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Separation of centre-of-mass motion for a charged two-body system in a homogeneous magnetic field

Daniel Baye

Physique Théorique et Mathématique CP 229, Université Libre de Bruxelles, Brussels, Belgium

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Abstract. Exact centre-of-mass separation is performed for the problem of a charged two-body system in a homogeneous magnetic field. Common eigenstates of three exact and one approximate constants of motion are constructed in the creation and annihilation operator formalism. Their expression as an infinite series in coordinate representation is obtained using two real linear canonical transformations. An expansion of the wavefunction in this eigenstate basis provides an infinite system of differential equations for the relative motion. This system of equations differs from the infinite nucleus mass approximation by the existence of small terms which couple states with different values of the magnetic quantum number. The usual limitation of the number of electron Landau states leads to a finite number of coupled equations.

1. Introduction

The problem of simple atoms in strong magnetic fields has received considerable attention for many years (see Garstang (1977), Canuto and Ventura (1977), Johnson *et al* (1983) for reviews and for the implications in solid-state physics and in astrophysics). Most of the work has been devoted to the accurate determination of atomic spectra in the different field regions, the nucleus being considered as infinitely massive (infinite-mass approximation). When accurate energy levels are obtained for the neutral hydrogen atom in this approximation, the spectrum of hydrogen-like ions is simply given by the scaling law (Surmelian and O'Connell 1974, Garstang 1977)

$$E(Z, B) = Z^2 E(1, B/Z^2) \tag{1.1}$$

where B is the magnetic field and Z the charge number of the nucleus. Implicit in the infinite-mass approximation is the assumption that nucleus-mass corrections are negligible, like in the low-field limit. Recently however, Virtamo and Simola (1978) and Wunner *et al* (1980) have shown that this assumption is incorrect for the hydrogen atom in the high-field region ($B > 10^6$ T).

An important basic quantum mechanical question is raised: can the separation of centre-of-mass (CM) motion in a homogeneous magnetic field be performed exactly? For a neutral two-body system, a full solution to this problem has recently been given (Avron *et al* 1978, Herold *et al* 1981). The CM motion can be separated out exactly and the treatment of the reduced Hamiltonian is not more difficult than in the

infinite-proton-mass approximation when the CM motion is parallel to the field axis. In this case, the proton-mass correction can be accounted for, with good accuracy, by a constant energy shift proportional to the proton cyclotron energy. Therefore, the CM correction is small with respect to the total energy of the system (which includes the electron cyclotron energy) but is no longer negligible with respect to the Coulomb binding energy of the system for large magnetic field strengths.

The relative simplicity of the neutral two-body problem arises from the existence of four constants of motion which commute with each other: the three components of the pseudomomentum (Avron *et al* 1978) and an operator which, for particular gauge choices, becomes identical to the orbital momentum component along the field axis. For a charged two-body system, the transverse components of the pseudomomentum cannot be made sharp simultaneously. The problem is then more complicated since one of the constants of motion becomes useless. However, Avron *et al* have shown that a notion of reduced Hamiltonian still exists in this case. Besides, they found that the spectrum of the system is infinitely degenerate.

The aim of this paper is to present an exact analytical treatment of CM separation for a *charged* two-body system in a homogenous magnetic field. Recently, we have proved the existence of an approximate constant of motion for the charged case (Baye 1982). This approximate constant of motion commutes with the three exact ones and with all but a small term of the Hamiltonian: the nucleus kinetic energy term. With four constants of motion (exact and approximate), the CM motion can be separated out in the charged problem also. Intuitively, we expect the electron-plus-nucleus system to behave like a charged particle with mass near to the nucleus mass. This 'particle' should have a spectrum similar to a harmonic Landau spectrum (the infinite degeneracy of such a spectrum corresponds to the degeneracy found by Avron *et al*). Since the nucleus cyclotron energy is about half the proton cyclotron energy, and since the Coulomb energy of a charged system is enhanced with respect to the hydrogen energy (see (1.1)), the CM corrections are expected to play, for low-lying CM states, a smaller role than the constant correction of the neutral case. However, the existence of a full (more or less harmonic) excitation spectrum should allow higher CM excitation energies and makes an exact study of the problem worthy of interest.

In § 2, the problem of a single particle in a homogeneous magnetic field is summarised, with particular emphasis on charge-sign dependence. The two-body problem and its exact and approximate constants of motion are presented in § 3. Section 4 is devoted to the construction of a common eigenstate basis of the constants of motion. In § 5, the matrix elements of the interaction potential are shown to be strikingly simple in this basis. An exact system of coupled differential equations is derived in § 6 and discussed. Concluding remarks are presented in § 7.

2. Charged particle in a homogeneous magnetic field

The quantum mechanical problem of a single particle in a magnetic field has been treated by many authors (see e.g. Cohen-Tannoudji *et al* 1973, Virtamo and Jauho 1975, Garstang 1977, Canuto and Ventura 1977, Avron *et al* 1978). In most cases, however, the authors have focused on the problem of a negatively charged particle. In the present work, we shall need formulae and notations with an explicit reference to the sign of the particle charge. For this reason, this section is devoted to a summary of single-particle properties and to a presentation of appropriate notations.

Let $\boldsymbol{r}$ and $\boldsymbol{p}$ be respectively the coordinate and momentum of a particle with mass m and charge q. In a homogeneous magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$, the non-relativistic spinless Hamiltonian is

$$H = (2m)^{-1}\boldsymbol{\pi}^2 \tag{2.1}$$

where the kinetic momentum $\boldsymbol{\pi}$ reads

$$\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A} \tag{2.2}$$

where $\boldsymbol{A}$ is the vector potential. With the gauge (which we shall use throughout)

$$\boldsymbol{A} = \tfrac{1}{2}\boldsymbol{B} \times \boldsymbol{r}, \tag{2.3}$$

the pseudomomentum (Johnson and Lippmann 1949, Avron *et al* 1978) can be written

$$\boldsymbol{k} = \boldsymbol{p} + q\boldsymbol{A}. \tag{2.4}$$

Its components and the component l_z of the angular momentum are constants of motion. The commutator of k_x and k_y is $-\mathrm{i}\hbar qB$. Since k_x and k_y do not commute, the most useful constants of motion are $\boldsymbol{k}_\perp^2 = k_x^2 + k_y^2$, p_z and l_z.

In the following sections, we need the expression of the above-mentioned operators in creation and annihilation form. In this formalism, it is convenient to introduce the Larmor frequency

$$\omega = |q|B/2m \tag{2.5}$$

(i.e. half the cyclotron frequency) and the Larmor radius

$$b = (2\hbar/|q|B)^{1/2} = (\hbar/m\omega)^{1/2}. \tag{2.6}$$

Then we define (Cohen-Tannoudji *et al* 1973, Canuto and Ventura 1977, Avron *et al* 1978, Johnson *et al* 1983)

$$\begin{aligned} a_\pm^\dagger &= \tfrac{1}{2}(x/b - b\,\partial/\partial x) \pm \tfrac{1}{2}\mathrm{i}(y/b - b\,\partial/\partial y) \\ a_\pm &= \tfrac{1}{2}(x/b + b\,\partial/\partial x) \mp \tfrac{1}{2}\mathrm{i}(y/b + b\,\partial/\partial y) \end{aligned} \tag{2.7}$$

with the algebra

$$[a_\pm, a_\pm^\dagger] = 1 \tag{2.8}$$

all the other commutators being zero.

With these operators, the spherical components of $\boldsymbol{\pi}$ and $\boldsymbol{k}$ can be written $[\pi_\pm = 2^{-1/2}(\pi_x \pm \mathrm{i}\pi_y)]$

$$\pi_\pm^{(\pm)} = k_\pm^{(\mp)} = -\mathrm{i}(\hbar|q|B)^{1/2} a_\mp \qquad \pi_\mp^{(\mp)} = k_\mp^{(\mp)} = \mathrm{i}(\hbar|q|B)^{1/2} a_\mp^\dagger. \tag{2.9}$$

In (2.9), the superscript denotes the sign of charge q. With (2.7) and (2.9), the transverse part of the Hamiltonian and the constants of motion take the form

$$\boldsymbol{\pi}_\perp^{(\pm)2} = \boldsymbol{k}_\perp^{(\mp)2} = \hbar|q|B(2a_\mp^\dagger a_\mp + 1) \tag{2.10}$$

$$l_z = (2qB)^{-1}(\boldsymbol{k}_\perp^{(\pm)2} - \boldsymbol{\pi}_\perp^{(\pm)2}) = \hbar(a_+^\dagger a_+ - a_-^\dagger a_-). \tag{2.11}$$

The common eigenstates of these operators are readily obtained as

$$|ns\rangle^{(\pm)} = (n!\,s!)^{-1/2}(a_\mp^\dagger)^n (a_\pm^\dagger)^s |0\rangle \tag{2.12}$$

where $|0\rangle$ is a boson vacuum defined by $a_\pm|0\rangle = 0$, with the properties

$$\begin{aligned} &H_\perp^{(\pm)}|ns\rangle^{(\pm)} = (2n+1)\hbar\omega|ns\rangle^{(\pm)} \\ &\boldsymbol{k}_\perp^{(\pm)2}|ns\rangle^{(\pm)} = (2s+1)\hbar|q|B|ns\rangle^{(\pm)} \\ &l_z|ns\rangle^{(\pm)} = \pm(s-n)\hbar|ns\rangle^{(\pm)}. \end{aligned} \tag{2.13}$$

In coordinate representation, the expressions of the eigenstates (2.12) are given for a negative charge by equation (43) of Virtamo and Jauho (1975), equation (5) of Simola and Virtamo (1978) and equation (A.25) of Canuto and Ventura (1977).

3. The charged two-body problem

From now on, we specialise to the following problem: we consider two particles with masses m_0 and m_1 and charges q_0 and q_1 verifying the conditions

$$q_0 > 0 \qquad q_1 < 0 \qquad q_0 > |q_1| \tag{3.1a}$$

$$m_0 \gg m_1. \tag{3.1b}$$

Condition (3.1*a*) is not a real restriction since the neutral problem has been treated by Avron *et al* (1978) and Herold *et al* (1981) and since the other cases might be treated like in the following (the treatment is even simpler if both charges have the same sign—see § 4). On the contrary, condition (3.1*b*) is essential for the existence of an approximate constant of motion (Baye 1982). If this condition were not met, the equations derived in § 6 would remain valid but would be much more complicated to solve.

The Hamiltonian of the system is

$$H = (2m_0)^{-1}\boldsymbol{\pi}_0^2 + (2m_1)^{-1}\boldsymbol{\pi}_1^2 + V \tag{3.2}$$

where V is a translation-invariant interaction potential with a cylindrical symmetry around the field axis. We also make use of the decomposition

$$H = H_\perp + H_z + V \tag{3.3}$$

where $H_\perp$ and H_z are the transverse and parallel interaction-free parts of the Hamiltonian.

Besides parity, the constants of motion are the total pseudomomentum

$$\boldsymbol{K} = \boldsymbol{k}_0 + \boldsymbol{k}_1 \tag{3.4}$$

and the z component of the total angular momentum

$$L_z = l_{0z} + l_{1z}. \tag{3.5}$$

The operator K_z is identical to the z component of the CM momentum $\boldsymbol{P} = \boldsymbol{p}_0 + \boldsymbol{p}_1$. Since K_x and K_y do not commute, the number of commuting constants of motion is three, i.e. one less than in the neutral case. The operator (Baye 1982)

$$\boldsymbol{C} = (1 + q_1/q_0)\boldsymbol{\pi}_0 - (q_1/q_0)\boldsymbol{k}_0 + \boldsymbol{k}_1 \tag{3.6}$$

is readily seen to commute with $\boldsymbol{K}$, condition (3.1*a*) being here unnecessary. Moreover, $\boldsymbol{C}$ commutes with V and $\boldsymbol{\pi}_1^2/2m_1$ but not with the small term $\boldsymbol{\pi}_0^2/2m_0$. The operators $P_z, \boldsymbol{K}_\perp^2, L_z$ and $\boldsymbol{C}_\perp^2$ are thus four commuting, exact or approximate, constants of motion.

In the direction parallel to the field, the situation is not different from the neutral case: the CM motion is free and can easily be separated out. In the rest of this section, and in §§ 4 and 5, we shall restrict the discussion to the problems related to the transverse motion.

A natural basis for the study of $H_\perp$ is the independent-particle basis. Let us thus introduce the boson operators (2.7) for particles 0 and 1. With this formalism, $H_\perp$ reads (see (2.5), (2.10) and (3.1*a*))

$$H_\perp = \hbar\omega_0(2a_{0-}^\dagger a_{0-} + 1) + \hbar\omega_1(2a_{1+}^\dagger a_{1+} + 1). \tag{3.7}$$

With (2.11) and (3.5), operator L_z also takes a simple form, involving number operators only. Both operators are diagonal in the basis

$$|n_1 n_0 s_1 s_0\rangle = (n_1! n_0! s_1! s_0!)^{-1/2}(a_{1+}^\dagger)^{n_1}(a_{0-}^\dagger)^{n_0}(a_{1-}^\dagger)^{s_1}(a_{0+}^\dagger)^{s_0}|0\rangle \tag{3.8}$$

where $|0\rangle$ is a two-particle vacuum defined by $a_{0\pm}|0\rangle = a_{1\pm}|0\rangle = 0$. However, this basis is not very convenient since the quantum numbers s_0 and s_1 are not related to constants of motion whereas the constants of motion $\boldsymbol{K}_\perp^2$ and $\boldsymbol{C}_\perp^2$ are not diagonal. A more appropriate basis is introduced in § 4.

4. Common eigenstates of the exact and approximate constants of motion

Let us introduce the creation and annihilation operators $A_+^\dagger$ and A_+ associated with the total pseudomomentum $\boldsymbol{K}$. With (2.9) and (2.10), one has

$$\boldsymbol{K}_\perp^2 = \hbar QB(2A_+^\dagger A_+ + 1) \tag{4.1}$$

where

$$Q = q_0 - |q_1| \tag{4.2}$$

is the total charge. With (3.4), (2.9) and the notation

$$\varepsilon = (|q_1|/q_0)^{1/2} \tag{4.3}$$

the operators $A_+^\dagger$ and A_+ are expressed as

$$A_+^\dagger = (1-\varepsilon^2)^{-1/2}(a_{0+}^\dagger - \varepsilon a_{1-}) \qquad A_+ = (1-\varepsilon^2)^{-1/2}(a_0 + \varepsilon a_{1-}^\dagger). \tag{4.4a}$$

Because of condition (3.1*a*), ε is smaller than unity. Obviously, $A_+^\dagger$ commutes with $a_{0-}^\dagger$ and $a_{1+}^\dagger$. In order to complete the canonical set, let us also define the canonically conjugate operators

$$a_-^\dagger = (1-\varepsilon^2)^{-1/2}(-\varepsilon a_{0+} + a_{1-}^\dagger) \qquad a_- = (1-\varepsilon^2)^{-1/2}(-\varepsilon a_{0+}^\dagger - a_{1-}) \tag{4.4b}$$

which commute with the other operators of the set. Equations (4.4) express a linear canonical transformation (Moshinsky and Quesne 1971, Wolf 1979). Notice that it is not a point transformation (i.e. a transformation involving the coordinates only) since the right-hand sides of (4.4) mix creation and annihilation operators. This emphasises the complication introduced by condition (3.1*a*). If q_0 and q_1 were both positive or negative, the canonical transformation would be point-like.

Besides $H_\perp$ (equation (3.7)) and $\boldsymbol{K}_\perp^2$ (equation (4.1)), L_z also takes a simple form with the new canonical set

$$L_z = \hbar(a_{1+}^\dagger a_{1+} - a_{0-}^\dagger a_{0-} - a_-^\dagger a_- + A_+^\dagger A_+). \tag{4.5}$$

The Hamiltonian and the two exact transverse constants of motion are thus diagonal in the basis (hereafter called intermediate basis)

$$|n_1 n_0 s S\rangle = (n_1! n_0! s! S!)^{-1/2} (a_{1+}^\dagger)^{n_1} (a_{0-}^\dagger)^{n_0} (a_-^\dagger)^s (A_+^\dagger)^S |\bar{0}\rangle \tag{4.6}$$

where a new vacuum $|\bar{0}\rangle$ is defined by $a_{1+}|\bar{0}\rangle = a_{0-}|\bar{0}\rangle = a_-|\bar{0}\rangle = A_+|\bar{0}\rangle = 0$. This vacuum is related to $|0\rangle$ by

$$|\bar{0}\rangle = (1-\varepsilon^2)^{1/2} \exp(\varepsilon a_{0+}^\dagger a_{1-}^\dagger)|0\rangle \tag{4.7}$$

as shown from (4.4) and from the definition of the new vacuum.

However, the basis (4.6) still presents a drawback: the approximate constant of motion $\boldsymbol{C}_\perp^2$ is not diagonal. Indeed, using (2.9), (3.6) and (4.4), one obtains

$$\boldsymbol{C}_\perp^2 = \hbar Q B \{2[\varepsilon a_-^\dagger + (1-\varepsilon^2)^{1/2} a_{0-}^\dagger][\varepsilon a_- + (1-\varepsilon^2)^{1/2} a_{0-}] + 1\}. \tag{4.8}$$

This is of course not surprising since $\boldsymbol{C}_\perp^2$ does not commute exactly with $H_\perp$.

Let us introduce a second canonical transformation

$$\alpha_0^\dagger = (1-\varepsilon^2)^{1/2} a_{0-}^\dagger + \varepsilon a_-^\dagger \qquad \alpha^\dagger = -\varepsilon a_{0-}^\dagger + (1-\varepsilon^2)^{1/2} a_-^\dagger \tag{4.9}$$

and the corresponding relations for α_0 and α. The first relation (4.9) is inspired by the expression (4.8) of $\boldsymbol{C}_\perp^2$. The second one ensures that the canonical commutation relations are verified. Notice that, contrarily to (4.4), the present canonical transformation is point-like and conserves the vacuum $|\bar{0}\rangle$.

Now, the three exact or approximate constants of motion take simultaneously simple forms. Besides (4.1), one obtains

$$\boldsymbol{C}_\perp^2 = \hbar Q B (2\alpha_0^\dagger \alpha_0 + 1) \tag{4.10}$$

and

$$L_z = \hbar (a_{1+}^\dagger a_{1+} - \alpha_0^\dagger \alpha_0 - \alpha^\dagger \alpha + A_+^\dagger A_+). \tag{4.11}$$

The corresponding basis states are

$$|n_1 \nu_0 \sigma S\rangle = (n_1! \nu_0! \sigma! S!)^{-1/2} (a_{1+}^\dagger)^{n_1} (\alpha_0^\dagger)^{\nu_0} (\alpha^\dagger)^\sigma (A_+^\dagger)^S |\bar{0}\rangle. \tag{4.12}$$

Their expressions in coordinate representation are not simple. The principle of their derivation is explained in the appendix.

Since $\boldsymbol{C}_\perp^2$ is not an exact constant of motion, $H_\perp$ becomes more complicated but only slightly non-diagonal:

$$\begin{aligned} H_\perp = {} & \hbar\omega_1 (2a_{1+}^\dagger a_{1+} + 1) + (1-\varepsilon^2)\hbar\omega_0 (2\alpha_0^\dagger \alpha_0 + 1) \\ & + \varepsilon^2 \hbar\omega_0 (2\alpha^\dagger \alpha + 1) - \varepsilon (1-\varepsilon^2)^{1/2} \hbar\omega_0 (\alpha^\dagger \alpha_0 + \alpha_0^\dagger \alpha). \end{aligned} \tag{4.13}$$

The first two terms resemble expression (3.7). The other terms are small and the non-diagonal term arises from the fact that $\boldsymbol{C}_\perp^2$ does not commute with $\boldsymbol{\pi}_{0\perp}^2$.

The eigenstate basis receives a clear interpretation in terms of two nearly decoupled pseudoparticles. A first pseudoparticle has $\boldsymbol{K}$ as pseudomomentum and $\boldsymbol{C}$ as kinetic momentum. Its charge is easily obtained to be the total charge Q by inspecting the commutation relations of the components of $\boldsymbol{C}_\perp$ and $\boldsymbol{K}_\perp$. With (2.11), one can even define the z component of its orbital momentum as $\hbar(A_+^\dagger A_+ - \alpha_0^\dagger \alpha_0)$. Hence, the difference of quantum numbers $S - \nu_0$ can be interpreted as its magnetic quantum number. The second pseudoparticle is very similar to the light particle 1. Its kinetic momentum is $\boldsymbol{\pi}_1$ but its pseudomomentum is $\boldsymbol{k}_1 - (q_1/q_0)(\boldsymbol{k}_0 - \boldsymbol{\pi}_0)$. Its charge is found to be q_1 and (2.11) provides the orbital-momentum z component

$\hbar(a_{1+}^{\dagger}a_{1+}-\alpha^{\dagger}\alpha)$. The magnetic quantum number of this negatively charged particle is then $n_1-\sigma$. Notice that the expression (4.11) of L_z can be reinterpreted as the sum of the orbital momenta of the two pseudoparticles. Finally, the masses of the pseudoparticles can be derived from the coefficients of the number operators $\alpha_0^{\dagger}\alpha_0$ and $a_{1+}^{\dagger}a_{1+}$ in (4.13). These masses are respectively m_0 and m_1. The pseudoparticle description is accurate if the last two terms of (4.13) are small, i.e. if conditions (3.1*b*) or $q_0 \gg |q_1|$ are satisfied.

5. Potential matrix elements in the eigenstate basis

The interaction potential V is assumed to be an analytical function of $\boldsymbol{r}_{\perp}^2$ ($\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_0$), the relative coordinate z in the direction parallel to the field axis being considered as a parameter. Using (2.7), (4.4) and (4.9), one obtains

$$(\boldsymbol{r}_{1\perp}-\boldsymbol{r}_{0\perp})^2 = b_1^2(a_{1+}^{\dagger}+\alpha)(a_{1+}+\alpha^{\dagger}). \tag{5.1}$$

The potential does not depend on operators $\alpha_0^{\dagger}$, α_0 and $A_+^{\dagger}$, A_+. Therefore, its matrix elements in the eigenstate basis read

$$\langle n_1\nu_0\sigma S|V|n_1'\nu_0'\sigma' S'\rangle$$
$$= \delta_{\nu_0\nu_0'}\delta_{SS'}(n_1!n_1'!\sigma!\sigma'!)^{-1/2}\langle\bar{0}|(\alpha)^{\sigma}(a_{1+})^{n_1}V(a_{1+}^{\dagger})^{n_1'}(\alpha^{\dagger})^{\sigma'}|\bar{0}\rangle.$$

The Kronecker symbols arise naturally from the fact that V commutes with the operators $\boldsymbol{C}_{\perp}^2$ and $\boldsymbol{K}_{\perp}^2$. Moreover, the matrix element can still be simplified as

$$\langle n_1\nu_0\sigma S|V|n_1'\nu_0'\sigma' S'\rangle = \delta_{\nu_0\nu_0'}\delta_{SS'}V_{n_1n_1'}^{\sigma\sigma'}(z) \tag{5.2}$$

with

$$V_{n_1n_1'}^{\sigma\sigma'}(z) = \langle\phi_{n_1\sigma}(\boldsymbol{r}_{\perp}')|V(\boldsymbol{r}_{\perp}'^2, z)|\phi_{n_1'\sigma'}(\boldsymbol{r}_{\perp}')\rangle. \tag{5.3}$$

We have taken advantage of the particular form of $\boldsymbol{r}_{\perp}^2$ in (5.1) to introduce a coordinate representation (see (2.7)) associated with the light pseudoparticle, namely

$$x'+iy' = b_1(a_{1+}^{\dagger}+\alpha) \qquad x'-iy' = b_1(a_{1+}+\alpha^{\dagger}). \tag{5.4}$$

The most striking property of the eigenstate basis is exhibited in (5.3): the matrix element is identical to the expression encountered in the infinite-mass approximation. Indeed, the wavefunction $\phi_{n_1\sigma}(\boldsymbol{r}_{\perp}')$ in (5.3) is the usual wavefunction of a particle with mass m_1 and charge q_1 (references giving its explicit form have been quoted in § 2). Explicit analytic expressions or techniques of numerical computation of the matrix elements $V_{n_1n_1'}^{\sigma\sigma'}$ have been discussed by many authors (e.g. Ventura 1973, Canuto and Ventura 1977, Simola and Virtamo 1978, Pröschel *et al* 1982). Let us only quote the important selection rule due to the cylindrical symmetry of the potential

$$n_1-\sigma = n_1'-\sigma'. \tag{5.5}$$

The magnetic quantum number of the light pseudoparticle is conserved.

6. Exact separation of CM motion

The exact constants of motion of the problem are P_z, $\boldsymbol{K}_{\perp}^2$, L_z and parity. The eigenstates Ψ of the problem can be labelled by the corresponding good quantum numbers K, S

and M (the parity quantum number has been dropped because it does not play any role here; it becomes important when solving the equations we shall derive). Let us introduce the expansion

$$\Psi^{KSM} = \sum_{n_1\nu_0\sigma} |n_1\nu_0\sigma S\rangle \, e^{iKZ} \varphi_{n_1\sigma}(z). \tag{6.1}$$

A mixed notation is employed in (6.1) to emphasise the fact that the basis states need not be given in coordinate representation. The three summation indices are not independent; (4.11) shows that they are related by

$$\nu_0 + \sigma - n_1 = S - M. \tag{6.2}$$

To simplify the notations, the unknown functions $\varphi_{n_1\sigma}$ are not labelled by the good quantum numbers nor by the redundant index ν_0.

Introducing (6.1) in a Schrödinger equation with Hamiltonian (3.3) and using (4.12), (4.13), (5.2) and (5.5), one obtains the infinite system of coupled equations

$$\begin{aligned}\Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2} &+ V^{\sigma\sigma}_{n_1n_1}(z) + \hbar\omega_1(2n_1+1) \\ &+ \hbar\omega_0[(1-\varepsilon^2)(2\nu_0+1)+\varepsilon^2(2\sigma+1)] + \frac{\hbar^2K^2}{2(m_0+m_1)} - E\Big)\varphi_{n_1\sigma}(z) \\ &+ \sum_{n_1'\neq n_1} V^{\sigma\sigma+n_1-n_1'}_{n_1n_1'}(z)\varphi_{n_1'\sigma+n_1-n_1'}(z) \\ &- \hbar\omega_0\varepsilon(1-\varepsilon^2)^{1/2}[\sigma^{1/2}(\nu_0+1)^{1/2}\varphi_{n_1\sigma-1}(z) + (\sigma+1)^{1/2}\nu_0^{1/2}\varphi_{n_1\sigma+1}(z)] = 0\end{aligned} \tag{6.3}$$

where μ is the reduced mass. Equations (6.3) depend in a trivial way on the good quantum number K. They also depend implicitly on the difference of good quantum numbers $S-M$ through ν_0 and (6.2). The infinite degeneracy announced by Avron *et al* (1978) (see also Baye (1982)) is thus explicitly obtained here. Only the difference of good quantum numbers $S-M$ has an influence on the solution.

The physically interesting energies correspond to light-particle Landau states with $n_1 = 0$ since $\hbar\omega_1(2n_1+1)$ is the dominant term in (6.3). For a given value of $S-M$, (6.2) provides the condition $n_1 \geqslant M-S$. Hence, low energy states are restricted to

$$S - M \geqslant 0. \tag{6.4}$$

In order to have a better insight into (6.3), let us consider the limiting case of highly charged hydrogen-like atoms ($q_0 \gg |q_1|$). Then ε is small and (6.3) can be approximated by

$$\begin{aligned}\Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dz^2} &+ V^{\sigma\sigma}_{n_1n_1}(z) + \hbar\omega_1(2n_1+1) + \hbar\omega_0(2\nu_0+1) + \frac{\hbar^2K^2}{2(m_0+m_1)} - E\Big)\varphi_{n_1\sigma}(z) \\ &+ \sum_{n_1'\neq n_1} V^{\sigma\sigma+n_1-n_1'}_{n_1n_1'}(z)\varphi_{n_1'\sigma+n_1-n_1'}(z) = 0.\end{aligned} \tag{6.5}$$

Equation (6.5) can also be derived from the approximate Hamiltonian

$$H_c = (2m_0)^{-1}\boldsymbol{C}^2 + (2m_1)^{-1}\boldsymbol{\pi}_1^2 + V \tag{6.6}$$

introduced in Baye (1982). A comparison with (3.2) shows that the kinetic energies of the particles are replaced by the kinetic energies of the pseudoparticles defined in § 4. Operators L_z, P_z, $\boldsymbol{K}_\perp^2$ and $\boldsymbol{C}_\perp^2$ are four *exact* constants of motion of H_c. The

orbital momentum components $\hbar(a_{1+}^{\dagger}a_{1+}-\alpha^{\dagger}\alpha)$ and $\hbar(A_{+}^{\dagger}A_{+}-\alpha_0^{\dagger}\alpha_0)$ of the pseudoparticles are linear combinations of these operators (see (2.11) and (4.11)) and are thus also constants of motion. In this approximation, ν_0 and the magnetic number $n_1-\sigma$ of the light pseudoparticle are good quantum numbers. The former is the Landau energy quantum number of the heavy pseudoparticle. The latter closely corresponds to the magnetic quantum number of the infinite-mass approximation. The coupled equations (6.5) differ from the infinite-mass approximation for a given magnetic quantum number $n_1-\sigma$ by trivial CM corrections and by the cyclotron energy term $\hbar\omega_0(2\nu_0+1)$. The intuitive picture discussed in the introduction, of an harmonic Landau spectrum of the nucleus superimposed as a fine structure on the infinite-nucleus-mass spectrum, is thus valid when $q_0 \gg |q_1|$.

Now, we have an obvious interpretation of the terms of (6.3) which have been neglected in (6.5). These small coupling terms arise from the fact that $\boldsymbol{C}_{\perp}^2$ is not an exact constant of motion. They introduce a coupling between states corresponding to different values of the approximate magnetic quantum number $n_1-\sigma$. The largest correcting terms are proportional to $\hbar\omega_0\varepsilon = (m_1/m_0\varepsilon)\hbar\omega_1$.

Finally, let us discuss briefly the principle of the approximation necessary to solve the system of equations (6.3). The usual approximation for such an infinite set of coupled equations is to truncate it with the condition $n_1 \leqslant N$ (Simola and Virtamo 1978). With this restriction and with (6.2), the number of coupled equations is $(N+1)(S-M+1+N/2)$. Although this number is larger than the number $N+1$ of coupled equations in the infinite-mass approximation, the search for approximate numerical solutions remains feasible. In particular, in the adiabatic approximation ($N=0$), the number of coupled equations is $S-M+1$ in place of unit for an infinitely massive nucleus.

7. Conclusion

The existence of an approximate constant of motion $\boldsymbol{C}$ for the charged two-body problem (Baye 1982) allowed us to reinterpret the tranverse interaction-free Hamiltonian in terms of two weakly coupled pseudoparticles. The first pseudoparticle is characterised by the total charge of the system and the nucleus mass. The second pseudoparticle has the same charge and mass as the electron but has a modified pseudomomentum. These pseudoparticles are represented by the common eigenstates of the exact and approximate constants of motion $\boldsymbol{K}_{\perp}^2$, $\boldsymbol{C}_{\perp}^2$ and L_z. In the creation and annihilation operator formalism, these eigenstates are very easy to handle and lead to strikingly simple expressions for the matrix elements of several useful operators. On the contrary, their expression in coordinate representation which can be obtained by performing two linear canonical transformations, is much more complicated.

The main result of the present paper is that CM motion can be separated out exactly for the charged problem with an expansion of the wavefunction in the eigenstate basis. (Here we use the abbreviation 'CM' in spite of the fact that the usual notion of centre-of-mass is valid in the direction parallel to the field axis only.) The technique of separation is more complicated than in the neutral problem but the resulting system of differential equations is in some respects simpler: the Coulomb matrix elements are those of the infinite-mass approximation, while they may involve displaced Landau states in the neutral case, if the CM motion is not parallel to the field axis (Herold *et al* 1981). The solutions depend on the good quantum numbers S and M through

their difference. An infinite Landau degeneracy is thus found for charged two-body systems (Avron *et al* 1978). If the system is truncated by limiting the number of allowed electron Landau states, the number of remaining equations is larger by a factor close to $S-M+1$ than in the neutral problem or in the infinite-mass approximation.

In the case of highly charged ions, an obvious generalisation (equation (6.5)) of the infinite-mass approximation should provide fair results. A nucleus Landau spectrum is superimposed on the electron energies of the infinite-mass approximation. This approximation, described by the modified Hamiltonian H_c (equation 6.6)), supports the naive picture of completely decoupled CM and relative motions. In this case, the corrections are very small with respect to the large electronic energies (see (1.1)). On the contrary, for low-charge ions like He^+, the correction is more important and should deviate significantly from a purely harmonic spectrum. The quantitative study of these deviations requires a detailed analysis of the truncated system of equations (6.3).

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Appendix

The boson operator form of the basis states is very convenient for the present study. It may, however, be desirable for the physical understanding to express these states in coordinate representation. This can be achieved by relations connecting the intermediate and eigenstate bases to the independent-particle basis since the latter has simple expressions in coordinate representation. These relations can be obtained from irreducible representations of the group of real linear canonical transformations, i.e. for two-boson transformations, the symplectic group Sp(4, R) (Moshinsky and Quesne 1971). However, the present canonical transformations ((4.4) or (4.9)) belong to simpler subgroups of this group.

Inspection of (4.9) shows that the second canonical transformation, as a point transformation, belongs to the SU(2) subgroup of Sp(4, R). The generators of SU(2) are

$$J_+ = a_-^\dagger a_{0-} \qquad J_- = a_- a_{0-}^\dagger \qquad J_0 = \tfrac{1}{2}(a_-^\dagger a_- - a_{0-}^\dagger a_{0-}). \tag{A1}$$

These generators obey the familiar SU(2) commutation relations (Hamermesh 1962). The basis states $|n_1 n_0 s S\rangle$ are eigenstates $|jm\rangle$ of the Casimir operator $J_0^2 + \frac{1}{2}(J_+J_- + J_-J_+)$ and of J_0 with respective eigenvalues $j(j+1)$ and m where

$$j = \tfrac{1}{2}(s+n_0) \qquad m = \tfrac{1}{2}(s-n_0). \tag{A2}$$

For a given j-value, the symmetric tensor product states $|n_1 n_0 s S\rangle$ carry a unitary irredicuble representation of dimension $2j+1$ of SU(2). The canonically transformed states $|n_1 \nu_0 \sigma S\rangle$ corresponding to the same j-value are thus related to the intermediate

basis states by

$$|n_1\nu_0\sigma S\rangle = \sum_{\substack{sn_0 \\ (s+n_0=\sigma+\nu_0)}} d^{(\sigma+\nu_0)/2}_{(s-n_0)/2,(\sigma-\nu_0)/2}(2\sin^{-1}\varepsilon)|n_1n_0sS\rangle \tag{A3}$$

where the $d^j_{mm'}$ are the usual SU(2) d-functions (Hamermesh 1962) and the 'rotation angle' only depends on the charge ratio.

The canonical transformation (4.4) belongs to the Sp(2, R) subgroup of Sp(4, R). The generators of this subgroup are

$$\bar{J}_+ = a^\dagger_{1+}a^\dagger_{0-} \qquad \bar{J}_- = a_{1+}a_{0-} \qquad \bar{J}_0 = \tfrac{1}{2}(a^\dagger_{1+}a_{1+} + a^\dagger_{0-}a_{0-} + 1) \tag{A4}$$

and obey the commutation relations

$$[\bar{J}_0, \bar{J}_\pm] = \pm\bar{J}_\pm \qquad [\bar{J}_+, \bar{J}_-] = -2\bar{J}_0.$$

The basis states $|n_1n_0s_1s_0\rangle$ are eigenstates $|\bar{j}\bar{m}\rangle$ of the Casimir operator $\bar{J}_0^2 - \frac{1}{2}(\bar{J}_+\bar{J}_- + \bar{J}_-\bar{J}_+)$ and of $\bar{J}_0$ with respective eigenvalues $\bar{j}(\bar{j}-1)$ and $\bar{m}$ where

$$\bar{j} = \tfrac{1}{2}(|s_1 - s_0| + 1) \qquad \bar{m} = \tfrac{1}{2}(s_1 + s_0 + 1). \tag{A5}$$

Equations (A5) show that the weight $\bar{m}$ exceeds the minimal weight $\bar{j}$ by an integer value. For a given $\bar{j}$-value, the tensor product states $|n_1n_0s_1s_0\rangle$ carry a unitary irreducible representation of Sp(2, R). Since this group is non-compact, its unitary irreducible representations are infinite dimensional. Like in (A3), the transformed states $|n_1n_0sS\rangle$ with the same $\bar{j}$-value are related to the independent-particle states by

$$|n_1n_0sS\rangle = \sum_{\substack{s_0s_1 \\ (|s_0-s_1|=|s-S|)}} \bar{d}^{(|s-S|+1)/2}_{(s_0+s_1+1)/2,(s+S+1)/2}(-2\tanh^{-1}\varepsilon)|n_1n_0s_1s_0\rangle \tag{A6}$$

where $\bar{d}^j_{m'm}$ is a d-function of the *unitary* irreducible representations of Sp(2, R). Explicit formulae for the representations of the locally isomorphic group SU(1, 1) can be found in (Ui 1970)†. Notice that (3.8), (4.4), (4.6), (4.7) and (A6) provide an alternative method of calculation of the $\bar{d}$-functions. For example, (4.7) and (3.8) immediately lead to

$$\bar{d}^{1/2}_{n+1/2,1/2}(\beta) = (\cosh\tfrac{1}{2}\beta)^{-1}(-\tanh\tfrac{1}{2}\beta)^n. \tag{A7}$$

With (A7), (A6) can be summed and provides a coordinate representation of $|\bar{0}\rangle$ in closed form. Then closed expressions can be derived for all other states. With (A3) and (A6), the wavefunctions can also be represented by series of products of Landau wavefunctions.

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† A factor $(-)^{m'-m}$ is missing in the expression (3.15) of $\bar{d}^j_{m',m}$ in Ui (1970).

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