground and first excited state is  $\Delta E = 5.38 \times 10^{-9}$  a.u. =  $1.46 \times 10^{-4}$  meV. The frequency corresponding to this energy is 35.3 MHz. The ground-state energy  $E_S$  of the completely separated, ionized, system, i.e., free electron and proton in the magnetic field, is given by the sum of the cyclotron energies of electrons and protons respectively. That is,

$$E_S = \frac{\omega_p}{2} + \frac{\omega_e}{2} = \frac{B}{2\mu}.$$

For  $B = 10^{-5}$  this energy has the value  $E_S = 5.0027 \times 10^{-6}$  a.u. Therefore, the binding energy of the ground state in the potential well is  $E_B = E_S - E_0 = 1.0079 \times 10^{-5}$  a.u. =  $0.274$  meV. Even though the binding of the states in the well is relatively weak they should be stable as long as collisional interaction is prevented.

Let us consider now the deviation of the exact energies from those of the harmonic approximation as a function of the level number. In Fig. 4 we have plotted the energy difference between the harmonic approximation and the exact energies of the hydrogen atom in units of  $\omega_-$ . We see that the difference grows stepwise while neighboring states show very different deviations from the harmonic approximation. To explain these features let us look at

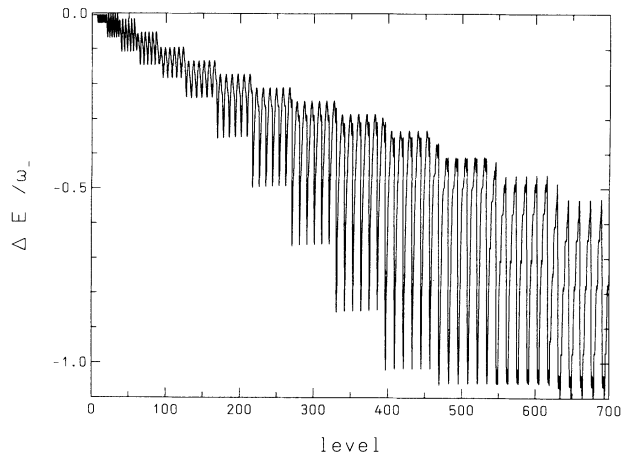


FIG. 4. Difference between harmonic approximated and exact energies of a hydrogen atom in a magnetic field in units of the frequency  $\omega_-$  as a function of the energy level. Parameters:  $B = 10^{-5}$ ,  $K = 1.0$ .

the energy level 331. We see that the difference between exact and approximated energies for this level is much larger than for the levels below 331. The level 331 has the quantum numbers  $n_+ = n_- = 0$  and  $n_z = 10$ , i.e., the quantum number  $n_z = 10$  appears for the first time. Looking at higher levels there are maxima of energy differences  $\Delta E / \omega_-$  every 11th level above 331 up to level 397. For these levels (342, 353, etc.) the quantum number  $n_z$  is 10 and  $n_- = 1, 2, \dots$ . Between two levels with  $n_z = 10$  there are levels with  $n_z < 10$ , and apparently the energy difference for these is smaller. That is, the difference between harmonic and exact energies is mostly determined by the quantum number  $n_z$ . Hence, the anharmonicity of the exact potential is most pronounced in the  $z$  direction. This can also be seen in perturbation theory for higher terms of the expansion of the Coulomb potential where the major contributions to the energy corrections are due to those terms containing high powers of  $z$ .

Let us now turn to the wave functions of the hydrogen atom in the well. In Table I we have listed the expectation value of  $x$  and the rms in  $x$ ,  $y$ , and  $z$  for some states with either  $n_z = 0$  or  $n_- = 0$ . The expectation values of  $y$  and  $z$  are zero for all these states. We see that for  $n_z = 0$  the wave function is centered near the minimum of the well. For increasing  $n_z$  the center of the wave function is

TABLE I. Expectation value  $x$  and root mean square in  $x$ ,  $y$ , and  $z$  for the wave functions of several states of the hydrogen atom in a magnetic field. Parameters:  $B = 10^{-5}$ ,  $K = 1.0$ . All values are given in atomic units.

Level	$n_+$	$n_-$	$n_z$	$\langle x \rangle$	$\sigma_x$	$\sigma_y$	$\sigma_z$
1	0	0	0	-4.71095	318.58000	313.93060	3907.19293
6	0	5	0	-4.50334	785.13007	764.23782	3907.30007
8	0	0	1	-14.17108	318.56584	313.94488	6775.21516
259	0	52	0	-2.54988	2336.01108	2268.85775	3908.30698
331	0	0	10	-97.10453	318.44277	314.11091	17679.04028
603	0	81	0	-1.34276	2905.81473	2821.96546	3908.92810
704	0	0	15	-141.50304	318.37772	314.23178	21061.14429

shifted towards negative values of  $x$ . This is due to the increasing extension of the wave function in  $z$  which makes these states be affected by the potential in regions of larger  $z$  where the minimum of the well is shifted to negative  $x$  values. In Table I we also see that the extension of the wave functions in  $x$  and  $y$  is the same for states with the same  $n_+$  and  $n_-$  and that the extension in  $z$  is the same for states with the same  $n_z$ . This shows that excitations in the plane perpendicular to the magnetic field are almost independent from those in the  $z$  direction. Furthermore, in general, the extension of the wave functions in the  $x$ - $y$  plane is much smaller than parallel to the field. Note that the extension of the wave functions in the  $x$ - $y$  plane is also much smaller than it would be in the same potential without the presence of a magnetic field. Apparently, the form of the wave function is determined substantially by the field-dependent kinetic energy.

Looking at the form of the wave functions we restrict ourselves to intersections perpendicular to the field. In

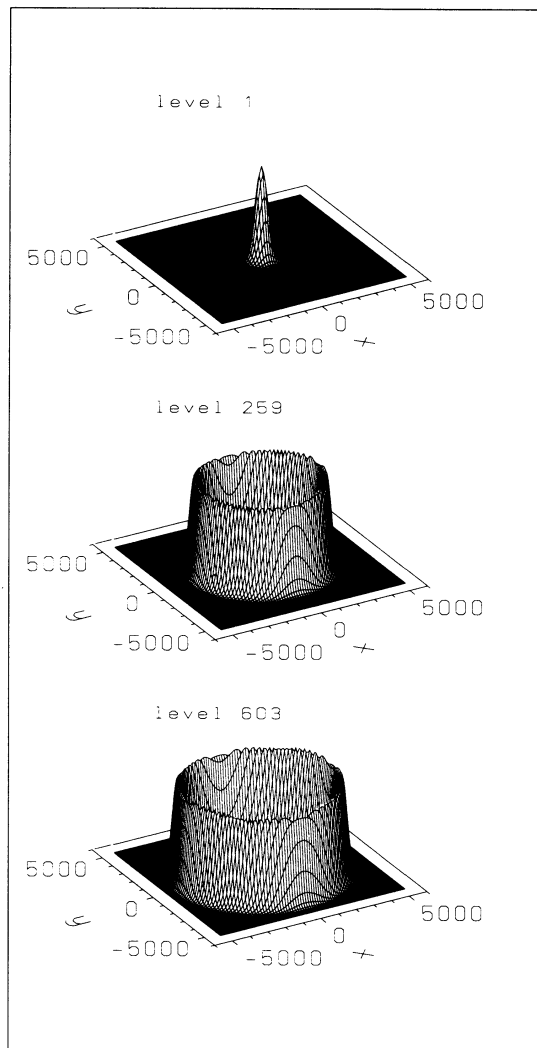


FIG. 5. Square of the absolute value of the wave functions of the hydrogen atom in a magnetic field. Shown are intersections in the plane perpendicular to the magnetic field. Parameters:  $B = 10^{-5}$ ,  $K = 1.0$ .

the  $z$  direction the form of the wave function is almost that of a harmonic oscillator changed only slightly by small corrections due to higher terms of the  $1/|r|$  expansion. Figure 5 shows the square of the absolute value of the wave functions of three states of the hydrogen atom in the well. They look almost the same as the corresponding wave function of the harmonic approximation. The small changes of the wave function due to the slightly anharmonic form of the potential well are only very hardly visible on the scale given in Fig. 5. This is different for smaller values of the pseudomomentum as will be seen in the following section.

## 2. $K = 0.06$

Let us now investigate the eigenvalues and wave functions of the hydrogen atom in the magnetic field  $B = 10^{-5}$  with pseudomomentum  $K = 0.6$ . As can be seen in Fig. 3 the deviation of the exact potential from the harmonic approximation is larger than for  $K = 1.0$ . Therefore, we expect larger energy differences and differences between the wave functions of the exact and approximated states.

In the following we discuss results of a calculation with parameters  $N = 3$ ,  $M_{\min} = -190$ ,  $M_{\max} = 10$ , and  $N_z = 17$ . By comparison with calculations with smaller basis sets we can assume that at least 400 energies and wave functions are converged. The energies are given in at least ten significant digits. The ground-state energy in the well is  $E_0 = -1.2499 \times 10^{-5}$  a.u.  $= -0.3399$  meV. Since the ground-state energy of the free electron and proton,  $E_S$ , is the same as in the case  $K = 1$ , the binding energy of the ground state in the well  $E_B = E_S - E_0 = 1.75 \times 10^{-5}$  a.u.  $= 0.476$  meV is larger than for  $K = 1$ .

Figure 6 illustrates the difference between the exact and approximated energies. We see the same features as in the case  $K = 1$ . However, the differences are larger than in the above case.

Also the size and location of the wave functions, given for some states in Table II, show similar features as those in the case  $K = 1$ . However, the shift in the  $x$  direction of

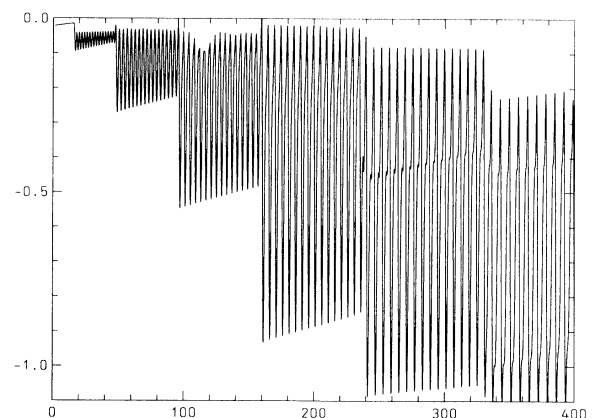


FIG. 6. Difference between harmonic approximated and exact energies of a hydrogen atom in a magnetic field in units of the frequency  $\omega_-$  as a function of the energy level. Parameters:  $B = 10^{-5}$ ,  $K = 0.6$ .

TABLE II. Expectation value  $x$  and root mean square in  $x$ ,  $y$ , and  $z$  for the wave functions of several states of the hydrogen atom in a magnetic field. Parameters:  $B = 10^{-5}$ ,  $K = 0.6$ . All values are given in atomic units.

Level	$n_+$	$n_-$	$n_z$	$\langle x \rangle$	$\sigma_x$	$\sigma_y$	$\sigma_z$
1	0	0	0	-26.497 73	332.505 94	302.149 89	2479.887 90
17	0	0	1	-80.215 99	332.304 20	302.304 03	4304.264 09
108	0	50	0	9.810 08	2484.797 75	2053.088 07	2480.842 26
204	0	72	0	26.027 74	2974.399 46	2454.927 62	2481.254 15
238	0	0	5	-288.591 24	331.534 17	302.928 65	8196.028 81
306	0	90	0	39.409 60	3322.071 03	2739.965 62	2481.587 40

the center of the wave functions is more pronounced for  $K = 0.6$  than for  $K = 1$ .

A major difference between the states for  $K = 0.6$  and 1 appears in the *form* of the wave functions. In Fig. 7 we have plotted the square of the absolute value of the wave functions of two states that are highly excited in the plane perpendicular to the field. The ground state and less highly excited states are not shown since they do not exhibit major differences to the harmonic approximation. Shown are the results in the harmonic approximation, this approximation plus corrections from first-order perturbation theory for higher terms of the  $1/|r|$  expansion, and the numerical results for the exact wave functions. We see that the harmonic approximation leads to a wave

function whose intensity is evenly distributed over an elliptical ring surrounding the minimum of the well. In contrast, due to corrections from anharmonic terms the intensity of the wave functions of the hydrogen atom for states that are highly excited in the plane perpendicular to the magnetic field is largely reduced close to the  $x$  axis both in the perturbation calculation and the exact results. Apparently, this deviation from the wave functions of the harmonic approximation is due to the anharmonicity of the potential. In the perturbation calculation we included only a few terms of the  $1/|r|$  expansion. That is why the decrease of intensity of the wave functions appears on the level of perturbation theory for even smaller values of the label  $n_-$  than in the exact calculation.

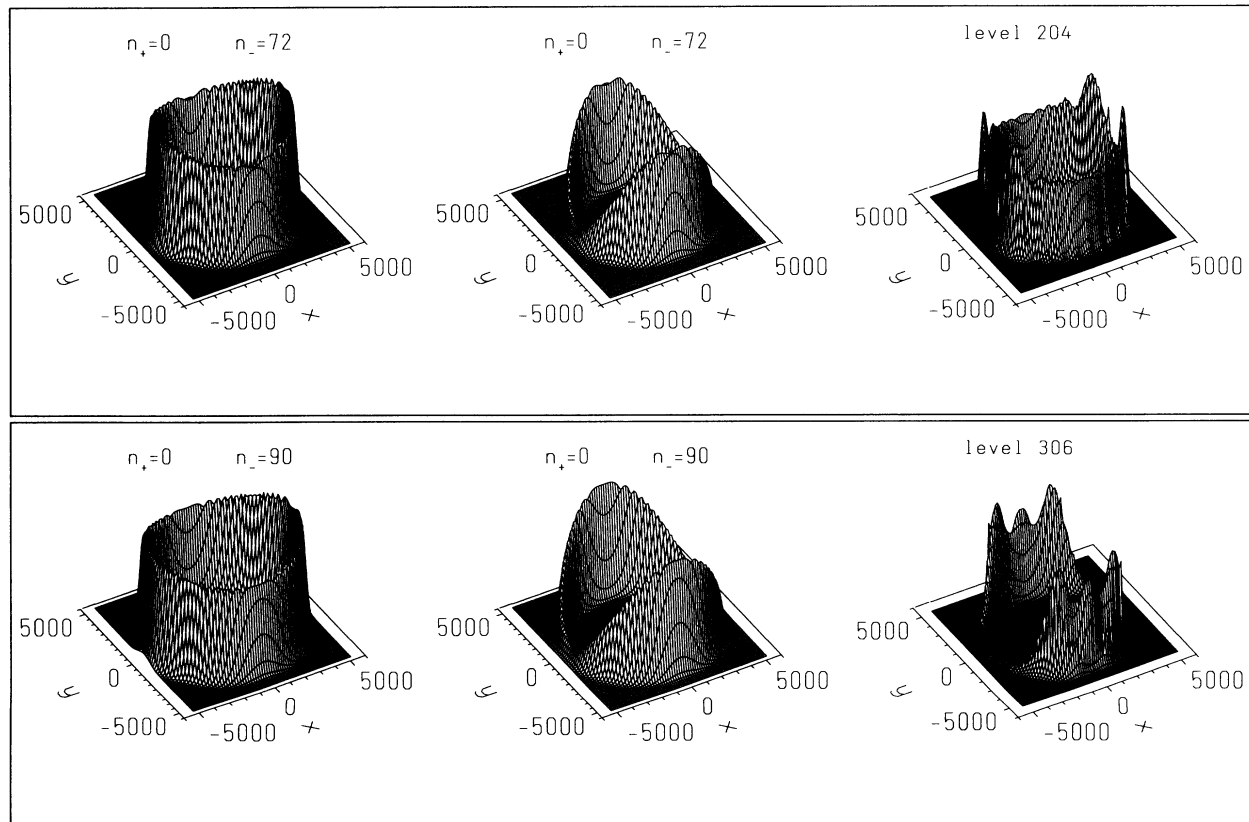


FIG. 7. Square of the absolute value of the wave functions of the hydrogen atom in a magnetic field. Shown are intersections in the plane perpendicular to the magnetic field for the harmonic approximation, for perturbation theory, and for the exact Hamiltonian (from left to right). Parameters:  $B = 10^{-5}$ ,  $K = 0.6$ .

### E. Summary and conclusions

In the present paper we have performed a gauge-independent pseudoseparation of the center-of-mass motion for a neutral two-body system with translation-invariant interaction in crossed fields. In the resulting Hamiltonian we were able to identify terms that depend on a (gauge-dependent) vector potential and belong to the kinetic energy of the internal motion. The complementary terms of the Hamiltonian are gauge independent and can, therefore, be assigned to an effective potential of the internal motion of the atom. The transformed Hamiltonian has been investigated for two different cases of interaction between the two particles. First, the Hamiltonian of a two-particle system with *anisotropic* harmonic interaction was further transformed to the form of a one-particle Hamiltonian of a charged harmonic particle in a magnetic field. We have calculated the eigenenergies and presented a complete analytical solution for the eigenfunctions of this charged particle in a magnetic field and an anisotropic harmonic potential.

The second two-particle system in a magnetic field which we investigated was the hydrogen atom in crossed fields. We were able to present a potential picture for the relative motion of the electron and proton. Due to the influence of the center-of-mass motion there is a potential well for large separations (typically several 10 000 Å) of the electron and proton. A method has been introduced to numerically compute the eigenvalues and the corresponding wave functions in this potential well. These calculations proved to be very efficient allowing us to calculate several hundred eigenstates to a very high accuracy even though the energy spacing between neighboring states is extremely small (of the order of a few MHz) and consequently the density of states is very high. Due to the large separation of the well from the Coulomb singularity the hydrogen atom in the well has a very large dipole moment. For laboratory field strengths we investigated two different cases ( $K=1.0$  and  $0.6$  a.u.) for which the density of states and the anharmonicity of the potential are different. We compared the states in the well to those of a harmonic approximated potential. It became apparent that, in particular for the case  $K=0.6$ , both the energies and the form of the wave functions of the hydrogen atom exhibit major differences to those of the harmonic approximated potential. First-order perturbation theory for the leading anharmonic terms of the expansion of the exact Hamiltonian proved that the differences between the energies and wave functions of the exact and the harmonic Hamiltonian are due to the lowest anharmonic terms. We remark that the pseudomomentum  $K$

emerges either from the induced electric field due to the motion of the center of mass of the hydrogen atom or/and an external electric field which is oriented perpendicular to the magnetic one. The values of  $K=1.0, 0.6$  a.u. used above correspond to an external electric field strength of  $2.8 \times 10^3$  and  $1.7 \times 10^3$  V/m, respectively.

For an experimental verification of the existence of the states in the well, for which the separation of the electron and the proton is extremely large, there are, in principle, two possibilities of investigation. The first one is the spectroscopical observation of the state-to-state transitions which belong to the radio-frequency regime. A second, probably more promising, approach to experimental verification of the existence of states in the well is the measurement of their dipole moment. The distance between the electron and proton is much larger than the extension of the wave function in the well. Therefore, to calculate the dipole moment of the hydrogen atom for states in the well we approximate the distance between the electron and proton by the distance between the minimum of the well and the Coulomb singularity which is approximately given by  $x_0 \approx -K/B$ . Using this expression for the separation of the electron and proton the dipole moment is  $d = |x_0|$ . For typical laboratory conditions  $B=10^{-5}$  a.u. and  $K=1$  a.u. we get  $d \approx 10^5$  a.u.  $\approx 2.4 \times 10^5$  D. For comparison, the dipole moment of NaCl is only about 9 D.<sup>2</sup> The unanswered question and experimental challenge in both methods is the preparation of states in the well, i.e., with a defined value of the pseudomomentum.

There have been experiments that indicate the existence of atoms with very large dipole moments in magnetic fields [36,37] for energies above the saddle-point energy. Fauth, Walter, and Werner [36] published results of experiments with Rydberg atoms in magnetic fields ( $B \approx 0.1 \times 10^{-5}$  a.u.). Their rough estimate for the dipole moment of these atoms is  $1.9 \times 10^4$  D. This value of the dipole moment is roughly of the order of magnitude to be expected.

### ACKNOWLEDGMENTS

It is a pleasure for us to thank H.-D. Meyer for many fruitful and illuminating discussions and in particular for his most useful suggestions concerning the mathematical and computational aspects of the present work.

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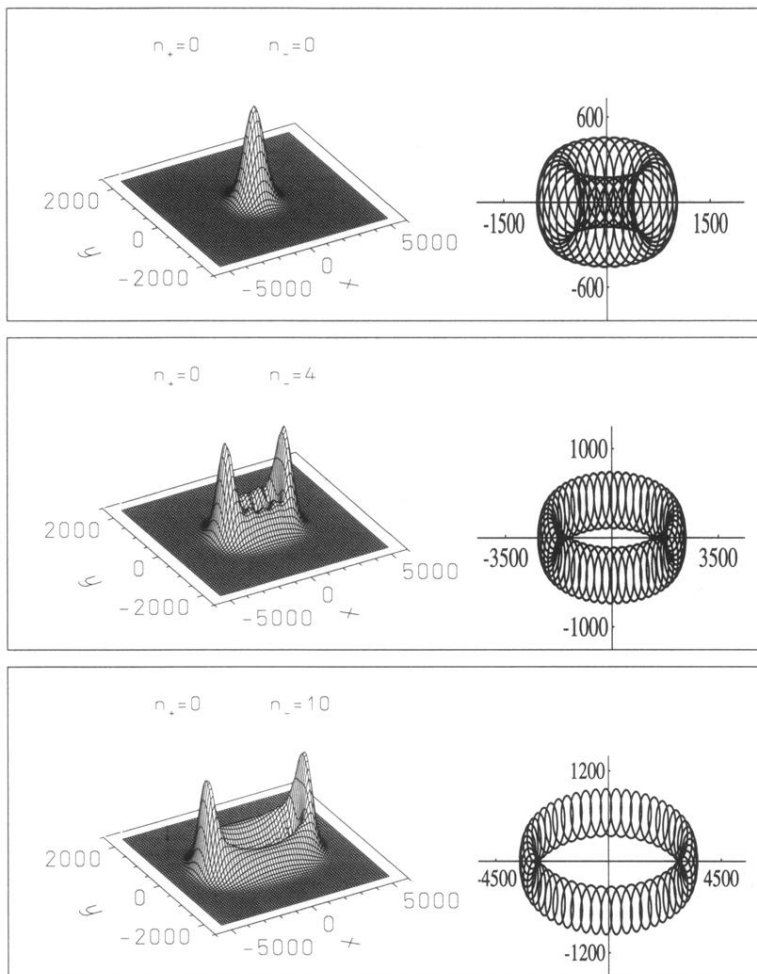


FIG. 1. Square of the absolute values of the wave functions of  $H_{xy}$  and corresponding classical trajectories. Quantum numbers are indicated in the plots. Parameters:  $B=10^{-5}$ ,  $\omega_x=10^{-7}$ , and  $\omega_y=5\times 10^{-7}$ . All values are given in atomic units.



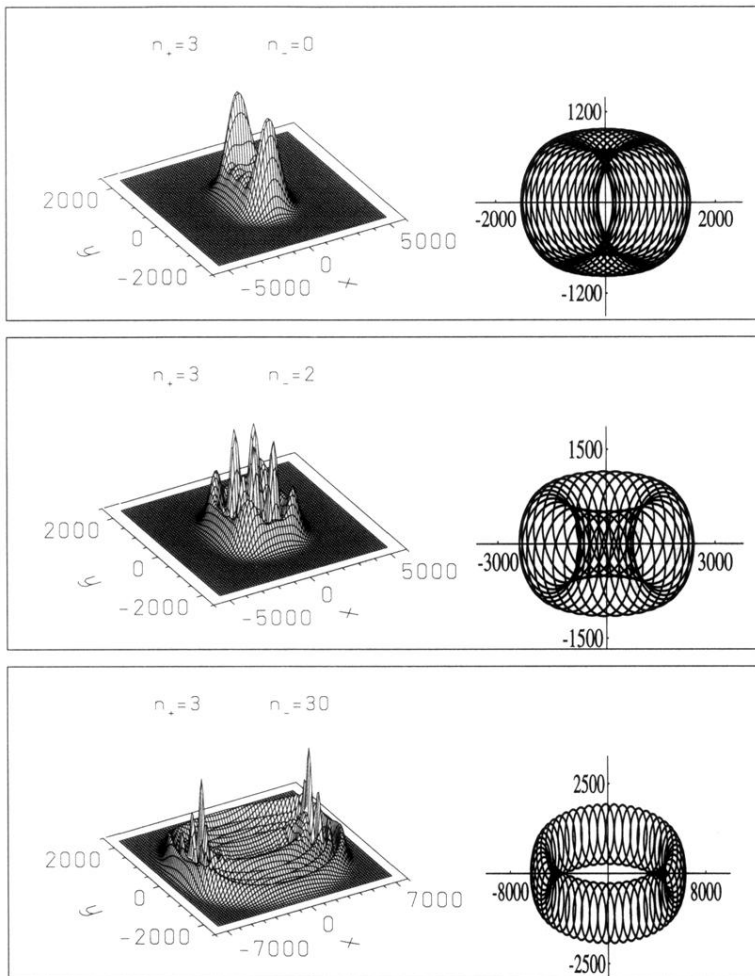
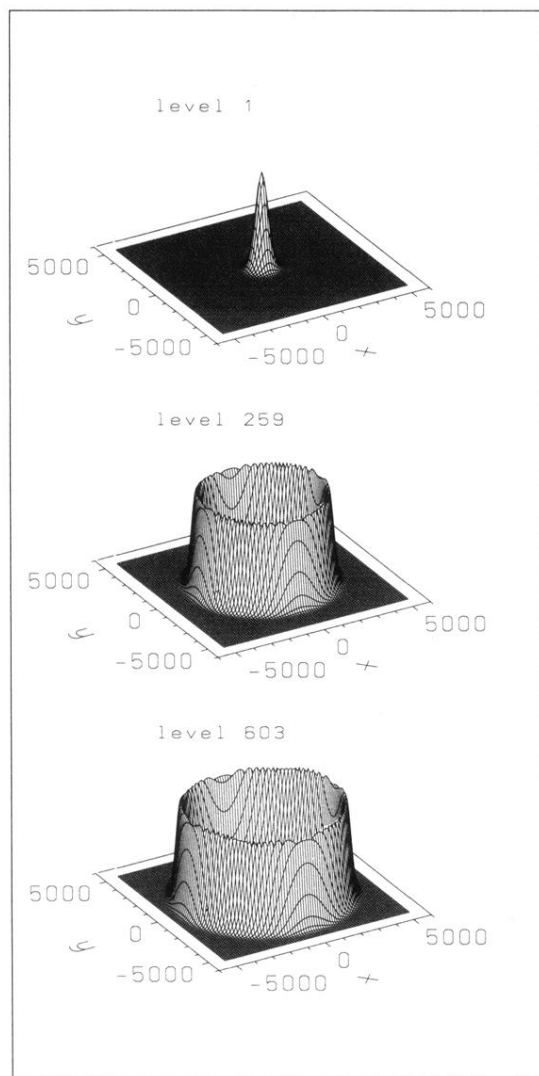
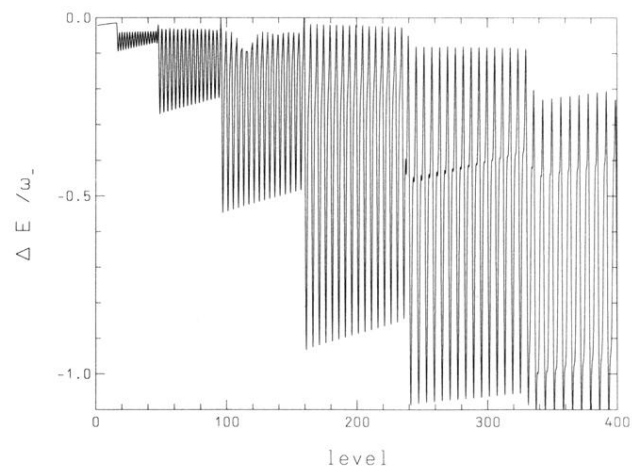


FIG. 2. Square of the absolute values of the wave functions of  $H_{xy}$  and corresponding classical trajectories. Quantum numbers are indicated in the plots. Parameters:  $B = 10^{-5}$ ,  $\omega_x = 10^{-7}$ , and  $\omega_y = 5 \times 10^{-7}$ .



**FIG. 5.** Square of the absolute value of the wave functions of the hydrogen atom in a magnetic field. Shown are intersections in the plane perpendicular to the magnetic field. Parameters:  $B = 10^{-5}$ ,  $K = 1.0$ .



**FIG. 6.** Difference between harmonic approximated and exact energies of a hydrogen atom in a magnetic field in units of the frequency  $\omega_-$  as a function of the energy level. Parameters:  $B=10^{-5}$ ,  $K=0.6$ .

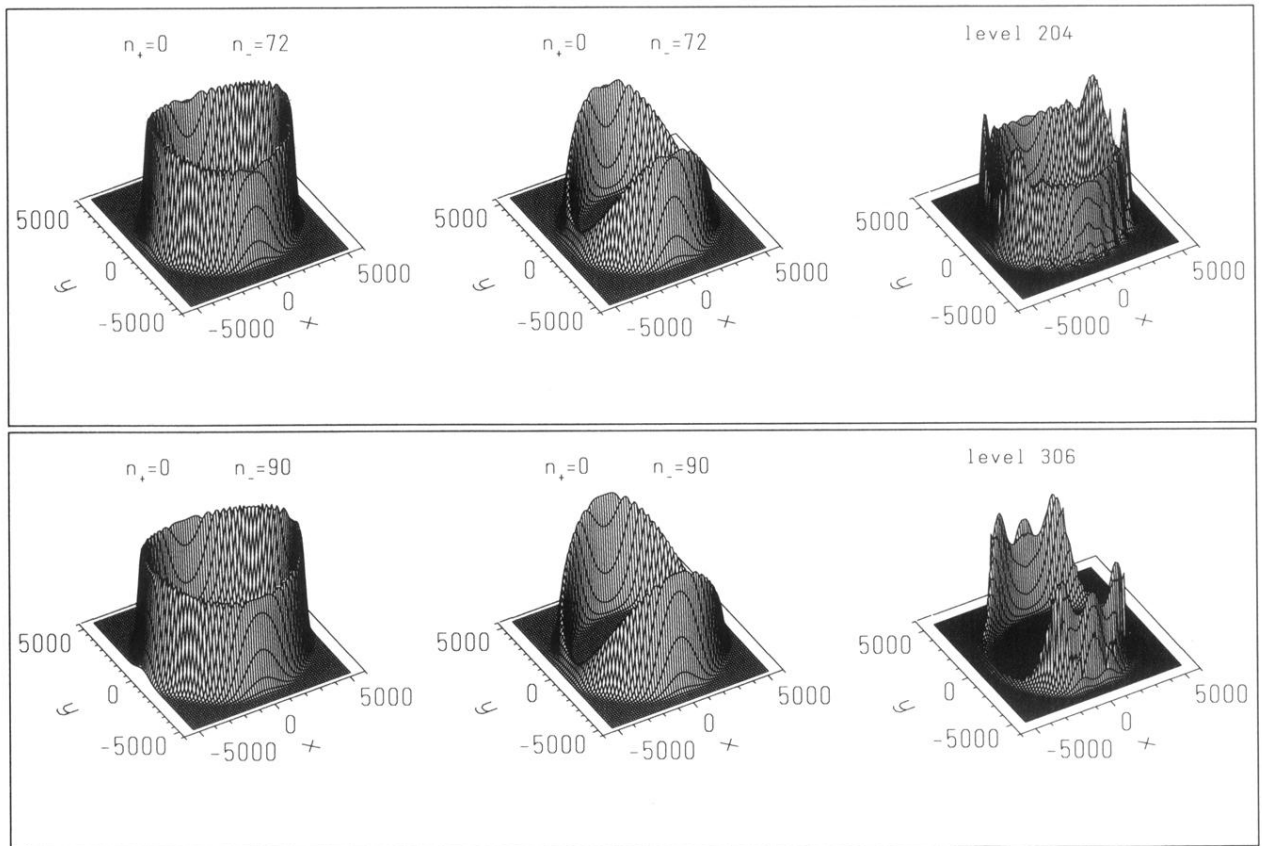


FIG. 7. Square of the absolute value of the wave functions of the hydrogen atom in a magnetic field. Shown are intersections in the plane perpendicular to the magnetic field for the harmonic approximation, for perturbation theory, and for the exact Hamiltonian (from left to right). Parameters:  $B = 10^{-5}$ ,  $K = 0.6$ .