Center-of-mass problem in a magnetic field: Unified treatment of charged and neutral systems

D. Baye and M. Vincke
Physique Théorique et Mathématique, Code Postal 229, Université Libre de Bruxelles, B1050 Brussels, Belgium
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The approximate constant of motion introduced previously for the description of a charged system in a homogeneous magnetic field is interpreted physically as the kinetic momentum of the collective motion. The algebra satisfied by this operator and by the exact constants of motion describes the behavior in a magnetic field of a single particle possessing the total charge of the system. With this algebra, we generalize the approximate constant of motion and obtain a family of operators depending on arbitrary parameters. Canonical transformations based on these new operators separate the Hamiltonian into collective, internal, and coupling terms. These terms take the same form for charged and neutral systems although the collective energy represents different physical behaviors. The coupling between the internal and collective motions is small for some choices of the parameters if at least one particle is much heavier than the other ones.

I. INTRODUCTION

In the presence of a magnetic field, the center-of-mass (c.m.) separation becomes a complicated problem whose solution is not exactly known.[1] In fact, the notion of a center of mass needs be generalized and the abbreviation c.m. should in some cases be more appropriately understood as meaning "collective motion." Center-of-mass corrections *qualitatively* modify some atomic properties when the magnetic field is strong enough, i.e., in the vicinity of neutron stars for low-lying levels or in the laboratory for Rydberg states. Binding energies are reduced by c.m. effects[2–4] and can render states unstable.[5,6] The c.m. problem also questions our understanding of basic quantum mechanics and forces us to develop new approaches.

Intuitively, one expects a very different behavior of a neutral system, such as an atom, and of a charged system, such as an atomic ion. In the former case, the collective motion is free whereas in the latter case, a cyclotron motion arises. This difference appears clearly in the detailed mathematical study of Avron *et al.*[1] These authors show that a notion of c.m. separation exists for neutral systems. Three commuting constants of motion are provided by the components of an operator called the total pseudomomentum, or the total generalized momentum. The process is called a "pseudoseparation" because the resulting internal Hamiltonian still depends on the eigenvalues of the pseudomomentum. In the charged case, two components of the pseudomomentum do not commute and an exact c.m. separation does not appear to be possible.

An approximate constant of motion initially introduced for atomic ions[7] but valid for arbitrary charged systems[8] provides an approximate c.m. separation.[9,10] This approximate constant of motion is useful for systems in which at least one particle is much heavier than the other ones. The separation process is then performed approximately with a perturbation expansion whose parameter is the cyclotron energy of the system in typical energy units of the field-free problem. This method allowed us to perform a detailed comparison of the charged and neutral cases.[6] Surprisingly, the properties of both kinds of systems exhibit a number of close similarities. In both cases, the same internal Hamiltonian and the same type of coupling between the internal and collective motions are found. Only the collective energies differ in the intuitively expected manner. The analogies between both kinds of systems become even more apparent in an exactly solvable model.[8]

The striking similarity between the charged and neutral systems raises the following question: Is a simultaneous treatment of both cases possible? In the present paper, we answer positively to this question. In order to develop this treatment, we first generalize the definition of the approximate constant of motion introduced in Ref. 7. To this end, as in our preliminary report,[11] we start from a physical definition of this approximate constant of motion in terms of a generalized kinetic momentum, associated with the total generalized momentum. On physical grounds, these operators have to satisfy the same commutation relations as those of a single (neutral or charged) particle in a magnetic field. With the generalized approximate constant of motion, we perform a canonical transformation which separates the collective motion from the internal motion, except for small coupling terms which can be treated perturbatively. The resulting treatment remains valid if the system is neutral or even in the absence of magnetic field.

The operators characterizing a single particle in a magnetic field and their algebra are recalled in Sec. II. An analog algebra for the collective motion is taken as definition of an approximate constant of motion in Sec. III. Solutions are presented and discussed in Sec. IV. In Sec. V a linear canonical transformation is performed to separate approximately the internal and collective

motions. The atomic case is treated as an example in Sec. VI. Concluding remarks are presented in Sec. VII.

II. PARTICLE IN A MAGNETIC FIELD

Let $\mathbf{r}$ and $\mathbf{p}$ be the coordinate and momentum of a particle with mass m and charge q in a homogeneous magnetic field $\mathbf{B}$. Its kinetic momentum is

$$\boldsymbol{\pi}=\mathbf{p}-q\,\mathbf{A}(\mathbf{r})\ , \tag{1}$$

where $\mathbf{A}$ is the vector potential in an arbitrary gauge.

The nonrelativistic spinless Hamiltonian

$$H=\boldsymbol{\pi}^2/2m \tag{2}$$

possesses several constants of motion. The pseudomomentum[1,12,13]

$$\mathbf{k}=\boldsymbol{\pi}+q\mathbf{B}\times\mathbf{r} \tag{3}$$

commutes with $\boldsymbol{\pi}$ and H. Classically, it is related to the center $\mathbf{r}_c$ of the orbit through $\mathbf{k}=q\mathbf{B}\times\mathbf{r}_c$. Another constant of motion generalizes the parallel component of the orbital momentum[14,9]

$$\mathcal{L}_{\parallel}=\hat{\mathbf{B}}\cdot\mathbf{r}\times\tfrac{1}{2}(\mathbf{k}+\boldsymbol{\pi})=(2qB)^{-1}(\mathbf{k}^2-\boldsymbol{\pi}^2)\ , \tag{4}$$

where $\hat{\mathbf{B}}$ is a unit vector in the field direction. The second form is valid only for $q\neq 0$. The operators $\mathbf{k}$ and $\boldsymbol{\pi}$ verify with $\mathcal{L}_{\parallel}$ the commutation relations

$$\begin{aligned}&[\pi_\lambda,k_\mu]=0\ ,\\ &[\pi_\lambda,\pi_\mu]=i\hbar q\epsilon_{\lambda\mu\nu}B_\nu,\quad [k_\lambda,k_\mu]=-i\hbar q\epsilon_{\lambda\mu\nu}B_\nu\ ,\\ &[\boldsymbol{\pi},\mathcal{L}_{\parallel}]=i\hbar\hat{\mathbf{B}}\times\boldsymbol{\pi},\quad [\mathbf{k},\mathcal{L}_{\parallel}]=i\hbar\hat{\mathbf{B}}\times\mathbf{k}\ ,\end{aligned} \tag{5}$$

where the indices vary from 1 to 3 and $\epsilon_{\lambda\mu\nu}$ is the antisymmetric tensor. The components of $\mathbf{k}$ and $\boldsymbol{\pi}$ parallel to the field are identical and commute with the transverse components. They also commute with $\mathcal{L}_{\parallel}$. The relations (5) show that $\mathbf{k}$ and $\boldsymbol{\pi}$ provide a convenient and natural basis for a gauge-independent description of charged particles in a magnetic field.[15]

In the neutral case ($q=0$), $\boldsymbol{\pi}$ and $\mathbf{k}$ become identical and their common transverse components satisfy with $\mathcal{L}_{\parallel}$ the two-dimensional Euclidian algebra. We note here an important difference between the neutral and charged cases: if $q=0$, all the operators belonging to the algebra (5) are constants of motion; if $q\neq 0$, $\boldsymbol{\pi}$ is not a constant of motion. This property has important consequences in the c.m. problem.

III. SYSTEM OF PARTICLES IN A MAGNETIC FIELD

Let us consider a system of $N+1$ particles (labeled from $i=0$ to $i=N$)) with charges q_i and masses m_i. During the c.m. separation process, all particles, but one, are treated in a symmetric way. The asymmetrical role is attributed to particle 0. Let us however emphasize that this particle can be chosen arbitrarily. Of course, in some cases, physical reasons may suggest a natural choice for particle 0 but this choice is by no means obligatory. In an atom, for example, the nucleus is an obvious candidate as particle 0.

The Hamiltonian of $N+1$ particles reads

$$H=\sum_{i=0}^{N}(2m_i)^{-1}\pi_i^2+V(\mathbf{r}_i-\mathbf{r}_0,\mathbf{r}_i-\mathbf{r}_j)\ , \tag{6}$$

where V is rotation invariant. Translation invariance of the potential is explicitly displayed in (6). The constants of motion are the total pseudomomentum

$$\mathbf{K}=\sum_{i=0}^{N}\mathbf{k}_i \tag{7}$$

and the generalized parallel component of the total orbital momentum

$$\mathcal{L}_{\parallel}=\sum_{i=0}^{N}\mathcal{L}_{i\parallel}\ . \tag{8}$$

The components of the total pseudomomentum $\mathbf{K}$ satisfy

$$[K_\lambda,K_\mu]=-i\hbar Q\epsilon_{\lambda\mu\nu}B_\nu\ , \tag{9}$$

where Q is the total charge. The transverse components commute with the parallel component but do not commute with each other if Q differs from zero. This commutation relation confirms that significant differences will appear according to whether Q is zero or not. The commutator of $\mathbf{K}$ with $\mathcal{L}_{\parallel}$ is

$$[\mathbf{K},\mathcal{L}_{\parallel}]=i\hbar\hat{\mathbf{B}}\times\mathbf{K}\ . \tag{10}$$

In the neutral case ($Q=0$) the transverse component of $\mathbf{K}$ and $\mathcal{L}_{\parallel}$ satisfy the Euclidean algebra.[11] The center of mass behaves as a free particle with $\mathbf{K}$ playing the role of a momentum. Since all the operators appearing in (9) and (10) are then constants of motion, a c.m. separation is possible.[1] The charged case ($Q\neq 0$) is different: if a separation were possible, the system should behave collectively as a single charged particle and relations similar to (5) should exist. But full separation implies that these relations would involve only constants of motion. However, we know that this possibility is already ruled out in the single-particle case.

Now, we generalize the approximate constant of motion by searching for a family of operators $\mathbf{C}(\boldsymbol{\alpha})$ presenting the physical behavior of a kinetic momentum whose commutator with H is "small." These operators depend on several linear parameters represented by the vector notation $\boldsymbol{\alpha}$. Their number as well as their definition will be made more precise in Sec. IV. However, we already choose that $\boldsymbol{\alpha}=\mathbf{0}$ corresponds to the approximate constant of motion employed in our earlier works.

Hermitian operators $\mathbf{C}$ presenting the physical behavior of a kinetic momentum must satisfy with $\mathbf{K}$ and $\mathcal{L}_{\parallel}$ the commutation relations

$$[C_\lambda,K_\mu]=0\ , \tag{11}$$

$$[C_\lambda,C_\mu]=i\hbar Q\epsilon_{\lambda\mu\nu}B_\nu\ , \tag{12}$$

$$[\mathbf{C},\mathcal{L}_{\parallel}]=i\hbar\hat{\mathbf{B}}\times\mathbf{C}\ , \tag{13}$$

with the additional translation invariance condition

$$[\mathbf{C},V]=0 \ . \tag{14}$$

An obvious solution to Eqs. (11) to (14) is the total kinetic momentum

$$\mathbf{\Pi}=\sum_{i=0}^{N}\boldsymbol{\pi}_i \tag{15}$$

but its commutator with the kinetic energy is not small. Another solution is given by the operator[7]

$$\mathbf{C}(\mathbf{0})=\mathbf{K}-Q\mathbf{B}\times\mathbf{r}_0 \ , \tag{16}$$

which has been successfully employed in the calculation of c.m. corrections for atomic ions.[10] In fact, (16) shows clearly that $\mathbf{C}$ cannot be an exact constant of motion, such as $\mathbf{K}$: it precesses with the coordinate $\mathbf{r}_0$ (Ref. 16) but this motion is slow if particle 0 is heavy. Indeed, the commutator with H is

$$[H,\mathbf{C}(\mathbf{0})]=i\hbar Q\mathbf{B}\times\boldsymbol{\pi}_0/m_0 \ . \tag{17}$$

In the atomic case, if we choose the nucleus as particle 0, the commutator (17) can be considered as small since it involves the inverse of the mass of the heaviest particle.

IV. GENERALIZED APPROXIMATE CONSTANT OF MOTION

Let us now search for more general solutions of (11) to (14). We choose to write them as linear combinations of the $\boldsymbol{\pi}_i$ and $\mathbf{k}_i$. Equation (13) is then automatically satisfied because of (5). Now we require translation invariance. Up to a multiplicative factor which is discussed below, the most general combination which satisfies (14) is

$$\mathbf{C}(\boldsymbol{\alpha})=\mathbf{K}+Q\sum_{i=0}^{N}(\alpha_i/q_i)(\boldsymbol{\pi}_i-\mathbf{k}_i) \ , \tag{18}$$

where the α_i ($i=0$ to N) are real parameters and $\boldsymbol{\alpha}$ represents $(\alpha_1,\alpha_2,\ldots,\alpha_N)$ as explained below. With (3), the fact that $\mathbf{C}(\alpha)$ commutes with V also appears clearly in the equivalent expression

$$\mathbf{C}(\boldsymbol{\alpha})=\mathbf{K}-Q\mathbf{B}\times\sum_{i=0}^{N}\alpha_i\mathbf{r}_i \ . \tag{19}$$

Notice that (19) is now valid even if some q_i are zero. The commutation relation (11) of $\mathbf{C}$ with $\mathbf{K}$ imposes the condition

$$\sum_{i=0}^{N}\alpha_i=1 \ . \tag{20}$$

Finally, one easily checks that the relations (12) are fulfilled so that the overall factor is $+1$ or -1. The fact that $\mathbf{C}$ is defined up to a global sign is without practical importance.

The condition (20) shows that one of the parameters α_i is not free. Let us now define more precisely the notation $\mathbf{C}(\boldsymbol{\alpha})$: this operator is a function of N *arbitrary* real parameters which we choose to be α_1 to α_N. We can rewrite (19) as

$$\mathbf{C}(\boldsymbol{\alpha})=\mathbf{K}-Q\mathbf{B}\times\mathbf{R}(\boldsymbol{\alpha}) \ , \tag{21}$$

with

$$\mathbf{R}(\boldsymbol{\alpha})=\sum_{i=0}^{N}\alpha_i\mathbf{r}_i=\mathbf{r}_0+\sum_{i=1}^{N}\alpha_i(\mathbf{r}_i-\mathbf{r}_0) \ . \tag{22}$$

Comparing (21) with (3) shows that $\mathbf{R}(\alpha)$ has a simple physical interpretation. It is the coordinate associated with the collective motion, i.e., the generalization of the c.m. coordinate. It differs from $\mathbf{r}_0$ by an arbitrary translation invariant expression.

With (16) and (21), $\mathbf{C}(\boldsymbol{\alpha})$ can be rewritten as

$$\mathbf{C}(\boldsymbol{\alpha})=\mathbf{C}(\mathbf{0})-Q\mathbf{B}\times[\mathbf{R}(\boldsymbol{\alpha})-\mathbf{r}_0] \ . \tag{23}$$

Generalizations of $\mathbf{C}(\mathbf{0})$ differ from it by the vector product of $\mathbf{B}$ by an arbitrary translation invariant coordinate vector. Interesting particular cases of (23) are obtained for $\boldsymbol{\alpha}=\mathbf{0}$ where the original approximate constant of motion is recovered and, if $Q\neq 0$, for $\alpha_i=q_i/Q$ since

$$\mathbf{C}(\mathbf{q}/Q)=\mathbf{\Pi} \ , \tag{24}$$

where $\mathbf{q}=(q_1,\ldots,q_N)$. In the former case, the coordinate $\mathbf{R}(\mathbf{0})$ is the particle-0 coordinate $\mathbf{r}_0$. In the latter, $\mathbf{R}(\mathbf{q}/Q)$ is the center of charge coordinate. If the system is neutral, $\mathbf{C}(\boldsymbol{\alpha})$ becomes independent of the α_i and identical to $\mathbf{K}$ (and therefore distinct from $\mathbf{\Pi}$). If B vanishes, $\mathbf{C}(\boldsymbol{\alpha})=\mathbf{K}$ is nothing but the total momentum.

The commutator of $\mathbf{C}(\boldsymbol{\alpha})$ with the Hamiltonian is

$$[H,\mathbf{C}(\boldsymbol{\alpha})]=i\hbar Q\mathbf{B}\times\sum_{i=0}^{N}(\alpha_i/m_i)\boldsymbol{\pi}_i \ . \tag{25}$$

The important point is that the constraint (20) on the α_i forbids the commutator (25) to vanish if Q or B is not zero. This commutator can, however, be made "small" if some m_i are much larger than the other ones. Then the corresponding α_i can be chosen large enough to satisfy (20) and the remaining α_i can be arbitrarily small. If particle 0 is much heavier than most other ones, the commutator is small if

$$\alpha_{i>0}=O\left[\frac{1}{m_0}\right] \ . \tag{26}$$

This case is typical of an atom.

Before closing this section, let us add the useful relation generalizing (12)

$$[C_\lambda(\boldsymbol{\alpha}),C_\mu(\boldsymbol{\alpha}')]=i\hbar Q\epsilon_{\lambda\mu\nu}B_\nu \tag{27}$$

for any sets $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}'$.

V. CANONICAL TRANSFORMATION

As in our previous works, we shall make use of a linear canonical transformation involving $\mathbf{K}$ and $\mathbf{C}(\boldsymbol{\alpha})$ to separate as much as possible the internal and collective motions. Unlike our previous works, we do not introduce a separate treatment of charged and neutral systems. Also, we do not need any more to treat differently the transverse and longitudinal terms. The derived equations are valid in the direction parallel to the field. However,

in applications, it might be useful to choose different values for the free parameters α_i in the parallel and transverse directions. This possibility remains open in the present approach but does not deserve any additional complication in the notations. The properties of $\mathbf{C}(\boldsymbol{\alpha})$ allow us to perform a linear canonical transformation in which the approximate constant of motion and the total pseudomomentum respectively become the kinetic momentum and the pseudomomentum associated with the collective motion, i.e., with the new particle 0.

In close analogy with Ref. 10 [Eq. (2.7)], Ref. 11 [Eq. (12)], and Ref. 8 [Eqs. (27) and (28)], we perform the linear canonical transformation for the *transverse* components ($i=1,\ldots,N$)

$$\boldsymbol{\pi}'_{0\perp}=\mathbf{C}_\perp(\boldsymbol{\alpha}) , \tag{28}$$

$$\mathbf{k}'_{0\perp}=\mathbf{K}_\perp , \tag{29}$$

$$\boldsymbol{\pi}'_{i\perp}=\boldsymbol{\pi}_{i\perp}-\alpha_i\mathbf{C}_\perp(\tfrac{1}{2}\boldsymbol{\alpha}) , \tag{30}$$

$$\mathbf{k}'_{i\perp}=\mathbf{k}_{i\perp}+\frac{q_i}{q_0}(\boldsymbol{\pi}_{0\perp}-\mathbf{k}_{0\perp})-\alpha_i\mathbf{C}_\perp(\tfrac{1}{2}\boldsymbol{\alpha}) . \tag{31}$$

Some general properties of this type of canonical transformations which belong to the $SO(N+1,N+1)$ group are discussed in the Appendix. The main difference with the earlier works—which correspond to $\boldsymbol{\alpha}=\mathbf{0}$—is that $\boldsymbol{\pi}'_{i\perp}$ now differs from $\boldsymbol{\pi}_{i\perp}$. However, the expressions (28) to (31) are not valid for the parallel components. Therefore, we prefer to rewrite and extend them as

$$\boldsymbol{\pi}'_0=\mathbf{C}(\boldsymbol{\alpha}) , \tag{32}$$

$$\mathbf{r}'_0=\mathbf{R}(\boldsymbol{\alpha}) , \tag{33}$$

$$\boldsymbol{\pi}'_i=\boldsymbol{\pi}_i-\alpha_i\mathbf{C}(\tfrac{1}{2}\boldsymbol{\alpha}) , \tag{34}$$

$$\mathbf{r}'_i=\mathbf{r}_i-\mathbf{r}_0 . \tag{35}$$

Now, the transformation is valid for the parallel components as well. The hybrid system of coordinates $\boldsymbol{\pi}_i$ and $\mathbf{r}_i$ is more physical but the canonical character of the transformation is less obvious. It is most easily checked by observing that all the components of the $\mathbf{r}'_i$ commute, that the components of the $\boldsymbol{\pi}'_i$ have the same commutation relations as the $\boldsymbol{\pi}_i$ [with (27)], and so on. Anyway, choosing a gauge allows one to write the canonical transformation in a more standard form involving momenta and coordinates.

The physical interpretation of (32) to (35) is obvious. The approximate constant of motion $\mathbf{C}(\boldsymbol{\alpha})$ is the collective kinetic momentum and is associated to the collective coordinate $\mathbf{R}(\boldsymbol{\alpha})$. The internal kinetic momenta $\boldsymbol{\pi}'_i$ are associated to relative coordinates with respect to particle 0. This transformation takes its simplest form when $\boldsymbol{\alpha}=\mathbf{0}$.

More general canonical transformations can be defined. For example, one can replace (34) by

$$\boldsymbol{\pi}'_i=\boldsymbol{\pi}_i-\alpha_i\mathbf{C}(\tfrac{1}{2}\boldsymbol{\alpha})+\tfrac{1}{2}\mathbf{B}\times\sum_{j=1}^{N}Q_{ij}(\mathbf{r}_j-\mathbf{r}_0) , \tag{36}$$

with

$$Q_{ij}=Q_{ji} ,$$

without affecting the canonical character of the transformation. However, here, we do not make use of this additional generality.

In order to determine the transformed Hamiltonian, we have to inverse (32) to (35). In fact, (35) allows one to transform easily the potential term. Moreover, one has

$$\boldsymbol{\pi}_0=\alpha_0\boldsymbol{\pi}'_0-\sum_{j=1}^{N}\mathbf{k}'_j+\tfrac{1}{2}(1+\alpha_0)Q\mathbf{B}\times\sum_{j=1}^{N}\alpha_j\mathbf{r}'_j , \tag{37}$$

$$\boldsymbol{\pi}_i=\boldsymbol{\pi}'_i+\alpha_i\boldsymbol{\pi}'_0+\tfrac{1}{2}\alpha_iQ\mathbf{B}\times\sum_{j=1}^{N}\alpha_j\mathbf{r}'_j . \tag{38}$$

Hence, the transformed Hamiltonian reads

$$H'=H_{\text{c.m.}}+H_{\text{int}}+H_c , \tag{39}$$

where

$$H_{\text{c.m.}}=\left[\sum_{j=0}^{N}\frac{\alpha_j^2}{2m_j}\right]\boldsymbol{\pi}'^2_0 \tag{40}$$

is the collective term. The internal Hamiltonian is

$$\begin{aligned}H_{\text{int}}=&\frac{1}{2m_0}\left[\sum_{i=1}^{N}[\mathbf{k}'_i-\tfrac{1}{2}(1+\alpha_0)Q\alpha_i\mathbf{B}\times\mathbf{r}'_i]\right]^2\\&+\sum_{i=1}^{N}\frac{1}{2m_i}\left[\boldsymbol{\pi}'_i+\tfrac{1}{2}\alpha_iQ\mathbf{B}\times\sum_{j=1}^{N}\alpha_j\mathbf{r}'_j\right]^2\\&+V(\mathbf{r}'_i,\mathbf{r}'_i-\mathbf{r}'_j) .\end{aligned} \tag{41}$$

The coupling term reads

$$\begin{aligned}H_c=&\sum_{i=1}^{N}\left[\frac{\alpha_i}{m_i}-\frac{\alpha_0}{m_0}\right]\boldsymbol{\pi}'_0\cdot\boldsymbol{\pi}'_i\\&+\sum_{i=1}^{N}\left[\frac{1}{2}\left[\sum_{j=0}^{N}\frac{\alpha_j^2}{m_j}+\frac{\alpha_0}{m_0}\right]Q\alpha_i-\frac{\alpha_0}{m_0}q_i\right]\boldsymbol{\pi}'_0\cdot\mathbf{B}\times\mathbf{r}'_i .\end{aligned} \tag{42}$$

These expressions are valid for any choice of the N arbitrary parameters α_i. In fact, these parameters should be chosen in such a way that H_c can be treated as a perturbation[9,10,6] up to high values of the magnetic field. Let us now consider possible choices of these parameters which lead to simplifications.

The simplest choice

$$\alpha_0=1, \quad \alpha_{i>0}=0 \tag{43}$$

provides the usual operator $\mathbf{C}(\mathbf{0})$. This leads to a drastic simplification of H_{int} (see Ref. 10). The coupling term may be rewritten as

$$H_c=-\frac{1}{m_0}\boldsymbol{\pi}'_0\cdot\sum_{i=1}^{N}\mathbf{k}'_i . \tag{44}$$

This expression has been employed in our treatment of the transverse Hamiltonian of hydrogenic ions [Eq. (2.11) of Ref. 10]. It has not been used yet in the neutral case. A second obvious choice is ($i=0$ to N)

$$\alpha_i = m_i / N \ , \tag{45}$$

where M is the total mass. In this case, an example of $H_{\rm int}$ is given by Eq. (11) of Ref. 6. The coordinate $\mathbf{R}(\alpha)$ is then the usual c.m. coordinate and H_c reduces to

$$H_c = \frac{1}{M} \boldsymbol{\pi}_0' \cdot \mathbf{B} \times \sum_{i=1}^{N} \left[Q \frac{m_i}{M} - q_i \right] \mathbf{r}_i' \ . \tag{46}$$

The choice (45), which is traditional in the absence of external field, has been employed in our treatment of neutral atoms [compare (46) with Eq. (12) of Ref. 6]. The coupling term, with $\boldsymbol{\pi}_0'$ replaced by its eigenvalue, is then well known to represent the "motional Stark effect."[17] Such an effect also occurs in the charged case with the present treatment. The only difference is that $\boldsymbol{\pi}_0'$ is not an exact constant of motion. The choice (45) allows a simultaneous treatment of the longitudinal and transverse motions. In our previous treatment of the charged case,[10] the choices (43) and (45) were applied respectively to the transverse and parallel motions. However, the values (45) lead, when Q differs from zero, to a much more complicated internal Hamiltonian. Other choices are possible. For example, it is possible to eliminate the second term of (42); in this case α_0 is solution of a cubic equation.

VI. AN EXAMPLE: THE ATOMIC CASE

In the atomic case, one has

$$m_{i>0} = m \ll m_0 \ ,$$

$$q_{i>0} = q \ .$$

If we make the symmetric choice

$$\alpha_{i>0} = \alpha \ , \tag{47}$$

$$\alpha_0 = 1 - N\alpha \ ,$$

the generalized constant of motion takes from (22)–(24) the simple form

$$\mathbf{C}(\alpha) = \left[1 - \frac{Q}{q} \alpha \right] \mathbf{C}(\mathbf{0}) + \frac{Q}{q} \alpha \boldsymbol{\Pi} \ . \tag{48}$$

Obviously, it is a single-parameter mixing of the two simple operators which possess the properties of a total kinetic momentum. In fact, any $\mathbf{C}(\alpha)$ possesses these properties. However, its commutator with H is not always small and approximate constants of motion are restricted to α values of the order of m/m_0.

The coupling term between the internal and c.m. motion becomes

$$H_c = \left[\frac{\alpha}{m} - \frac{\alpha_0}{m_0} \right] \boldsymbol{\pi}_0' \cdot \sum_{i=1}^{N} \boldsymbol{\pi}_i' + \frac{1}{2m_0} \left[\left[\alpha_0^2 + \alpha_0 + N\alpha^2 \frac{m_0}{m} \right] Q\alpha - 2q\alpha_0 \right] \boldsymbol{\pi}_0' \cdot \mathbf{B} \times \sum_{i=1}^{N} \mathbf{r}_i' \ , \tag{49}$$

which is small for α of the order of m/m_0. We note that the additional parameter α does not allow a significant simplification of the problem with respect to the treatment of Refs. 9, 10, and 6.

VII. CONCLUSION

In the present work, we show that the close similarities observed in analytical[8] or numerical[6] studies of the c.m. problem for charged and neutral systems in a magnetic field, are not fortuitous. A unified treatment of the apparently disconnected charged and neutral cases is possible. Simultaneously, this treatment unifies the descriptions of the longitudinal and transverse motions. It includes the zero-field problem as a particular case.

The definition of the approximate constant of motion introduced in Ref. 7 is not unique. This operator must behave as a kinetic momentum associated with the total pseudomomentum. This physical definition fixes the algebra satisfied by this operator.[11] More general linear combinations of the $\boldsymbol{\pi}_i$ and $\mathbf{k}_i$ involving N arbitrary parameters (the number of particles minus one) are possible. However, these expressions behave as approximate constants of motion only if they are not too different from the original operator $\mathbf{C}(\mathbf{0})$. Hence, while the additional freedom explains the apparently fortuitous similarities between the c.m. separation in charged and neutral systems, it does not introduce practical simplifications in the atomic case. The parameter choice leading to the simplest expressions (especially for the internal Hamiltonian) remains the original one. However, the new flexibility of the approximate constant of motion might be useful for the more complicated molecular case which has recently received attention.[18]

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APPENDIX

The canonical transformations encountered in Sec. V are not displayed in a standard form.[19] In this appendix, their canonical character is emphasized. They are shown to belong to the $SO(N+1,N+1)$ subgroup of the symplectic group.

In order to simplify the presentation, we first discuss the particular case of a single charged particle in a magnetic field (see Sec. II). The operators $\boldsymbol{\pi}$ and $\mathbf{k}$ are redefined by dividing them by $(\hbar|q|B)^{1/2}$. We choose the z axis along the field direction $\hat{\mathbf{B}}$. With these choices, (5) provides

$$[\pi_x, \pi_y] = i \ \mathrm{sgn}(q) \ ,$$
$$[k_x, k_y] = -i \ \mathrm{sgn}(q) \ . \tag{A1}$$

The remaining commutators between the components of $\boldsymbol{\pi}$ and $\mathbf{k}$ are zero. From (A1), it appears that the canonically conjugate operators are on one hand π_x, π_y and on the other hand k_y, k_x if q is positive. If q is negative, they

become π_y, π_x and k_x, k_y. Therefore, it is meaningful to apply a canonical transformation to the components of $\boldsymbol{\pi}_\perp$ and $\mathbf{k}_\perp$. However, the physical context requires transformations which preserve the vector character and the Hermiticity of $\boldsymbol{\pi}_\perp$ and $\mathbf{k}_\perp$, i.e.,

$$\begin{pmatrix} \boldsymbol{\pi}'_\perp \\ \mathbf{k}'_\perp \end{pmatrix} = \underline{A} \begin{pmatrix} \boldsymbol{\pi}_\perp \\ \mathbf{k}_\perp \end{pmatrix} , \tag{A2}$$

where $\underline{A}$ is a real 2×2 matrix. With (A1), $\underline{A}$ must satisfy

$$\underline{A}^T \underline{\sigma}_z \underline{A} = \underline{\sigma}_z \tag{A3}$$

where $\underline{\sigma}$ represents the Pauli matrices. The general form of matrices satisfying (A3) and connected with the identity is

$$\underline{A} = (\cosh\alpha)\underline{1} + (\sinh\alpha)\underline{\sigma}_z \tag{A4}$$

where α is a real parameter. The canonical transformation (A2) therefore belongs to the SO(1,1) group. The transformation (A2) can be realized with the operator

$$T(\alpha) = \exp[-i\alpha\,\mathrm{sgn}(q)\hat{\mathbf{B}}\cdot(\mathbf{k}\times\boldsymbol{\pi})] . \tag{A5}$$

Now, we extend the transformation to a system of $N+1$ *charged* particles. Again, we redefine the $\boldsymbol{\pi}_i$ and $\mathbf{k}_i$ by dividing them by $(\hbar|q_i|B)^{1/2}$. The vectors $\boldsymbol{\pi}_{i\perp}$ and $\mathbf{k}_{i\perp}$ are arranged in a column matrix $\underline{\mathbf{M}}$ in the following order

$$\begin{aligned} &\boldsymbol{\pi}_{i\perp}(q_i>0),\quad \mathbf{k}_{i\perp}(q_i<0) , \\ &\mathbf{k}_{i\perp}(q_i>0),\quad \boldsymbol{\pi}_{i\perp}(q_i<0) . \end{aligned} \tag{A6}$$

Physically interesting transformations take the form

$$\underline{\mathbf{M}}' = \underline{A}\,\underline{\mathbf{M}} \tag{A7}$$

with $\underline{A}$ real. It is readily shown that this matrix belongs to the $\mathrm{SO}(N+1,N+1)$ group, since it satisfies (A3) with the elements of $\underline{\sigma}_z$ replaced by zero or unit matrices. The generators of the corresponding algebra are given by the $(N+1)(2N+1)$ operators

$$\hat{\mathbf{B}}\cdot(\boldsymbol{\pi}_i\times\mathbf{k}_j) \quad (i,j=0,\ldots,N)$$

and

$$\hat{\mathbf{B}}\cdot(\boldsymbol{\pi}_i\times\boldsymbol{\pi}_j),\quad \hat{\mathbf{B}}\cdot(\mathbf{k}_i\times\mathbf{k}_j) \quad (i>j=0,\ldots,N) .$$

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