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The classical centre-of-mass separation for two particles in a homogeneous magnetic field

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Abstract. We investigate classically the problem of the centre-of-mass separation for a two-body system with net charge in a homogeneous magnetic field. With a view to general atomic physics applications, particular attention is paid to the case where one particle is much heavier than the other. Using a series of canonical transformations we introduce constants of the motion as the new momenta and determine the conjugate coordinates. Alternative momenta involving a suggested near-constant of the motion are investigated for use with a translation-invariant internal potential. These lead to a 'near separation' in terms of two coupled particles characterised by vectors which possess a simple classical interpretation, even in the presence of an interaction potential. However we find that the coupling is not small and is not reduced when one of the particles is much heavier than the other, although the frequencies of the two motions then differ widely.

1. Introduction

The problem of the motion of systems of charged particles in a homogeneous magnetic field has long been of interest, particularly with regard to its quantum mechanical implications (see Johnson *et al* (1983) for a general comprehensive review and Baye (1982, 1983) and the references therein for a detailed study of the two-body case).

Here we investigate the centre-of-mass (CM) separation for a two-body system with non-zero net charge and arbitrary masses. In particular we concentrate on the case typical in atomic physics where one of the particles is very much heavier than the other. We follow the quantal analysis of Baye (1983), in which he proposes for a strong magnetic field a separation in terms of two weakly coupled pseudoparticles. This is achieved through the introduction of a suggested near-constant, C closely related to the total kinetic momentum of the system, and characteristic of one of the pseudoparticles.

It is hoped that a classical approach may provide a view of the problem complementary to the formal quantal picture in terms of creation and annihilation operators (Baye 1983), thus giving additional insight into the behaviour of C. Further, while a quantal solution is required for the low-lying atomic states, a classical approach may be useful for Rydberg states where the strong-field regime can be achieved with laboratory fields.

We seek to describe the problem making maximum use of constants of the motion as canonical momenta since this makes Hamilton's equations relatively simple and facilitates comparison with the quantum results.

Although generally the vector potential $\boldsymbol{A}$ couples relative and CM variables in the Hamiltonian, the CM motion is still separable for the neutral two-body system, such as atomic hydrogen (see Johnson *et al* 1983). Strictly this is termed a 'pseudoseparation' since the resulting one-body problem takes, as a parameter, the magnitude of the constant total pseudomomentum (Johnson *et al* 1983). However for a system with non-zero total charge Q such a separation can be made only for motion parallel to the magnetic field.

Transverse to the field the usual notion of CM separation is seen to require some modification, the constant pseudomomentum above now supplying one less canonical momentum than in the neutral system. Baye (1983) suggests that this reduction from a separable problem can be countered by utilising $\boldsymbol{C}$, which for non-zero values of Q is completely independent of the constant pseudomomentum. It is expected that $\boldsymbol{C}$ will furnish an additional near-constant transverse canonical momentum to permit an analogue of CM separation for the $Q \neq 0$ problem, whereby the internal motion is affected by weak coupling to the CM motion. Then we have replaced the two-body two-dimensional problem by two weakly coupled one-body problems.

Section 2.1 summarises the Hamiltonian description of the motion of a single charged particle in a homogeneous magnetic field and introduces the relevant constants of the motion for future reference. In § 2.2 we extend this treatment to the two-body, $Q \neq 0$ system with a view to accommodating the effect of a typical interaction potential. Canonical sets for use with such a potential are derived in § 3, notably one yielding an approximate CM-like separation for the transverse motion. We also consider the inclusion of the potential, which takes a relatively compact form in the latter representation. Section 4 outlines an alternative approach to the general $Q \neq 0$ problem, useful for relatively weak magnetic fields. Concluding remarks are presented in § 5.

2. Motion of charged particles in a homogeneous magnetic field

2.1. One-body problem

Consider a particle of mass m, charge e, position vector $\boldsymbol{r}$ and conjugate momentum $\boldsymbol{p}$. Then the non-relativistic Hamiltonian in the presence of a vector potential $\boldsymbol{A}(\boldsymbol{r})$ is

$$H = (\boldsymbol{p} - e\boldsymbol{A})^2/2m = \boldsymbol{\pi}^2/2m$$

with $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}$ the kinetic momentum. With the static symmetric gauge $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r}$, used throughout this paper, the transverse kinetic momentum $\boldsymbol{\pi}_\perp$ now reads

$$\boldsymbol{\pi}_\perp = \boldsymbol{p}_\perp - (e/2)\boldsymbol{B} \times \boldsymbol{r}_\perp \tag{1}$$

where $\boldsymbol{r}_\perp$ is the component of $\boldsymbol{r}$ perpendicular to the field $\boldsymbol{B}$. The motion parallel and perpendicular to the field uncouples

$$H = H_\parallel + H_\perp = p_z^2/2m + \pi_\perp^2/2m \tag{2}$$

with $\boldsymbol{B} = B\hat{\boldsymbol{z}}$, where the parallel motion corresponds to that of a free particle. For the transverse motion, Hamilton's equations have the general solution

$$\boldsymbol{p}_\perp = -(e/2)\boldsymbol{B} \times \boldsymbol{r}_\perp + \boldsymbol{k}_\perp \tag{3}$$

where $\boldsymbol{k}_\perp$ is a constant (momentum-like) vector in the xy plane. The constant can equally be written in the convenient forms

$$\boldsymbol{k}_\perp = e\boldsymbol{B}\times\boldsymbol{r}_c = \boldsymbol{\pi}_\perp + e\boldsymbol{B}\times\boldsymbol{r}_\perp \tag{4}$$

such that $\boldsymbol{r}_c$ is a constant (displacement-like) vector, also in the xy plane. Using equations (1) and (3) we then obtain

$$\dot{\boldsymbol{r}}_\perp = \boldsymbol{\pi}_\perp/m = (e/m)[(\boldsymbol{r}_\perp - \boldsymbol{r}_c)\times\boldsymbol{B}] \tag{5}$$

and so the transverse motion is identified as precession of angular frequency eB/m about a fixed centre $\boldsymbol{r}_c$ termed the 'guiding centre' (Landau and Lifshitz 1975, § 21) of the classical Landau orbit of radius $|\boldsymbol{r}_\perp - \boldsymbol{r}_c|$. Combining this with the uniform motion in the z direction produces a helical trajectory about an axis parallel to $\boldsymbol{B}$ passing through $\boldsymbol{r}_c$.

From equation (3) we define $\boldsymbol{k} = \boldsymbol{p} + (e/2)\boldsymbol{B}\times\boldsymbol{r}$ to be the (constant) pseudomomentum of the charged particle in a constant $\boldsymbol{B}$ field. (Note that parallel to the field $k_z = p_z$.) The other constants of the motion are $\pi_\perp^2$ and l_z, the z component of angular momentum. However not all these constants are independent since from equations (1) and (3) we obtain

$$2eBl_z = k_\perp^2 - \pi_\perp^2. \tag{6}$$

Further, on inspecting the Poisson bracket (PB) algebra of k_x and k_y, the constant $\boldsymbol{k}_\perp$ provides only one canonical momentum, which we shall take to be $k_\perp^2 = k_x^2 + k_y^2$. The possible canonical momenta are then $(l_z, k_\perp^2, \pi_\perp^2, p_z)$ and, by virtue of equation (6) above, one of $(l_z, k_\perp^2, \pi_\perp^2)$ must be discarded to form a canonical set. (This freedom to choose alternative canonical momenta will be exploited again below in the two-body case.)

Choosing the constants $(k_\perp^2, \pi_\perp^2, p_z)$ as momenta we have the following canonical set $(\boldsymbol{q}, \boldsymbol{p})$ where

$$\begin{aligned} q_1 &= \tan^{-1}(k_y/k_x) & p_1 &= k_\perp^2/2eB \\ q_2 &= \tan^{-1}(\pi_y/\pi_x) & p_2 &= -\pi_\perp^2/2eB \\ q_3 &= z & p_3 &= p_z. \end{aligned} \tag{7}$$

While one can employ $k_\perp$ and $\pi_\perp$ and conjugate distances, the use here of angle-action coordinates (Goldstein 1980) for the transverse variables facilitates comparison with the quantal approach of Baye (1983).

Alternatively we may choose the constants $(k_\perp^2, l_z, p_z)$ and, using a simple point transformation suggested by equation (6), obtain the corresponding canonical set $(\boldsymbol{q}', \boldsymbol{p}')$

$$\begin{aligned} q_1' &= \tan^{-1}(k_y/k_x) - \tan^{-1}(\pi_y/\pi_x) & p_1' &= k_\perp^2/2eB \\ q_2' &= \tan^{-1}(\pi_y/\pi_x) & p_2' &= l_z \\ q_3' &= z & p_3' &= p_z. \end{aligned} \tag{8}$$

The Hamiltonian may now be written in these two representations as

$$H = p_3^2/2m - (eB/m)p_2 = p_3'^2/2m + (eB/m)(p_1' - p_2').$$

We see that H is independent of p_1 and that the vector $\boldsymbol{\pi}_\perp$ precesses with uniform angular frequency of magnitude eB/m. We note from the primed representation, equation (8), that q_2' acts as a reference angle to which the relative angle q_1' is referred. It is this representation, in particular, which goes over most readily to the final two-body description of § 3.

2.2. *Two-body problem with non-zero net charge*

Consider two particles with charges, masses and position vectors e_0, m_0, $\boldsymbol{r}_0$ and e_1, m_1, $\boldsymbol{r}_1$ respectively and non-zero total charge $Q = e_0 + e_1$. The Hamiltonian may be decomposed as in § 2.1 into

$$H = H_\parallel + H_\perp + V(\boldsymbol{r}_0, \boldsymbol{r}_1) \tag{9}$$

with interaction-free components:

$$H_\parallel = p_{0z}^2/2m_0 + p_{1z}^2/2m_1 \qquad H_\perp = \pi_{0\perp}^2/2m_0 + \pi_{1\perp}^2/2m_1 \tag{10}$$

and an interaction potential V.

For strong magnetic fields the separate treatment of the parallel and transverse motions becomes advantageous. By strong fields here we imply for electrons fields $B \gg B_0$ where $B_0 = \alpha^2 m^2 c^2/e\hbar = 2.35 \times 10^5$T is the conventional atomic unit of field strength.

We concentrate then on the transverse motion since the parallel motion is no different from the well understood field-free case. Neglecting, initially, the interaction V the canonical set given in equations (7) may be adopted for each particle independently:

$$\begin{aligned}
q_1 &= \tan^{-1}(k_{0y}/k_{0x}) & p_1 &= k_{0\perp}^2/2e_0B \\
q_2 &= \tan^{-1}(k_{1y}/k_{1x}) & p_2 &= k_{1\perp}^2/2e_1B \\
q_3 &= \tan^{-1}(\pi_{0y}/\pi_{0x}) & p_3 &= -\pi_{0\perp}^2/2e_0B \\
q_4 &= \tan^{-1}(\pi_{1y}/\pi_{1x}) & p_4 &= -\pi_{1\perp}^2/2e_1B
\end{aligned} \tag{11}$$

with constants analogous to the one-body problem (§ 2.1) for each particle (i.e. all quantities except q_3 and q_4 are constant).

More realistically, in the presence of a potential $V(\boldsymbol{r}_0, \boldsymbol{r}_1)$, none of the individual momenta are constant since the relative transverse coordinates $\boldsymbol{r}_{0\perp}$, $\boldsymbol{r}_{1\perp}$ depend on all the q and p:

$$\boldsymbol{r}_{0\perp} = (\boldsymbol{k}_{0\perp} - \boldsymbol{\pi}_{0\perp}) \times \boldsymbol{B}/e_0B^2 \tag{12}$$

using equation (4), and similarly for $\boldsymbol{r}_{1\perp}$.

However for particular potentials some constants are retained. Specifically for a translation-invariant potential $V = V(\boldsymbol{r})$, $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_0$, the total (transverse) pseudomomentum $\boldsymbol{K}_\perp$ is conserved (see Johnson *et al* 1983), where

$$\boldsymbol{K}_\perp = \boldsymbol{k}_{0\perp} + \boldsymbol{k}_{1\perp}. \tag{13}$$

If we now define $\boldsymbol{R}_c$ by $\boldsymbol{K}_\perp = Q\boldsymbol{B} \times \boldsymbol{R}_c$, as in equation (4), one may view this as the charge centroid of the guiding centres

$$\boldsymbol{R}_c = (e_0\boldsymbol{r}_{0c} + e_1\boldsymbol{r}_{1c})/Q \tag{14}$$

which remains fixed, in contrast to the now-drifting individual guiding centres ($\boldsymbol{r}_{0c}$, $\boldsymbol{r}_{1c}$).

As in § 2.1, because $[K_x, K_y] \neq 0$, the constant transverse pseudomomentum $\boldsymbol{K}_\perp$ contributes only one useful canonical momentum, unlike the special case of zero net charge where it yields two (Avron *et al* 1978, Herold *et al* 1981).

Further, if V is invariant under rotations about the field direction, then the z component of the total angular momentum L_z is also conserved, and by equations (6) and (11)

$$L_z = l_{0z} + l_{1z} = \sum_{i=1}^{4} p_i. \tag{15}$$

It is straightforward to verify that the PB of the set ($K_\perp^2$, L_z, $\pi_{0\perp}^2$ and $\pi_{1\perp}^2$) all vanish. In the next section we derive a full set of generalised coordinates including these momenta and discuss the problems in separating the transverse CM motion.

3. Use of constants of the motion as canonical momenta

3.1. Use of the constants $K_\perp^2$, L_z

The theory of canonical transformations (e.g. Goldstein 1980) provides a method whereby the canonical set including certain specified momenta may be obtained from an existing set. The constants $K_\perp^2$, L_z can be written in terms of the single-particle set of § 2.1 and so may be systematically introduced by canonical transformations. However since the PB of $K_\perp^2$ and either $k_{0\perp}^2$ or $k_{1\perp}^2$ is non-vanishing we require to introduce L_z first.

Using (14) we can perform a simple point momentum transformation replacing (arbitrarily) p_1 by $p_1' = L_z$ to yield the set

$$q_1' = q_1 \qquad q_i' = q_i - q_1 \qquad p_i' = p_i \qquad i = 2, 3, 4. \tag{16}$$

The constant $K_\perp^2$ now satisfies

$$K_\perp^2 = k_{0\perp}^2 + k_{1\perp}^2 + 2k_{0\perp}k_{1\perp}\cos q_2' \tag{17}$$

with $k_{0\perp}^2$ implicitly defined through equation (15). A further transformation $(\boldsymbol{q}', \boldsymbol{p}') \to (\boldsymbol{Q}, \boldsymbol{P})$ replaces $p_2' (= k_{1\perp}^2/2e_1B)$ by $P_2 (= K_\perp^2/2QB)$ using an $F_4(\boldsymbol{p}', \boldsymbol{P})$-type generating function (Goldstein 1980) given by

$$F_4 = -\int q_2' \, \mathrm{d}p_2'$$

with $q_2' = q_2'(p_2', P_2; P_1, P_3, P_4)$ implicitly defined through equations (15) and (17).

To preserve the other momenta we adjoint the relevant identity generator F_2 and form the composite generating function (see Goldstein 1980, p 385):

$$F = F_4 + F_2 = -\int q_2' \, \mathrm{d}p_2' + (q_1'P_1 + q_3'P_3 + q_4'P_4). \tag{18}$$

After some analysis, the details of which are outlined in the appendix, the following canonical set $(\boldsymbol{Q}, \boldsymbol{P})$ is found

$$\begin{aligned}
Q_1 &= \tan^{-1}(k_y/k_x) & P_1 &= L_z \\
Q_2 &= \tan^{-1}(K_y/K_x) - \tan^{-1}(k_y/k_x) & P_2 &= K_\perp^2/2QB \\
Q_3 &= \tan^{-1}(\pi_{0y}/\pi_{0x}) - \tan^{-1}(k_y/k_x) & P_3 &= -\pi_{0\perp}^2/2e_0B \\
Q_4 &= \tan^{-1}(\pi_{1y}/\pi_{1x}) - \tan^{-1}(k_y/k_x) & P_4 &= -\pi_{1\perp}^2/2e_1B.
\end{aligned} \tag{19}$$

Here we have defined the charge-weighted relative pseudomomentum,

$$\boldsymbol{k}_\perp = (e_0\boldsymbol{k}_{1\perp} - e_1\boldsymbol{k}_{0\perp})/Q \tag{20}$$

interpreted through equation (4) as relating to the separation of the guiding centres of the particles (see figure 1):

$$\boldsymbol{k}_\perp = (e_0 e_1/Q)\boldsymbol{B}\times(\boldsymbol{r}_{1c}-\boldsymbol{r}_{0c}). \tag{21}$$

In contrast to $\boldsymbol{K}_\perp$, the relative pseudomomentum $\boldsymbol{k}_\perp$ is constant only in the absence of an interaction potential.

From the definitions of $\boldsymbol{K}_\perp$ and $\boldsymbol{k}_\perp$, equations (13) and (20) respectively, we obtain analogously to equation (6)

$$L_z = K_\perp^2/2QB + k_\perp^2/2eB - \pi_{0\perp}^2/2e_0B - \pi_{1\perp}^2/2e_1B \qquad 1/e = 1/e_0 + 1/e_1 \tag{22}$$

relating the magnitude of $k_\perp^2$ to the canonical momenta of equations (19).

Since we chose to preserve $(\pi_{0\perp}^2, \pi_{1\perp}^2)$ as canonical momenta the Hamiltonian is simply $H_\perp = H_\perp(P_3, P_4)$ in the set $(\boldsymbol{Q}, \boldsymbol{P})$ given in equations (19). Then Q_1 and Q_2 are constants while

$$Q_3(t) = -\omega_0 t + Q_3^0 \qquad Q_4(t) = -\omega_1 t + Q_4^0 \qquad \omega_i = e_i B/m_i \qquad i = 0, 1 \tag{23}$$

where Q_3^0 and Q_4^0 are constants. This set is equivalent to what Baye terms his 'intermediate' basis.

Under the influence of an internal potential $V(r)$, however, the number of constants is greatly reduced, the relative coordinate $\boldsymbol{r}_\perp = \boldsymbol{r}_{1\perp} - \boldsymbol{r}_{0\perp}$ appearing as

$$\boldsymbol{r}_\perp = (\boldsymbol{k}_\perp/e - \boldsymbol{\pi}_{1\perp}/e_1 + \boldsymbol{\pi}_{0\perp}/e_0)\times\boldsymbol{B}/B^2 \tag{24}$$

and so V depends on $(Q_3, Q_4; P_1, P_2, P_3, P_4)$.

Thus, for the Hamiltonian $\mathscr{H} = H_\perp + V$, only the momenta $P_1 = L_z$ and $P_2 = K_\perp^2/2QB$ are constant, and these are insufficient to permit a separation of relative motion and CM motion.

3.2. *Properties of Baye's momentum* $\boldsymbol{C}_\perp$

Baye (1982, 1983) has suggested that the vector

$$\boldsymbol{C}_\perp = (1 + e_1/e_0)\boldsymbol{\pi}_{0\perp} - (e_1/e_0)\boldsymbol{k}_{0\perp} + \boldsymbol{k}_{1\perp} \tag{25a}$$

$$= \boldsymbol{K}_\perp - Q\boldsymbol{B}\times\boldsymbol{r}_{0\perp} = Q\boldsymbol{B}\times(\boldsymbol{R}_c - \boldsymbol{r}_{0\perp}) \tag{25b}$$

will be a near-constant of the motion when $m_0 \gg m_1$ and $e_0 > -e_1 > 0$. Clearly for the neutral problem, $\boldsymbol{C}_\perp$ reduces to $\boldsymbol{K}_\perp$. ($\boldsymbol{R}_c$ is given in equation (14).)

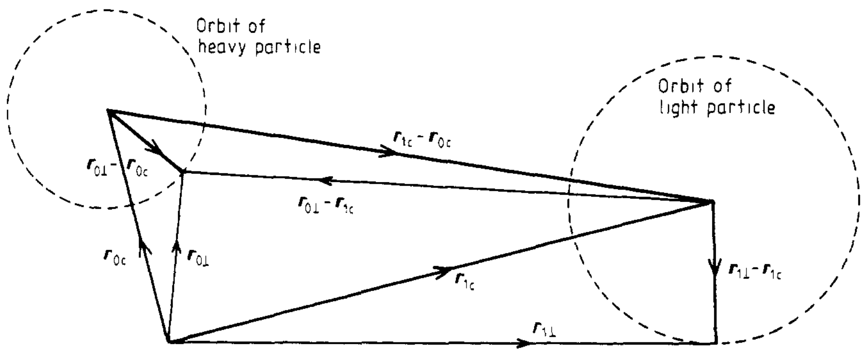

Figure 1. The broken circles represent the orbits of the particles in the absence of an interaction. The position vectors related to the momenta $\boldsymbol{k}_\perp$, $\tilde{\boldsymbol{k}}_\perp$, $\boldsymbol{\pi}_{0\perp}$ and $\boldsymbol{\pi}_{1\perp}$ (see text) are also shown.

From equations (20) and (25a) we have $\boldsymbol{C}_\perp = (Q/e_0)(\boldsymbol{k}_\perp + \boldsymbol{\pi}_{0\perp})$ or, explicitly, in terms of the set $(\boldsymbol{Q}, \boldsymbol{P})$

$$C_\perp^2 = (Q^2/e_0^2)(k_\perp^2 + \pi_{0\perp}^2 + 2k_\perp \pi_{0\perp} \cos Q_3) \tag{26}$$

i.e. $\boldsymbol{C}_\perp$ is the sum of a constant vector and a uniformly precessing vector. We see from equation (23) that $\boldsymbol{C}_\perp$ will be approximately constant only when $k_\perp \gg \pi_{0\perp}$ (see figure 2). The fact that $m_0 \gg m_1$ does not in fact affect whether $\boldsymbol{C}_\perp$ is constant or not but does ensure that $\boldsymbol{C}_\perp$ will change slowly compared to $\boldsymbol{\pi}_{1\perp}$, since Q_3 will then change slowly, see equation (23).

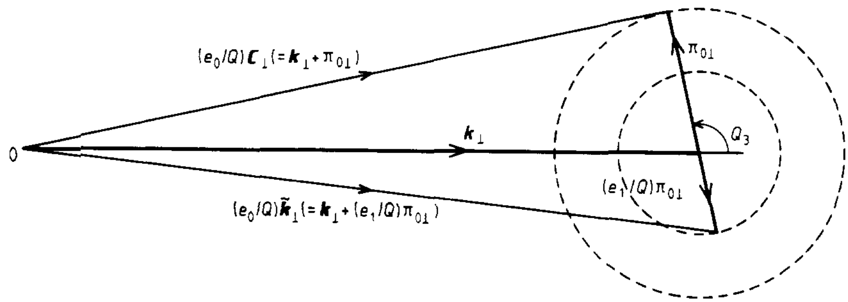

Figure 2. The variation of the momenta $\boldsymbol{C}_\perp$ and $\tilde{\boldsymbol{k}}_\perp$ is shown for the case $e_0 > -e_1 > 0$, assuming $|\boldsymbol{k}_\perp| > |\boldsymbol{\pi}_{0\perp}|$. Here 0 is a fixed point and the broken circles represent the loci of the (varying) ends of the vectors $(e_0/Q)\boldsymbol{C}_\perp$ and $(e_0/Q)\tilde{\boldsymbol{k}}_\perp$.

In terms of guiding centres, $\boldsymbol{C}_\perp$ will be a near-constant if the separation of the guiding centres (varying as $k_\perp$ from equation (21)) is very much larger than the radius of the heavy particle orbit (varying as $\pi_{0\perp}$ from equation (5)). Figure 1 illustrates the situation, but is to be strictly understood only in the limit of the interaction potential becoming negligible.

It is easily seen that $[\boldsymbol{r}_\perp, \boldsymbol{C}_\perp] = 0$, and so $\boldsymbol{C}_\perp$ is not affected directly by the presence of an interaction potential $V(r_\perp)$. Writing $\boldsymbol{\Pi}_\perp = \boldsymbol{\pi}_{0\perp} + \boldsymbol{\pi}_{1\perp}$, then $\boldsymbol{C}_\perp = \boldsymbol{\Pi}_\perp + e_1 \boldsymbol{B} \times (\boldsymbol{r}_{1\perp} - \boldsymbol{r}_{0\perp})$. In this way $\boldsymbol{C}_\perp$ corresponds closely to the CM kinetic momentum $\boldsymbol{\Pi}_\perp$. Also since $[C_x, C_y] \neq 0$, $\boldsymbol{C}_\perp$ (like $\boldsymbol{K}_\perp$) provides only one useful canonical momentum, which we take to be $C_\perp^2$.

The less restrictive condition for $C_\perp^2$ to be a near-constant is that $k_\perp \gg \pi_{0\perp}$, or vice versa. Neither criterion is directly influenced by the mass ratio but they do depend on the charge ratio $|e_1|/e_0$ (see equations (5) and (21)).

For $C_\perp^2$ to be a near-constant in the quantal picture requires that its off-diagonal matrix elements be small compared to its diagonal spacing with respect to basis states in which $H_\perp$ itself is diagonal, e.g. the 'intermediate' set of Baye (1983).

For a time-independent Hamiltonian such as that under discussion we have the standard result for the off-diagonal elements of some operator $\hat{O}$,

$$\langle \mathrm{f}|\hat{O}|\mathrm{i}\rangle = \langle \mathrm{f}|[\hat{H}, \hat{O}]|\mathrm{i}\rangle/(E_\mathrm{f} - E_\mathrm{i})$$

where $|\mathrm{i}\rangle$, $|\mathrm{f}\rangle$ are the (assumed non-degenerate) wavefunctions with respective energy eigenvalues E_i, E_f of a Hamiltonian $\hat{H}$.

In the intermediate basis of Baye (1983), analogous to our set $(\boldsymbol{Q}, \boldsymbol{P})$, it is seen that the only non-vanishing off-diagonal elements arise from adjacent states labelled by the quantum numbers n_0, s. (We follow the quantal notation of Baye (1983) except that ω_0 denotes the cyclotron frequency, see equation (23), and not the Larmor frequency as in Baye.) Then the appropriate energy difference is $\Delta E(=E_f - E_i) = \hbar\omega_0$.

Further, the corresponding off-diagonal elements of the commutator $[H_\perp, C_\perp^2]$ are

$$\langle n_0+1, s-1|[H_\perp, C_\perp^2]|n_0 s\rangle = 2\hbar\omega_0\varepsilon(1-\varepsilon^2)^{1/2}\hbar QB[s(n_0+1)]^{1/2}$$

and $\varepsilon = (|e_1|/e_0)^{1/2}$. Thus the off-diagonal elements of $C_\perp^2$ are

$$\langle n_0+1, s-1|C_\perp^2|n_0 s\rangle = 2\varepsilon(1-\varepsilon^2)^{1/2}\hbar QB[s(n_0+1)]^{1/2}$$

independent of m_1/m_0.

Hence the existence of a small commutator $[H_\perp, C_\perp^2]$, because m_0 is large, does not guarantee that the off-diagonal elements of $C_\perp^2$ are themselves small.

Finally the diagonal spacing of $C_\perp^2$ may be defined as

$$\Delta C^2_{\perp(n_0 s)} = \langle n_0 s|C_\perp^2|n_0 s\rangle - \langle n_0' s'|C_\perp^2|n_0' s'\rangle$$

where $n_0' = n_0+1$, $s' = s-1$. Then the ratio describing the variation of $C_\perp^2$ is typically

$$\frac{\langle n_0+1, s-1|C_\perp^2|n_0 s\rangle}{|\Delta C^2_{\perp(n_0 s)}|} = \varepsilon(1-\varepsilon^2)^{1/2}[s(n_0+1)]^{1/2}.$$

Thus the ratio is not directly affected by the mass condition $m_0 \gg m_1$ and is in general never small. However in the special case of highly charged hydrogen-like systems with $e_0 \gg |e_1|$ (such that we have a weak magnetic field relative to the Coulomb interaction) this ratio can be small. Note that $\varepsilon = 1$ corresponds to the well understood $Q = 0$ problem.

3.3. *Canonical momenta including* $C_\perp^2$

Because of the vanishing PB of $\boldsymbol{C}_\perp$ and $\boldsymbol{r}_\perp$ and the slow variation of $\boldsymbol{C}_\perp$ compared to $\boldsymbol{\pi}_{1\perp}$ it is useful to introduce $C_\perp^2$ as a momentum. The derivation of the corresponding canonical set follows that in § 3.1. Replacing $P_3 = -\pi_{0\perp}^2/2e_0B$ by $P_3' = -C_\perp^2/2QB$ yields (see appendix)

$$\begin{aligned}
Q_1' &= \tan^{-1}(\tilde{k}_y/\tilde{k}_x) & P_1' &= L_z \\
Q_2' &= \tan^{-1}(K_y/K_x) - \tan^{-1}(\tilde{k}_y/\tilde{k}_x) & P_2' &= K_\perp^2/2QB \\
Q_3' &= \tan^{-1}(C_y/C_x) - \tan^{-1}(\tilde{k}_y/\tilde{k}_x) & P_3' &= -C_\perp^2/2QB \\
Q_4' &= \tan^{-1}(\pi_{1y}/\pi_{1x}) - \tan^{-1}(\tilde{k}_y/\tilde{k}_x) & P_4' &= -\pi_{1\perp}^2/2e_1B
\end{aligned} \tag{27}$$

with the momentum $\tilde{\boldsymbol{k}}_\perp$ defined as

$$\tilde{\boldsymbol{k}}_\perp = (Q/e_0)\boldsymbol{k}_\perp + (e_1/e_0)\boldsymbol{\pi}_{0\perp} = \boldsymbol{k}_{1\perp} - (e_1/e_0)(\boldsymbol{k}_{0\perp} - \boldsymbol{\pi}_{0\perp}) = \boldsymbol{C}_\perp - \boldsymbol{\pi}_{0\perp} \tag{28}$$

$$= e_1\boldsymbol{B}\times(\boldsymbol{r}_{1c} - \boldsymbol{r}_{0\perp}) \tag{29}$$

interpreted (see figure 1) as relating to the position vector of the heavy particle referred to the guiding centre of the light particle.

From the definitions of $\boldsymbol{C}_\perp$ and $\tilde{\boldsymbol{k}}_\perp$ we have, in place of equation (22),

$$L_z = K_\perp^2/2QB - C_\perp^2/2QB + \tilde{k}_\perp^2/2e_1B - \pi_{1\perp}^2/2e_1B. \tag{30}$$

The transverse Hamiltonian is $H_\perp = H_c + H'$ where

$$H_c = \pi_{1\perp}^2/2m_1 + C_\perp^2/2m_0 \qquad H' = (1/2m_0)(\tilde{k}_\perp^2 - 2\tilde{k}_\perp C_\perp \cos Q_3') \tag{31}$$

with $\tilde{k}_\perp$ defined in terms of the other momenta through equation (30) and where the Q_3' dependence indicates that $C_\perp^2$ is not constant.

Replacing L_z by $\tilde{k}_\perp^2/2e_1B$ using equation (30) yields the alternative description

$$\begin{aligned} Q_1'' &= \tan^{-1}(\tilde{k}_y/\tilde{k}_x) & P_1'' &= \tilde{k}_\perp^2/2e_1B \\ Q_2'' &= \tan^{-1}(K_y/K_x) & P_2'' &= K_\perp^2/2QB \\ Q_3'' &= \tan^{-1}(C_y/C_x) & P_3'' &= -C_\perp^2/2QB \\ Q_4'' &= \tan^{-1}(\pi_{1y}/\pi_{1x}) & P_4'' &= -\pi_{1\perp}^2/2e_1B \end{aligned} \tag{32}$$

which is to be compared with the independent-particle set of equation (11). This set is equivalent to the final set introduced by Baye (1983).

The equations (30)–(32) now offer an interpretation (Baye 1983) in terms of two pseudoparticles with the following properties:

	(i)	(ii)	
mass	m_1	m_0	
charge	e_1	Q	(33)
pseudomomentum	$\tilde{\boldsymbol{k}}_\perp$	$\boldsymbol{K}_\perp$	
kinetic momentum	$\boldsymbol{\pi}_{1\perp}$	$\boldsymbol{C}_\perp$.	

Noting that in the set $(\boldsymbol{Q}'', \boldsymbol{P}'')$ the angle dependence of the Hamiltonian arises through the second term of

$$H' = (1/2m_0)[\tilde{k}_\perp^2 - 2\tilde{k}_\perp C_\perp \cos(Q_3'' - Q_1'')] \tag{34}$$

then all the momenta are constants in the 'unperturbed' Hamiltonian H_c. The effect of the 'perturbation' H' is both to cause $C_\perp^2$ and $\tilde{k}_\perp^2$ to vary and to couple the pseudoparticles, see equation (32).

For the coupling of the whole system to be small it is necessary that H' be much smaller than each of the remaining terms in the Hamiltonian. While H' varies as m_0^{-1} so does $C_\perp^2/2m_0$ and hence the condition is not directly influenced by the mass ratio. However H' can be much smaller when $|e_1| \ll e_0$, see equations (25*b*) and (29).

We note that the heavy pseudoparticle is characterised by an exact constant of the motion $K_\perp^2$ and a 'slowly varying' quantity $C_\perp^2$ and in this sense we have a CM-like separation of the heavy motion from the relatively fast motion of the light particle. We see below that this separation is not significantly altered by the presence of an interaction potential $V(r)$.

Finally we may also relate the time variation of the light particle pseudomomentum $\tilde{\boldsymbol{k}}_\perp$ to that of $\boldsymbol{\pi}_{0\perp}$, as for $\boldsymbol{C}_\perp$. Using the definition, equation (28), and referring to figure 2 the motion of the light pseudoparticle has a similar interpretation in terms of a constant and a slowly varying vector, $\tilde{\boldsymbol{k}}_\perp$ and $\boldsymbol{\pi}_{1\perp}$, respectively. However $\tilde{\boldsymbol{k}}_\perp$ and $\boldsymbol{\pi}_{1\perp}$ are directly affected when a potential $V(r)$ is introduced as we see below.

3.4. *The effect of the interaction potential*

We consider the effect of a spherically symmetric translation-invariant potential $V(r)$. Strictly we need only a cylindrically symmetric potential but this is unlikely to be encountered in practice. From equations (24) and (28) we have

$$\boldsymbol{r}_\perp = (1/e_1B^2)[(\tilde{\boldsymbol{k}}_\perp - \boldsymbol{\pi}_{1\perp}) \times \boldsymbol{B}] \tag{35}$$

so that V depends on $r_\perp$ where

$$e_1^2B^2r_\perp^2 = \pi_{1\perp}^2 + \tilde{k}_\perp^2 - 2\pi_{1\perp}\tilde{k}_\perp \cos(Q_4'' - Q_1''). \tag{36}$$

We see that the potential takes a very much simpler form in the set $(\boldsymbol{Q}'', \boldsymbol{P}'')$ of equations (32), compared to the previous two-body sets (see equations (12) and (24)), and is completely determined by the canonical quantities appropriate to the light pseudoparticle only. Thus the CM-like separation of the heavy pseudoparticle is not directly affected.

4. Alternative approach to the $Q \neq 0$ problem

For completeness we note the complementary treatment (Power and Zienau 1959, Woolley 1971) of the coupling in the $Q \neq 0$ problem appropriate for weaker magnetic fields, $B \ll B_0$, and for arbitrary masses. The Power-Zienau-Woolley (PZW) transformation (see Johnson *et al* 1983) seeks to minimise the coupling between the CM and internal variables. The classical analogue of the PZW transformation is a point transformation $(\boldsymbol{r}_0, \boldsymbol{r}_1; \boldsymbol{p}_0, \boldsymbol{p}_1) \to (\boldsymbol{R}, \boldsymbol{r}; \boldsymbol{P}_\mathrm{M}, \boldsymbol{p}_\mathrm{M})$ which uses the gauge freedom to specify new CM and internal momenta $\boldsymbol{P}_\mathrm{M}$ and $\boldsymbol{p}_\mathrm{M}$ respectively, while retaining the standard CM and relative coordinates, $\boldsymbol{R}\ [=(m_0\boldsymbol{r}_0+m_1\boldsymbol{r}_1)/M]$ and $\boldsymbol{r}\ (=\boldsymbol{r}_1-\boldsymbol{r}_0)$ respectively.

The required F_2 generating function is

$$F_2(\boldsymbol{r}_0, \boldsymbol{r}; \boldsymbol{P}_\mathrm{M}, \boldsymbol{p}_\mathrm{M}) = \boldsymbol{P}_\mathrm{M} \cdot \boldsymbol{R}(\boldsymbol{r}_0, \boldsymbol{r}_1) + \boldsymbol{p}_\mathrm{M} \cdot \boldsymbol{r}(\boldsymbol{r}_0, \boldsymbol{r}_1) + g(\boldsymbol{r}_0, \boldsymbol{r}_1) \tag{37}$$

where to obtain the PZW transformation we employ

$$g = (e_1 m_0 - e_0 m_1)\boldsymbol{r} \cdot \boldsymbol{B} \times \boldsymbol{R}/2M. \tag{38}$$

The Hamiltonian is then

$$H = \Pi_\mathrm{M}^2/2M + \pi_\mathrm{M}^2/2m + V \qquad M = m_0 + m_1 \qquad m = m_0 m_1/M \tag{39}$$

where the kinetic momenta are

$$\boldsymbol{\Pi}_\mathrm{M} = \boldsymbol{P}_\mathrm{M} - \tfrac{1}{2}Q\boldsymbol{B} \times \boldsymbol{R} - (e_1 m_0 - e_0 m_1)\boldsymbol{B} \times \boldsymbol{r}/M \tag{40a}$$

$$\boldsymbol{\pi}_\mathrm{M} = \boldsymbol{p}_\mathrm{M} - (e_1 m_0^2 + e_0 m_1^2)\boldsymbol{B} \times \boldsymbol{r}/2M^2. \tag{40b}$$

Here the only coupling between the CM and internal coordinates arises in the CM kinetic energy term, see equation (40a).

Referring the dipole moment of the two particles to the CM we note that this residual coupling may be regarded as a dipole contribution

$$\boldsymbol{\mu} = e_0(\boldsymbol{r}_0 - \boldsymbol{R}) + e_1(\boldsymbol{r}_1 - \boldsymbol{R}) = (e_1 m_0 - e_0 m_1)\boldsymbol{r}/M. \tag{41}$$

In contrast, the standard separation applied in field-free problems (corresponding to $g = 0$ in equation (37)) has additional coupling in the internal kinetic energy term.

5. Conclusions

For two particles (with arbitrary charges and masses) in the presence of a homogeneous magnetic field the standard (field-free) separation of the problem is not possible. The remedy offered by Baye (1983) for strong fields, through the introduction of the suggested near-constant $\boldsymbol{C}_\perp$, yields a separation in which there remains some coupling between the pseudoparticles, independent of the mass ratio. However for two particles of different masses the introduction of $\boldsymbol{C}_\perp$ is the natural starting point for the separation of slow and fast motions. In the representation $(\boldsymbol{Q}'', \boldsymbol{P}'')$ the momentum $P_3''\ (=-C_\perp^2/2QB)$ and the angle $Q_3''\ (=\tan^{-1}(C_y/C_x))$ may be regarded as constant even in the presence of an interaction potential $V(r)$ (see § 3.4) since such a potential affects only the light pseudoparticle. The equations may then be solved for the fast motion of the light pseudoparticle and subsequently for the relatively slow motion of the heavy pseudoparticle.

While we have concentrated mainly on the properties of the momentum $\boldsymbol{C}_\perp$ associated with the heavy pseudoparticle physically one is interested primarily in the light particle energies. In this respect the coupling term H' does indeed constitute a small perturbation of the remaining terms in the Hamiltonian H such that, to zeroth order, the light particle energies may be derived from the approximate Hamiltonian $H-H'$. One can then invoke a perturbation treatment, whose expansion parameter is m_1B/m_0B_0, to provide higher-order corrections valid even for fields $B>B_0$. (Here B_0 is determined by the charge and mass of the light particle, i.e. typically, but not necessarily, the electron parameters in the definition of B_0, see § 2.2.) In contrast H' is not a small perturbation of the heavy particle motion, except when $e_0 \gg |e_1|$.

Thus we see it is the slow variation of $\boldsymbol{C}_\perp$ which renders a convenient classical description of the transverse motion of two charged particles in a strong magnetic field. The description is particularly appropriate in the context of highly charged hydrogen-like ions ($e_0 \gg |e_1|$).

In contrast the PZW approach is useful for relatively weak magnetic fields for which a separation of the motion parallel and transverse to the field is not helpful. The effect of the CM coupling on the internal motion may be treated by a perturbation expansion in B/B_0 (Johnson *et al* 1983).

Further progress awaits numerical investigations.

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Appendix

The derivation of the canonical set $(\boldsymbol{Q}, \boldsymbol{P})$ from the set $(\boldsymbol{q}', \boldsymbol{p}')$ proceeds from the generator $F_4(\boldsymbol{p}', \boldsymbol{P})$

$$F_4 = -(1/2e_1B)\int^{k_{1\perp}^2} \cos^{-1}\left(\frac{K_\perp^2 - k_{0\perp}^2 - k_{1\perp}^{*2}}{2k_{0\perp}k_{1\perp}^*}\right) \mathrm{d}k_{1\perp}^{*2}. \tag{A1}$$

For completeness and for its possible use in semiclassical mechanics (Miller 1974) we obtain F_4 explicitly by integration by parts, yielding

$$F_4 = (P_2Q_2 - p_2'q_2') - [P_1 - (P_3 + P_4)](q_1' - Q_1) \tag{A2}$$

where the $\boldsymbol{Q}(\boldsymbol{p}', \boldsymbol{P})$ are given by equations (19), $q_2'(\boldsymbol{p}', \boldsymbol{P})$ by equation (17) and $q_1'(\boldsymbol{p}', \boldsymbol{P})$ by equations (15) and (20).

Alternatively, to provide a check we may derive the conjugate angles directly, by differentiating under the integral sign in equation (A1). With attention to the integration limits, this produces elementary integrals of the form

$$\int_0^x \mathrm{d}x'/R^{1/2}y' \tag{A3}$$

where R is a quadratic in x' $(=k_{1\perp}^2)$, and y' is linear in x'.

The lower limit, taken as zero in each case, yields an unimportant constant and the angles given in equations (19) are obtained by combining the various (inverse) circular functions, arising from F_4 and F_2, see equation (18), using suitable identities.

For illustration, the conjugate angle to P_2 of the set $(\boldsymbol{Q}, \boldsymbol{P})$ is obtained from

$$Q_2 = 2QB(\partial F_4/\partial K_\perp^2) = (Q/2e_1)\int^{k_{1\perp}^2} (k_{0\perp} k_{1\perp}^* \sin q_2')^{-1}\, \mathrm{d}k_{1\perp}^{*2}. \tag{A4}$$

Expressing $(k_{0\perp}, q_2')$ in terms of only one 'old' momentum $(k_{1\perp})$ and otherwise 'new' momenta $(K_\perp^2, L_z, \pi_{0\perp}^2, \pi_{1\perp}^2)$ through equations (15) and (17) gives

$$Q_2 = (Q/e_1)\int^{k_{1\perp}^2} \mathrm{d}k_{1\perp}^{*2}/R^{1/2} \tag{A5}$$

where R is a quadratic in the old momentum $k_{1\perp}^2$, and the coefficients are functions of the new momenta. Finally, casting the arguments of the resulting inverse circular functions in terms of the components of the individual particle momenta renders a particularly concise form and suggests the definition of the pseudomomentum $\boldsymbol{k}_\perp$ of equation (20).

The form of the second F_4-type generator used in deriving the final canonical set $(\boldsymbol{Q}', \boldsymbol{P}')$ of equations (27) is very similar

$$F_4' = (1/2e_0B)\int^{\pi_{0\perp}^2} \cos^{-1}\left(\frac{(e_0C_\perp/Q)^2 - \pi_{0\perp}^{*2} - k_\perp^2}{2\pi_{0\perp}^* k_\perp}\right)\mathrm{d}\pi_{0\perp}^{*2}. \tag{A6}$$

The conjugate angle to P_3' is expressible in integral form as

$$Q_3' = -(e_0/2Q)\int^{\pi_{0\perp}} (\pi_{0\perp}^* k_\perp \sin Q_3')^{-1}\, \mathrm{d}\pi_{0\perp}^{*2} \tag{A7}$$

the analysis proceeding by casting $(k_\perp, Q_3')$ in terms of one 'old' momentum $(\pi_{0\perp})$ and otherwise 'new' momenta $(K_\perp^2, L_z, C_\perp^2, \pi_{1\perp}^2)$, and the resulting angle being treated as above.

Analogously to $F_4(\boldsymbol{p}', \boldsymbol{P})$, one can obtain the generator $F_4'(\boldsymbol{P}, \boldsymbol{P}')$ explicitly:

$$F_4'(\boldsymbol{P}, \boldsymbol{P}') = (P_3'Q_3' - P_3Q_3) - [P_1' - (P_2' + P_4')](Q_1 - Q_1') \tag{A8}$$

with the angles taking a complicated form in terms of the momenta $(\boldsymbol{P}, \boldsymbol{P}')$.

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