PHYSICAL REVIEW A VOLUME 43, NUMBER 1 1 JANUARY 1991

Interaction of the Landau orbitals of atomic ions in a magnetic field with electronic motion

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(Received 16 August 1990)

For neutral particle systems in a homogeneous magnetic field, there exists a constant of motion, the pseudomomentum, which allows a complete pseudoseparation of the center-of-mass motion. For ions such a separation is not possible, and the Landau orbit of the center-of-mass and internal (electronic) motion are intimately coupled. We investigate different physical situations for which this interaction becomes strong at laboratory magnetic-field strengths. In particular, we find that the Landau orbit itself can change substantially upon this interaction.

I. INTRODUCTION

The behavior of matter in strong magnetic fields became in the past ten years a subject of great interest. In solid-state physics, for example, both of the revolutionary discoveries of the 1980s, the quantum Hall effect and the high-temperature superconductors, are the result of or at least intimately related to the action of a magnetic field on matter. On the other hand, the discovery of strong magnetic fields, unavailable in the laboratory, on astrophysical objects like white dwarfs ($\approx 10^4$ T) and neutron stars ($\approx 10^8$ T) was the motivation and the starting point for a rapid development of our knowledge on the behavior of atoms and molecules in the presence of a strong magnetic field. In atomic physics the main object of interest was the simplest of all atoms: the hydrogen atom.[1-4] With the increasing knowledge and especially the rapid improvement of the computational techniques it was, within the past five years, possible to calculate the eigenvalues and the eigenfunctions of the hydrogen atom in the presence of a magnetic field up to the field-free ionization threshold. For these Rydberg states of the hydrogen atom the magnetic energies become, already at laboratory magnetic-field strengths, comparable or even larger than the Coulomb binding energies. It was therefore possible to study the behavior of the hydrogen atom in the intermediate- and high-field regions, which are characterized by the ratio of the magnetic and Coulomb energies, by decreasing the Coulomb binding energies, i.e., by investigating highly excited states. The original interest in the behavior of the hydrogen atom in a strong magnetic field being motivated by astrophysical observations, it came now into the focus field of physics: the quantum chaos. The hydrogen atom is one of the simplest quantum-mechanical systems that allows an experimental as well as theoretical investigation of the transition of regularity to irregularity.[5-7]

The enormous increase in our knowledge of the behavior of atoms and molecules in strong magnetic fields should not obscure the fact that many of the *fundamental* problems are still unsolved. One of these problems, which is the subject of the present paper, is the mutual influence of the center-of-mass and internal motion of an atomic ion in a homogeneous magnetic field. Before going into the details of the treatment of the center-of-mass motion of a charged atom let us recall the situation for a neutral atom. In the neutral case there exist three exact constants of motion, the components of the total pseudomomentum **K**, which commute among each other and can be used to perform a pseudoseparation of the center-of-mass motion of the atom.[8-13] The residual influence of the center-of-mass motion on the internal motion is described by a motional Stark effect. The corresponding *constant* electric field is induced by the collective motion of the neutral atom in the magnetic field. The center of mass follows, more or less, a straight line or, in the language of quantum mechanics, the dependency of the total wave function on the center-of-mass coordinate is given by a plane wave. For a neutral particle system there exists no possibility for the system to change its state of collective motion. Once the constant total pseudomomentum is given it is fixed forever or intuitively spoken: there exists no real interaction between the center-of-mass and internal motion. Especially it is possible to eliminate the effects of the center-of-mass motion on the internal motion by choosing the pseudomomentum parallel to the magnetic-field axis. The abovementioned theoretical as well as experimental investigations of the hydrogen atom have used this fact in order to get rid of the motional Stark effect. The additional electric field, which is perpendicular to the magnetic field, provided for those investigations only an additional undesired complication.

For a charged-particle system the situation is completely different. Although the pseudomomentum is still an exact constant of motion it cannot be used for a *complete* pseudoseparation of the center-of-mass motion since its components do not commute. As a consequence an additional approximately conserved kinetic momentum has been introduced in the literature.[14,15] This quantity can be used, together with the total pseudomomentum, to perform a partial center-of-mass separation.[16,17] The resulting Hamiltonian has consequently been used to study the corrections to the collective and internal motion, arising from the coupling terms of the Hamiltonian between the center of mass and the internal degrees of freedom.[17,18] However, all these investigations were performed only for the ground and first few excited states of small atomic ions. The total ground state of the atom means that the internal as well as collective motion, including the couplings between them, are in the ground state. Considerable corrections due to the couplings appear then only for astrophysical magnetic-field strengths, i.e., for field strengths of the order of magnitude or larger than 10^5 T.

Within the present paper we choose an alternative way of performing a partial center-of-mass separation for an atomic ion (see also Ref. 19) and pay particular attention to excited states instead of to the ground state. We are able to show that the coupling between the center-of-mass and the internal motion becomes large at laboratory magnetic-field strengths if *either* the collective motion *or both* the collective and internal motion correspond to highly excited states. As a consequence we expect a variety of interesting new effects, whose detailed investigations go beyond the scope of this paper and will be the subject of future studies.

II. THEORY

Our starting point is the nonrelativistic Hamiltonian in Cartesian coordinates for an atomic ion in a homogeneous magnetic field:

$$H_c' = \sum_i \frac{1}{2m_e}(\mathbf{p}_i' - e\,\mathbf{A}_i')^2 + \frac{1}{2M_0}(\mathbf{P}' + eZ\,\mathbf{A}')^2 + V\ , \tag{1}$$

where we have omitted the rather trivial interaction of the spins with the magnetic field. m_e and M_0 are the electron and nuclear mass, respectively. e is the electron charge, Z the nuclear charge number. $\{\mathbf{p}_i'\}$ and $\mathbf{P}'$ are the canonical conjugated momenta of the electrons and the nucleus, respectively. V contains all the Coulomb interaction terms of the electrons and the nucleus. The vector potential will in the following be chosen in the symmetric gauge, i.e., $\mathbf{A}_i' = \frac{1}{2}\mathbf{B}\times\mathbf{r}_i'$ and $\mathbf{A}' = \frac{1}{2}\mathbf{B}\times\mathbf{R}'$. $\mathbf{B}$ is the magnetic-field vector. The total pseudomomentum

$$\mathbf{K}' = \sum_i (\mathbf{p}_i' + e\,\mathbf{A}_i') + (\mathbf{P}' - eZ\,\mathbf{A}') \tag{2}$$

is a constant of motion, i.e., it commutes with the Hamiltonian (1). The first step in our center-of-mass separation is the transformation of the Hamiltonian (1) from Cartesian coordinates to the coordinate system which contains the center-of-mass coordinate $\mathbf{R}_S$ and the relative coordinates $\{\mathbf{r}_i\}$ of the electrons with respect to the nucleus. The resulting Hamiltonian H' takes on the following appearance:

$$\begin{aligned} H' = \sum_i \frac{1}{2m_e} \Bigg[\mathbf{p}_i - \frac{e}{2}\mathbf{B}\times\mathbf{r}_i + \frac{e}{2}\frac{m_e}{M}\mathbf{B}\times\sum_j \mathbf{r}_j \\ + \frac{m_e}{M}\mathbf{P}_S - \frac{e}{2}\mathbf{B}\times\mathbf{R}_S \Bigg]^2 \\ + \frac{1}{2M_0}\Bigg[\sum_i \mathbf{p}_i + \frac{e}{2}\frac{Zm_e}{M}\mathbf{B}\times\sum_i \mathbf{r}_i \\ - \frac{M_0}{M}\mathbf{P}_S - \frac{e}{2}Z\mathbf{B}\times\mathbf{R}_S \Bigg]^2 + V\ , \end{aligned} \tag{3}$$

where M is the total mass of the atom. $\{\mathbf{p}_i\}$ and $\mathbf{P}_S$ are the canonical conjugated momenta of the coordinates $\{\mathbf{r}_i\}$ and $\mathbf{R}_S$, respectively. The total pseudomomentum reads as follows:

$$\mathbf{K} = \mathbf{P}_S + \frac{Q}{2}\mathbf{B}\times\mathbf{R}_S + \frac{e}{2}\alpha\mathbf{B}\times\sum_i \mathbf{r}_i\ , \tag{4}$$

where Q is the net charge of the ion and $\alpha = (M_0 + Zm_e)/M$. The reader should note that α is of the order of 1, i.e., $\alpha \approx 1$, for an ion and it is exactly 1, i.e., $\alpha = 1$, for the case of a neutral system. The Hamiltonian H' has a complicated structure. The terms involving only the center of mass or the internal degrees of freedom as well as the coupling terms between both types of motion have no simple interpretation. But what should be the aim of our transformations? From a physically intuitive picture we expect the part of the Hamiltonian which involves only the center-of-mass degrees of freedom to be the Hamiltonian for a free particle with mass M and charge Q in a homogeneous magnetic field. This is obviously not the case for the Hamiltonian H' in Eq. (3).

As a next step we transform the Hamiltonian H', in analogy to the case of a neutral particle system,[8-13] by a unitary gauge transformation

$$H = U^{-1}H'U \tag{5}$$

with

$$U = \exp\left[+i\frac{e}{2}\alpha(\mathbf{B}\times\mathbf{R}_S)\sum_i \mathbf{r}_i \right] .$$

After some algebra we arrive at the following final structure for our Hamiltonian H:

$$H = H_1 + H_2 + H_3\ , \tag{6}$$

where

$$H_1 = \frac{1}{2M}\left[\mathbf{P}_S - \frac{Q}{2}\mathbf{B}\times\mathbf{R}_S \right]^2 , \tag{6a}$$

$$H_2 = -\frac{e}{M}\alpha\left[\mathbf{P}_S - \frac{Q}{2}\mathbf{B}\times\mathbf{R}_S \right]\cdot\left[\mathbf{B}\times\sum_i \mathbf{r}_i \right] , \tag{6b}$$

$$\begin{aligned} H_3 = \sum_i \frac{1}{2m_e}\left[\mathbf{p}_i - \frac{e}{2}\mathbf{B}\times\mathbf{r}_i + \frac{Q}{2}\frac{m_e^2}{M^2}\mathbf{B}\times\sum_j \mathbf{r}_j \right]^2 \\ + \frac{1}{2M_0}\Bigg[\sum_i \mathbf{p}_i + \left[\frac{e}{2} - \frac{Q}{2M}\frac{m_e}{M}(M + M_0) \right] \\ \times\mathbf{B}\times\sum_i \mathbf{r}_i \Bigg]^2 + V\ . \end{aligned} \tag{6c}$$

The Hamiltonian H has indeed the structure we were looking for. The unitary transformation U decoupled, to some extent, the collective and internal motion. The pure center-of-mass Hamiltonian H_1 has the desired structure: it describes the motion of a free pseudoparticle with charge Q and mass M in a homogeneous magnetic field. H_2 is the coupling term between the collective and internal motion which is proportional to the velocity of the heavy pseudoparticle. H_3 describes the internal relative motion of the electrons and the nucleus. We remark that the above performed partial separation of the center-of-mass motion presumes the validity of the physical picture that the electrons somehow follow the nuclear motion, i.e., are bound to the nucleus by the potential V.

The Hamiltonian for the case of a neutral atom can be obtained from Eqs. (6a)–(6c) by setting $Q=0$ and replacing the operator $\mathbf{P}_S$ by its eigenvalue, the *constant* pseudomomentum $\mathbf{k}$. For a neutral atom the center of mass follows more or less a straight line and there exists no real interaction between the collective and internal motion. For an atomic ion, however, the situation is completely different. The center of mass performs in the plane perpendicular to the magnetic field in zeroth order a Landau motion which is described by the Hamiltonian H_1. The especially important novelty is that there exists a dynamical coupling term H_2 between this collective and the internal motion. This coupling term is proportional to the cross product of the center-of-mass velocity and the magnetic field which represents a rapidly *changing internal* electric field. Because of this "dynamical" electric field the collective and internal motion will, as we shall see later on, mix up heavily, i.e., it is possible for the ion to change its state of collective or internal motion through the coupling term H_2. Since the ion possesses at least a zero-point Landau energy the coupling term cannot vanish and is an inherent property of the center-of-mass motion of a charged-particle system in a magnetic field. This is in contrast to the case of a neutral system where the influence of the center-of-mass motion on the internal motion is given by a motional Stark effect with a *constant* electric field, which can be set equal to zero by choosing the *constant* total pseudomomentum parallel to the magnetic-field axis.

In order to investigate the significance and effects of the Hamiltonian H_2, which couples the collective and internal motion, we apply in the following a method for formally solving the total Schrödinger equation $H\Psi=E\Psi$. The most natural way is to expand the total wave function Ψ in a series of products

$$\Psi(\mathbf{R}_S;\{\mathbf{r}_i\})=\sum_{p,q} c_{pq}\Phi_p^L(\mathbf{R}_S)\psi_q(\{\mathbf{r}_i\}) , \tag{7}$$

where $\{c_{pq}\}$ are the coefficients of the product expansion. In Eq. (7) the trivial one-dimensional free motion of the center of mass along the magnetic-field axis has been omitted. The functions $\{\Phi_p^L\}$ obey the Schrödinger equation $H_1\Phi_p^L=E_p^L\Phi_p^L$ for a free particle with charge Q and mass M in a homogeneous magnetic field. These so-called Landau orbitals[20] read in cylindrical coordinates (ρ_S,φ_S) (the magnetic field is assumed to be oriented along the z axis) as follows:

$$\Phi_p^L=\left[\frac{(|\mu|+N)!}{(2\pi)2^{|\mu|}N!}\right]^{1/2}\frac{1}{|\mu|!a^{1+|\mu|}}\exp(\pm i\mu\varphi_S)$$
$$\times\rho_s^{|\mu|}\exp(-\rho_S^2/4a^2)F(-N,|\mu|+1,\rho_S^2/2a^2) , \tag{8}$$

where the sign ± corresponds to negative and positive charge Q, respectively. The simple index p stands for the quantum numbers N and μ. F is the confluent hypergeometric function which, in our special case, is equal to a generalized Laguerre polynomial. $a=(|Q|B)^{-1/2}$ is the typical length unit. The energy eigenvalues are given by

$$E_p^L=\frac{|Q|B}{M}\left[N+\frac{\mu+|\mu|+1}{2}\right] ,$$
$$N=0,+1,\ldots,\quad \mu=0,\pm1,\ldots, \tag{9}$$

which is, apart from the fact that each Landau level is infinitely degenerate, a harmonic oscillator spectrum.

The functions $\{\psi_q\}$ in Eq. (7) are chosen to be eigenfunctions of the electronic Hamiltonian, i.e., $H_3\psi_q=E_q^I\psi_q$ (q stands collectively for all electronic quantum numbers). If we insert the product expansion (7) for the total wave function Ψ in the total Schrödinger equation and project on a simple product $\Phi_{p'}^L\psi_{q'}$ we arrive at the following set of coupled equations for the coefficients $\{c_{pq}\}$:

$$(\underline{H}_2+\underline{E}^L+\underline{E}^I)\mathbf{c}=E\mathbf{c} , \tag{10}$$

where $\mathbf{c}$ is the column vector with components $\{c_{pq}\}$. $\underline{E}^L$ and $\underline{E}^I$ are the diagonal matrices which contain the Landau energies $\{E_p^L\}$ and internal energies $\{E_q^I\}$, respectively. $\underline{H}_2$ contains the matrix elements of the coupling term H_2 and has therefore the following structure:

$$\underline{H}_2=-\frac{e}{M}\alpha\left\langle\Phi_{p'}^L\middle|\left[\mathbf{P}_S-\frac{Q}{2}\mathbf{B}\times\mathbf{R}_S\right]\middle|\Phi_p^L\right\rangle\cdot\left[\mathbf{B}\times\left\langle\psi_{q'}\middle|\sum_i\mathbf{r}_i\middle|\psi_q\right\rangle\right] . \tag{11}$$

Each element of $\underline{H}_2$ is a product of two terms: the first term is a matrix element between Landau orbitals and the second one is a dipole matrix element between internal electronic wave functions. The first part of the coupling matrix $\underline{H}_2$, i.e., the matrix elements between Landau orbitals, can also be reduced to pure dipole matrix elements by the following calculation. Let us consider the quantity

$$\langle\Phi_{p'}^L|[\mathbf{R}_S,H_1]|\Phi_p^L\rangle . \tag{12}$$

This quantity can be evaluated in two different ways. The first way is to explicitly calculate the commutator. The second way uses the fact that $\Phi_{p'}^L$, Φ_p^L are eigenfunctions of the Hamiltonian H_1 with eigenvalues $E_{p'}^L$ and E_p^L, respectively. Combining the two results we arrive at the following relation:

$$\left\langle\Phi_{p'}^L\middle|\left[\mathbf{P}_S-\frac{Q}{2}\mathbf{B}\times\mathbf{R}_S\right]\middle|\Phi_p^L\right\rangle$$
$$=iM(E_{p'}^L-E_p^L)\langle\Phi_{p'}^L|\mathbf{R}_S|\Phi_p^L\rangle . \tag{13}$$

With the explicit expression for the Landau wave functions [see Eq. (8)] we can calculate the coupling term (13) by calculating the dipole matrix elements between different Landau orbitals. The results reads as follows:

$$\langle \Phi_{p'}^{L} | \mathbf{R}_S | \Phi_p^L \rangle = (1/\sqrt{2})a \left[\begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix} \delta_{\mu'-\mu,1} \times \begin{cases} \delta_{NN'}(\mu+N+1)^{1/2} - \delta_{N-1,N'} N^{1/2} & \text{for } \mu \geq 0 \\ \delta_{NN'}(N-\mu)^{1/2} - \delta_{N+1,N'}(N+1)^{1/2} & \text{for } \mu < 0 \end{cases} \right.$$
$$\left. + \begin{pmatrix} 1 \\ \mp i \\ 0 \end{pmatrix} \delta_{\mu-\mu',1} \times \begin{cases} \delta_{NN'}(\mu+N)^{1/2} - \delta_{N+1,N'}(N+1)^{1/2} & \text{for } \mu > 0 \\ \delta_{NN'}(-\mu+N+1)^{1/2} - \delta_{N-1,N'} N^{1/2} & \text{for } \mu \leq 0 \end{cases} \right] , \tag{14}$$

where the simple indices p' and p stand for the sets of quantum numbers (N,μ) and (N',μ'), respectively. Inserting Eq. (14) in Eq. (13) and finally in Eq. (11) we obtain the final, completely general, form of the coupling matrix $\underline{H}_2$:

$$\underline{H}_2 = -i\frac{e}{M}(|Q|B/2)^{1/2} \left[\left[\begin{pmatrix} 1 \\ \pm i \\ 0 \end{pmatrix} \delta_{\mu'-\mu,1}[(\mu+|\mu|)/2+N+1]^{1/2} \begin{cases} -\delta_{NN'} & \text{for } \mu \geq 0 \\ \delta_{N+1,N'} & \text{for } \mu < 0 \end{cases} \right. \right.$$
$$\left. \left. + \begin{pmatrix} 1 \\ \mp i \\ 0 \end{pmatrix} \delta_{\mu-\mu',1}[(\mu+|\mu|)/2+N]^{1/2} \begin{cases} +\delta_{NN'} & \text{for } \mu > 0 \\ -\delta_{N-1,N'} & \text{for } \mu \leq 0 \end{cases} \right] \alpha \left[\mathbf{B} \times \left\langle \psi_{q'} \middle| \sum_i \mathbf{r}_i \middle| \psi_q \right\rangle \right] \right] . \tag{15}$$

The above expression for $\underline{H}_2$ shows that couplings occur only between states which differ by one unit in the magnetic quantum number μ. For the Landau principal quantum number only transitions with $\Delta N = 0, \pm 1$ are allowed. These are the selection rules for dipole transitions between different Landau wave functions. Furthermore we have only nonvanishing coupling matrix elements between states with different energy. This means that an appreciable value of the coupling leads always to a strong mixing of different states of collective motion with different energies.

The original problem of the investigation of the significance and effects of the couplings is therefore reduced to the solution of the eigenvalue problem (10), i.e., the diagonalization of essentially the coupling matrix $\underline{H}_2$ in Eq. (15). The central subject of the present paper is to show and discuss physical situations for which the coupling terms become large already *at laboratory magnetic-field strengths.* To this end we have to specify our internal electronic wave functions. For the sake of simplicity we specialize to the case of one-electron ions, i.e., our internal wave functions $\{\psi_q\}$ are hydrogenlike functions which are eigenfunctions of H_3 in Eq. (6c) without the diamagnetic interaction term. The diamagnetic interaction will be taken into account by perturbation theory. We will, therefore, be able to draw at most qualitative conclusions for the region where the diamagnetic term in the Hamiltonian H_3 becomes important or even dominant for the internal motion.

The internal hydrogenlike electronic wave functions read in spherical coordinates (r,θ,φ) as follows:

$$\psi_{q'}(r,\theta,\varphi) = a_B^{-3/2} A_{nl} \left[\frac{r}{a_B} \right]^l \exp\left[-\frac{Zr}{a_B n} \right] \times L_{n+l}^{2l+1} \left[\frac{2Zr}{a_B n} \right] Y_l^m(\theta,\varphi) \tag{16}$$

where the index q' stands for the set of quantum numbers (n,l,m). a_B is the Bohr radius $(\mu_+ e^2)^{-1}$, where μ_+ is the reduced mass $(m_e M_0/M)$. L_{n+l}^{2l+1} is a generalized Laguerre polynomial. Y_l^m are the spherical harmonic functions and A_{nl} are the normalization constants

$$A_{nl} = \left[\left[\frac{2Z}{n} \right]^{2l+3} \frac{(n-l-1)!}{(n+l)!^3 2n} \right]^{1/2} . \tag{17}$$

In order to establish the coupling matrix $\underline{H}_2$ [see Eq. (15)] we have to calculate the dipole matrix elements between two electronic wave functions $\psi_{q'}$ and ψ_q. The calculation of the radial part of the general dipole matrix elements is rather lengthy and has been performed in the literature.[21–23] We give here only the final result for our coupling matrix $\underline{H}_2$ in Eq. (15):

$$\underline{H}_2 = +\frac{e}{M}\alpha B(|Q|B/2)^{1/2} \times \{ \delta_{\mu'-\mu,1}\delta_{m'-m,1}[N+(\mu+|\mu|)/2+1]^{1/2} \mathcal{L}(N,N',\mu)\mathcal{N}(-m,l,l',n,n')$$
$$+ \delta_{\mu-\mu',1}\delta_{m-m',+1}[N+(\mu+|\mu|)/2]^{1/2} \mathcal{L}(N-1,N',-\mu)\mathcal{N}(+m,l,l',n,n') \} , \tag{18}$$

where

$$\mathcal{L}(N,N',\mu) = \begin{cases} -\delta_{NN'} & \text{for } \mu \geq 0 \\ \delta_{N+1,N'} & \text{for } \mu < 0 \end{cases}$$

and

$$\mathcal{N}(m,l,l',n,n')=\left[\delta_{l+1,l'}\mathcal{M}^{l,l+1}_{nn'}\left[\frac{(l-m+2)(l-m+1)}{(2l+1)(2l+3)}\right]^{1/2}-\delta_{l-1,l'}\mathcal{M}^{l,l-1}_{nn'}\left[\frac{(l+m)(l+m-1)}{(2l-1)(2l+1)}\right]^{1/2}\right],$$

where the radial part $\mathcal{M}^{l,l-1}_{nn'}$ of the electronic dipole matrix element takes on the following appearance:

$$\mathcal{M}^{l,l-1}_{nn'}=\frac{(-1)^{n'-l}}{4(2l-1)!}\left[\frac{(n+l)!(n'+l-1)!}{(n-l-1)!(n'-l)!}\right]^{1/2}\frac{(4nn')^{l+1}(n-n')^{n+n'-2l-2}}{(n+n')^{n+n'}}(a_B/Z)$$
$$\times\left[F\left[-(n-l-1),-(n'-l);2l;-\frac{4nn'}{(n-n')^2}\right]-\frac{(n-n')^2}{(n+n')^2}F\left[-(n-l+1),-(n'-l);2l;-\frac{4nn'}{(n-n')^2}\right]\right].\tag{19}$$

F is the hypergeometric function which reduces in our special case to a polynomial. $\mathcal{M}^{l,l+1}_{nn'}$ can be obtained from Eq. (19) by permuting the indices. Equation (19) holds only for the case $n\neq n'$. For $n=n'$ we obtain the simple result

$$\mathcal{M}^{l,l-1}_{nn}=-\tfrac{3}{2}(a_B/Z)[n^2-l^2)]^{1/2}n\ .\tag{20}$$

We remark that the coupling matrix (18) exhibits the fact that $L_{\parallel}$, the component of the total angular momentum parallel to the magnetic field axis, is a constant of motion:

$$-\mu'+m'=-\mu+m$$

for all transition matrix elements. The matrix $\underline{H}_2$ can be calculated separately for each value of $\mu+m$. Furthermore Eq. (18) contains the well-known selection rules for a dipole transition between two two-electronic eigenstates of a one-electron atom $\Delta l=\pm1$ and $\Delta m=\pm1$.

In order to complete our eigenvalue problem from Eq. (10) we have to establish the matrix for the internal energies $\underline{E}^I$. Since our electronic hydrogenlike wave functions (16) are not exact eigenfunctions of the internal Hamiltonian $\underline{H}_3$ we obtain a nondiagonal matrix $\underline{E}^I$ which takes on the following structure:

$$\underline{E}^I=\delta_{pp'}\left[\left[-\frac{Z^2\mu_+e^4}{2n^2}-\frac{e}{2\mu_-}Bm\right]\delta_{qq'}\right.$$
$$\left.+\frac{e^2}{8\mu_0}B^2\delta_{mm'}S^m_{ll'}\langle R_{nl}(r)|r^2|R_{n'l'}(r)\rangle\right]\tag{21}$$

where

$$S^m_{ll'}=\left[2\delta_{ll'}\frac{(l^2+l+|m|^2-1)}{(2l-1)(2l+3)}-\delta_{l+2,l'}\left[\frac{(l-|m|+1)(l-|m|+2)(l+|m|+2)(l+|m|+1)}{(2l+1)(2l+5)(2l+3)^2}\right]^{1/2}\right.$$
$$\left.-\delta_{l-2,l'}\left[\frac{(l+|m|)(l+|m|-1)(l-|m|-1)(l-|m|)}{(2l+1)(2l-3)(2l-1)^2}\right]^{1/2}\right]$$

and

$$\mu_-=\left[\frac{m_eM_0}{M_0-\alpha m_e}\right],$$
$$\mu_0=\left[\frac{1}{m_e}\left[1-\frac{Q}{e}\frac{m_e^2}{M^2}\right]^2\right.$$
$$\left.+\frac{1}{M_0}\left[1-\frac{Q}{e}\frac{m_e}{M}\frac{M+M_0}{M}\right]^2\right]^{-1}.$$

For the following considerations the off-diagonal part of $\underline{E}^I$ will be of only marginal importance. We therefore refer the reader for the explicit complicated structure of the matrix elements $\langle R_{nl}(r)|r^2|R_{n'l'}(r)\rangle$ to the literature[22] and give here only its diagonal elements

$$\langle R_{nl}(r)|r^2|R_{nl}(r)\rangle=\frac{n^2}{2Z^2}a_B^2[5n^2+1-3l(l+1)]\ .\tag{22}$$

III. DISCUSSION

Having completely specified our eigenvalue problem (10) we are now able to investigate our original problem of the significance of the coupling terms. The relevant quantity is not the absolute value κ of the coupling elements of the matrix $\underline{H}_2$ but rather the quotient of this coupling κ and the energy spacing Δ of the corresponding diagonal matrix elements in $\underline{E}^L$ and $\underline{E}^I$.

Let us first consider two different electronic states of, for example, the helium ion which belong to the same n manifold and couple via the matrix $\underline{H}_2$. According to the selection rules [see Eq. (18)] these two electronic states must differ in both of their eigenvalues l,m, by one unit. The corresponding Landau levels of the center-of-mass motion differ also by one unit in the magnetic quantum number μ. Without loss of generality we assume further that $\mu<0$, i.e., that the Landau levels differ also by one unit in their principal quantum number N.

We begin with small principal quantum numbers n, for example, $n=2$. Within this n manifold and for strong laboratory magnetic-field strengths (≈1 T) the Zeeman effect dominates the spin-orbit coupling and determines the energy spacing between the electronic states with different m eigenvalues. The diamagnetic interaction is negligible in this range of magnetic-field strengths and principal quantum numbers. Our coupling matrix tells us that the ($l=1$, $m=1$) electronic state couples with the ($l=0$, $m=0$) state and the latter one with the ($l=1$, $m=-1$) state. But how large are these couplings? From the matrix $\underline{H}_2$ we obtain the value

$$\kappa_1=(e/M)\alpha B[|Q|B(N)]^{1/2}(3a_B/Z)$$

for the coupling between the state ($l=1$, $m=1$) and ($l=0$, $m=0$) and the value

$$\kappa_2=+(e/M)\alpha B[|Q|B(N-1)]^{1/2}(3a_B/Z)$$

for the coupling between the states ($l=0$, $m=0$) and $l=1$, $m=-1$). The energy spacing Δ is essentially given by the electronic Zeeman energy split $(e/2)(B/\mu_-)$ (the energy difference due to the change in the Landau principal quantum numbers is negligible). If we assume $N \gg 1$, i.e., $N \approx N-1 \approx N-2$, we arrive at the following estimation for the quotient (κ/Δ).

$$(\kappa/\Delta)\approx\frac{\sqrt{NB}}{M}\ , \tag{23}$$

where we have used atomic units ($B=2.35\times10^5$ T corresponds to 1 a.u.). For a typical laboratory magnetic-field strength $B=10^{-5}$ a.u. and the mass $M\approx7.3\times10^3$ a.u. of the helium ion we need N to be of the order of magnitude $N\approx6\times10^{11}$ in order to make the coupling κ as large as the energy spacing Δ, i.e., $(\kappa/\Delta)\approx1$. At first sight this seems to be an astronomical number. However, the energy of the center-of-mass motion belonging to this value of N is $E^L\approx10^3$ a.u., i.e., some 10 KeV. This is a kinetic energy which is without problem achievable in the laboratory and still far from the region where relativistic effects start to become significant. Since the number of quantums N in the pure center of mass Landau motion is very high, the center-of-mass motion is expected, apart from small fluctuations, to be well described by its classical path. The influence of the internal motion on the collective motion *in this special case* is therefore expected to be negligible. Since the above-mentioned coupled three levels of the $n=2$ manifold are energetically well separated from the $n=1$ and 3 manifold we can neglect the couplings of the states of the $n=2$ manifold to the states of other n manifolds.

The above discussion shows that significant values of the coupling of the center-of-mass motion to the internal motion appear already at laboratory magnetic-field strengths and even for low-lying electronic states. These couplings modify the internal wave function considerably, whereas, in our special case of low-lying electronic states, the reaction back on the collective motion is negligible. We remark that by increasing N it is possible to manipulate (κ/Δ) and therefore the mixing of the internal states over a wide range.

As a next step we investigate the behavior of the coupling terms for "intermediate" values of the principal quantum number n. "Intermediate" here means that the Zeeman energy is still dominant over the diamagnetic interaction energies. Since the diamagnetic energies are proportional to B^2n^4 we are for n up to approximately 15 and in the laboratory achievable magnetic-field strengths well within the above-mentioned region. The energy spacing Δ for two electronic states of the same n manifold is then again determined by the Zeeman energy difference. Let us specialize to the case $n \gg 1$. The quantity (κ/Δ) can be obtained from Eq. (18) together with Eq. (20) and its order of magnitude is determined by the expression

$$(\kappa/\Delta)\approx\frac{\sqrt{NB}}{M}n^2\ . \tag{24}$$

As an example we take $n=10$, $B=10^{-5}$ a.u., and the mass of the helium ion. If we again demand that the coupling κ is as large as the energy spacing Δ we arrive at a corresponding value of $N\approx10^8$. This means a kinetic energy of the ion of the order of magnitude of 1 a.u., i.e., some 10 eV. We conclude therefore that for typical strong laboratory magnetic-field strengths the coupling between the collective and internal motion becomes for states within a higher n manifold ($n\approx10$) already important for a center-of-mass energy of the ion of a few eV.

So far we have considered only the coupling of states within the same n manifold. For states belonging to different n manifolds and for intermediate values of n ($n \gg l$) the order of magnitude of the energy spacing [see Eq. (21)] is determined by the energy difference in the absence of a magnetic field, i.e., $\Delta\approx(-Z^2/n^3)$. For the evaluation of the couplings we have to use the fact that the matrix elements $\mathcal{M}_{nn'}^{l,l-1}$ are for large n, $n \gg l$, and $|n-n'| \ll n$ in the leading order proportional to n^2. A rough estimation yields then the following order of magnitude for our quantity (κ/Δ):

$$(\kappa/\Delta)\approx\frac{\sqrt{NB}}{M}Bn^5\ . \tag{25}$$

For a magnetic-field strength $B=10^{-4}$ a.u. and $n=10$ we obtain from our requirement that κ should be of the order of magnitude of Δ that $N\approx10^{10}$, i.e., a center-of-mass energy of the ion of a few keV. This means that the couplings become at these energies not only dominant for states within the same n manifold but also important for states belonging to adjacent n manifolds. The exact eigenfunction of the ion is therefore a sum of products of collective and internal wave functions which mixes the Landau orbitals of a certain range of the principal quantum number $N,\dots,N+\Delta N$ and the electronic wave functions over a certain range of their quantum numbers n,l, and m according to the selection rules of our coupling matrix $\underline{H}_2$.

In the preceding discussion we assumed zero temperature. For finite temperature we have to take into account the effect of the thermal motion of the ion. In order to obtain an estimation of the order of magnitude of the effects of the thermal motion we set the Landau energy in Eq. (9) (for $\mu<0$) equal to the mean thermal energy k_BT for the two degrees of freedom, where k_B is the Boltzmann constant and T the temperature. This yields the following relation between the Landau principal quantum number and the temperature (in K):

$$N\approx\frac{k_BTM}{|Q|B}\ . \tag{26}$$

As an example we again take the helium ion at a magnetic-field strength of $B=10^{-5}$ a.u. and for room temperature $T\approx 300$ K. As a result we obtain $N\approx 6\times 10^5$. For intermediate values of n the corresponding value of the coupling is still negligible, but for high n manifolds (see the discussion below) the kinetic energy due to the thermal motion of the ion at room temperature will be sufficient to cause significant values of the couplings and produce a strong interaction between the collective and internal motions.

The physical situation discussed so far changes dramatically if we go to higher values of the principal quantum number n. The diamagnetic term of the internal motion becomes more and more important and therefore our description of the electronic wave function in terms of hydrogenlike functions becomes inadequate. The n manifolds are no more well defined, i.e., they mix strongly and the internal wave function continuously changes its shape from initially Coulombic to finally electronic Landau character. These changes are accompanied by a phase transition from regularity to irregularity, i.e., the onset of quantum chaos.[5-7] The region where the internal motion is chaotic is also for our problem of the coupled collective and internal motion of special interest. Since the energy spacing of the electronic eigenstates becomes much smaller than the corresponding spacing of the levels in the field-free case and since the coupling between the electronic states is probably underestimated by the above considerations we expect to obtain a strong mixture of the collective and internal motion, i.e., strong couplings, already for $N\approx 10^4$ [see Eq. (25)]. As a consequence the mixing of many different states of collective motion, for example, $\Delta N\approx 10^2-10^3$, becomes essential for the collective motion and provides no more small fluctuations around a more or less classical center-of-mass orbit. We remark that this strong mixing appears automatically because of the finite temperature of the system ($N\approx 10^4$ corresponds to $T\approx 5$ K). To study this very interesting region where probably both the internal and collective motion become chaotic and couple strongly goes beyond the scope of this paper and will be left to future investigations.

ACKNOWLEDGMENTS

The Deutsche Forschungsgemeinschaft is acknowledged for financial support.

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