Classical and Quantum Mechanics of a Charged Particle in Oscillating Electric and Magnetic Fields

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The motion of a particle with charge q and mass m in a magnetic field given by $\mathbf{B} = \mathbf{k}B_0 + B_1[\mathbf{i}cos(\omega t) + \mathbf{j}sin(\omega t)]$ and an electric field which obeys $\nabla \times \mathbf{E} = -\partial\mathbf{B}/\partial t$ is analyzed classically and quantum-mechanically. The use of a *rotating coordinate system* allows the analytical derivation of the particle classical trajectory and its laboratory wavefunction. The motion exhibits two resonances, one at $\omega = \omega_c = -qB_0/m$, the *cyclotron frequency*, and the other at $\omega = \omega_L = -qB_0/2m$, the *Larmor frequency*. For ω at the first resonance frequency, the particle acquires a simple closed trajectory, and the effective hamiltonian can be interpreted as that of a particle in a *static* magnetic field. In the second case a term corresponding to an effective static electric field remains, and the particle orbit is an open line. The particle wave function and eigenenergies are calculated.

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I Introduction

The dynamics of charged particles in electric and magnetic fields is of both academic and practical interest. The areas where this problem finds applications include the development of cyclotron accelerators [1], free electron lasers [2], plasma physics [4] and so on.

In this paper one considers the classical and quantum dynamics of a particle with charge q and mass m acted by a magnetic field given by

$$\mathbf{B} = \mathbf{k}B_0 + B_1[\mathbf{i}cos(\omega t) + \mathbf{j}sin(\omega t)] \tag{1}$$

and an electric field which relates to $\mathbf{B}$ through the Faraday law:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{2}$$

Both fields can be derived from the vector potential:

$$\mathbf{A} = -\frac{1}{2}\mathbf{R} \times \mathbf{B} \tag{3}$$

When B_1 is given by two pairs of crossed Helmholtz coils, the approximation of homogeneity implicit in equation (1) is valid in a region of about 20% of the volume enclosed by the coils. Similar assumption have been taken by other authors [2, 3].

The classical equations of motion can be obtained from the lagrangian:

$$\mathcal{L} = \frac{m}{2}(\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2) + \frac{q}{2}\dot{X}[ZB_1 sin(\omega t) - YB_o] + \\ + \frac{q}{2}\dot{Y}[XB_o - ZB_1 cos(\omega t)] + \frac{q}{2}\dot{Z}[YB_1 cos(\omega t) - XB_1 sin(\omega t)] \tag{4}$$

whereas to study the quantum dynamics we need the hamiltonian:

$$\mathcal{H} = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) - \frac{q}{2m}[B_1 cos(\omega t)L_x + B_1 sin(\omega t)L_y + B_0 L_z] + \\ + \frac{q^2}{8m}\{B_0^2(X^2 + Y^2) + B_1^2 Z^2 - 2B_0 B_1 Z[X cos(\omega t) + Y sin(\omega t)] + \\ + B_1^2[Y cos(\omega t) - X sin(\omega t)]^2\} \tag{5}$$

II The classical motion

The classical equations of motion can be easily obtained from (4). In order to eliminate the time dependence of the lagrangian, we perform the following transformation of coordinates:

$$\mathbf{i} = \mathbf{i}' cos(\omega t) - \mathbf{j}' sin(\omega t)$$
$$\mathbf{j} = \mathbf{i}' sin(\omega t) + \mathbf{j}' cos(\omega t) \tag{6}$$
$$\mathbf{k} = \mathbf{k}'$$

In the nuclear magnetic resonance (NMR) literature [5] these transformations are interpreted as leading to a system of reference which rotates with angular frequency ω in respect to the laboratory coordinate system.

From (6), using lower case to indicate the variables in the rotating system, the effective lagrangian becomes:

$$\mathcal{L}_{eff} = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \frac{q}{2}\dot{x}y(B_o + \frac{2\omega}{\gamma}) + \frac{q}{2}\dot{y}[x(B_o + \frac{2\omega}{\gamma}) - zB_1] + + \frac{q\dot{z}yB_1}{2} + \frac{q\omega}{2}(B_o + \frac{\omega}{\gamma})(x^2 + y^2) - \frac{q\omega B_1 xz}{2} \tag{7}$$

This lagrangian can be written in the usual compact form:

$$\mathcal{L}_{eff} = T + q\dot{\mathbf{r}} \cdot \mathbf{A}_{eff} - q\phi_{eff} \tag{8}$$

where T is the particle kinetic energy, $\mathbf{A}_{eff}$ the *effective vector potential* given by:

$$\mathbf{A}_{eff}(\mathbf{r}) = -\frac{1}{2}\mathbf{r} \times \mathbf{B}_{eff}, \tag{9}$$

with $\mathbf{B}_{eff}$ being the *effective magnetic field* (defined below), and the *effective scalar potential*:

$$\phi_{eff}(\mathbf{r}) = \frac{1}{2}\omega B_1 xz - \frac{\omega}{2}(B_o + \frac{\omega}{\gamma})(x^2 + y^2) \tag{10}$$

where $\gamma = q/m$ is the particle charge-to-mass ratio. Thus, one has for the particle in the rotating frame the following equations of motion:

$$\ddot{x} = \gamma\left[\dot{y}(B_o + \frac{2\omega}{\gamma}) + x\omega(B_o + \frac{\omega}{\gamma}) - \frac{z\omega B_1}{2}\right]$$
$$\ddot{y} = \gamma\left[\dot{z}B_1 - \dot{x}(B_o + \frac{2\omega}{\gamma}) + y\omega(B_o + \frac{\omega}{\gamma})\right] \tag{11}$$
$$\ddot{z} = -\gamma\left[\dot{y}B_1 + \frac{x\omega B_1}{2}\right]$$

It is useful to define an *effective electric* field $\mathbf{E}_{eff}$. The expressions for the effective fields are:

$$\mathbf{E}_{eff} = \left[x\omega(B_o + \frac{\omega}{\gamma}) - \frac{z\omega}{2}B_1\right]\mathbf{i}' + + \left[y\omega(B_o + \frac{\omega}{\gamma})\right]\mathbf{j}' - \frac{x\omega B_1}{2}\mathbf{k}' \tag{12}$$

$$\mathbf{B}_{eff} = B_1\mathbf{i}' + (B_o + \frac{2\omega}{\gamma})\mathbf{k}' \tag{13}$$

Therefore, for a fixed value of ω, each particle with a given charge-to-mass ratio, γ, will feel different effective fields. Note that $\mathbf{B}_{eff}$ differs from that in the NMR case by a factor '2' in the "apparent field" ω/γ [5]. With these definitions, the form of the Lorentz force is preserved in the rotating system:

$$\mathbf{F}_{eff} = q\mathbf{E}_{eff} + q\mathbf{v} \times \mathbf{B}_{eff} \tag{14}$$

One can clearly see from (11) that there are two resonance frequencies in the motion: one at $\omega = \omega_c = -qB_0/m$, the cyclotron frequency, and another at $\omega_L = -qB_0/2m$, the Larmor frequency. For a frequency equal to the first one (ω_c) the particle feels the following effective fields:

$$\mathbf{E}_{eff} = -\frac{1}{2}\omega B_1[z\mathbf{i}' + x\mathbf{k}'] \quad (15)$$

$$\mathbf{B}_{eff} = B_1\mathbf{i}' - B_o\mathbf{k}' \quad (16)$$

and for the second frequency($\omega = \omega_L$),

$$\mathbf{E}_{eff} = \frac{1}{2}\left[x\omega B_o - z\omega B_1\right]\mathbf{i}' + \frac{1}{2}y\omega B_o\mathbf{j}' - \frac{1}{2}x\omega B_1\mathbf{k}' \quad (17)$$

$$\mathbf{B}_{eff} = B_1\mathbf{i}' \quad (18)$$

Now we consider a particle incident in region of fields B_0 and B_1, at the origin of the coordinate system, with initial velocity parallel to $\mathbf{B}_0$. That is, $x(0) = y(0) = z(0) = 0$, $v_x(0) = v_y(0) = 0$, and $v_z(0) = v_0$. As in usual NMR, one makes the approximation $B_0 \gg B_1$. In this limit, it is easy to verify by direct substitution the following solutions of (11), for $\omega = \omega_c$:

$$x(t) \approx \frac{\sqrt{3}v_o}{3\omega_c}sin(\frac{\sqrt{3}\omega_1 t}{2}) - \frac{\omega_1 v_o}{2\omega_c^2}sin(\omega_c t)$$

$$y(t) \approx -\frac{2v_o}{3\omega_1}\left[cos(\frac{\sqrt{3}\omega_1 t}{2}) - 1\right] - \frac{\omega_1 v_o}{2\omega_c^2}cos(\omega_c t) \quad (19)$$

$$z(t) \approx \frac{2\sqrt{3}v_o}{3\omega_1}sin(\frac{\sqrt{3}\omega_1 t}{2})$$

where $\omega_1 \equiv \gamma B_1$. For $\omega = \omega_L$:

$$x(t) \approx \frac{\omega_1 v_o}{\omega_L^2}sin(\omega_L t) - \frac{v_o}{\omega_L}sinh(\frac{\omega_1 t}{2})$$

$$y(t) \approx \frac{\omega_1 v_o}{2\omega_c^2}cos(\omega_L t) + \frac{v_o\omega_1}{\omega_L^2}cosh(\frac{\omega_1 t}{2}) \quad (20)$$

$$z(t) \approx \frac{2v_o}{\omega_1}sinh(\frac{\omega_1 t}{2})$$

The detailed calculation for the obtention of these solutions is given in ref. [8].

Then, we see that whereas for $\omega = \omega_c$ the solutions are purely trigonometric functions, for $\omega = \omega_L$ there is a mixture of trigonometric and hyperbolic functions. This means that the trajectory of the particle will be a closed path in the first case, and an open line in the second. For a general value of ω, which can be very close to ω_c, there will also be an exponential drift. As an example, Figure 1 shows the trajectories of particles in a beam containing triply ionized isotopes of uranium. The respective charge-to-mass ratios in MHz/T are as follow: $\gamma(^{233}\text{U}) = 1.242$; $\gamma(^{234}\text{U}) = 1.237$; $\gamma(^{235}\text{U}) = 1.231$; $\gamma(^{236}\text{U}) = 1.226$ and $\gamma(^{238}\text{U}) = 1.216$. For this simulation we set $v_0 = 10^4$ m/s, $B_0 = 1$ T, $B_1 = 0.01$ T. The oscillating field frequency is tuned to the cyclotron frequency of the isotope ^{235}U, that is, $\omega = -1.231$ MHz. The drawing is in the rotating system. One can have a picture of the trajectories in the laboratory system by rotating the figure about the z-axis. Note that each isotope, according to Eqs. (12) and (13), feels different effective fields. This causes the lighter isotopes to deviate in opposite directions in respect to the heavier ones.

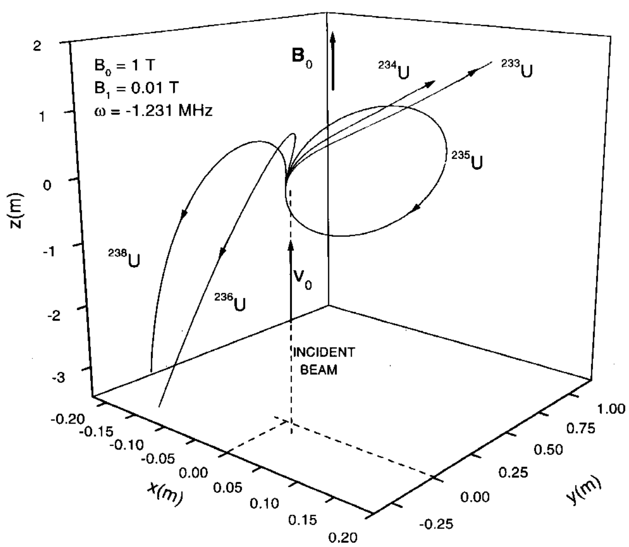

Figure 1. Trajectories of triply ionized Uranium isotopes in oscillating fields "tuned" to the ^{235}U isotope resonance (-1.231 MHz) in the rotating coordinate system. The static field is along the $+z$-axis, and the oscillating magnetic field is on the xy-plane. The initial velocity of the particles is $v_0 = 10^4$ m/s, along the direction of the static field. The orbit of the resonant particle is closed, whereas the non-resonant ones drift away. The trajectories in the laboratory system are obtained rotating the picture about the z-axis. These curves were produced for different lengths of time in order to make them all visible in the same scale.

III Quantum description

In this section we approach the problem from the quantum-mechanical point of view. The transformation to the rotating frame in this case, made directly on the Schrödinger equation, allows the derivation of the laboratory wave function and the particle eigenenergies.

Using the following straightforward relations:

$$(i)\quad X cos(\omega t) + Y sin(\omega t) = e^{-i\omega t L_z/\hbar} X e^{i\omega t L_z/\hbar}$$

$$(ii)\quad [Y cos(\omega t) - X sin(\omega t)]^2 = e^{-i\omega t L_z/\hbar} Y^2 e^{i\omega t L_z/\hbar}$$

$$(iii)\quad X^2 + Y^2 = e^{-i\omega t L_z/\hbar}(X^2+Y^2) e^{i\omega t L_z/\hbar}$$

$$(iv)\quad Z^2 = e^{-i\omega t L_z/\hbar} Z^2 e^{i\omega t L_z/\hbar}$$

$$(v)\quad L_x cos(\omega t) + L_y sin(\omega t) = e^{-i\omega t L_z/\hbar} L_x e^{i\omega t L_z/\hbar}$$

$$L_z = e^{-i\omega t L_z/\hbar} L_z e^{i\omega t L_z/\hbar}$$

where, L_x, L_y and L_z are the components of the canonical angular momentum of the particle, the hamiltonian $\mathcal{H}$ in Eq. (5) becomes[1]:

$$\begin{aligned} e^{i\omega t L_z/\hbar}\mathcal{H}(t) e^{-i\omega t L_z/\hbar} \equiv \mathcal{H}' = \frac{P^2}{2m} + \frac{m\gamma^2 B_0^2}{8}(X^2+Y^2) + \frac{m\gamma^2 B_1^2}{8}(Y^2+Z^2) \\ - \frac{m\gamma^2 B_0 B_1}{4} XZ - \frac{\gamma B_0}{2} L_z - \frac{\gamma B_1}{2} L_x \end{aligned} \tag{21}$$

This hamiltonian represents a charged particle moving in a *static* magnetic field $\mathbf{B} = B_1\mathbf{i} + B_0\mathbf{k}$. The above operation can be interpreted as the quantum-mechanical transformation of the hamiltonian to the rotating coordinate system.

Defining the wavefunction ψ' through the relation:

$$\psi = e^{-i\omega t L_z/\hbar}\psi'$$

and replacing into the Schrödinger equation one obtains:

$$(\mathcal{H}' - \omega L_z)\psi' = i\hbar\frac{\partial\psi'}{\partial t} \equiv \mathcal{H}'_{eff}\psi' \tag{22}$$

Since $\mathcal{H}'_{eff}$ is time-independent, the solution of (22) will be:

$$\psi'(t) = e^{-i(\mathcal{H}'-\omega L_z)t/\hbar}\psi(0) \tag{23}$$

and consequently the wavefunction *in the laboratory system* will be

$$\psi(t) = e^{-i\omega t L_z/\hbar} e^{-i(\mathcal{H}'-\omega L_z)t/\hbar}\psi(0) \tag{24}$$

Note that since $[L_z, \mathcal{H}'] \neq 0$, the two exponential operators in Eq. (24) cannot be gathered into one.

Now we shall analyze the properties of $\mathcal{H}'_{eff}$:

$$\begin{aligned} \mathcal{H}'_{eff} = \frac{P^2}{2m} + \frac{m\gamma^2 B_0^2}{8}(X^2+Y^2) + \frac{m\gamma^2 B_1^2}{8}(Y^2+Z^2) \\ - \frac{m\gamma^2 B_0 B_1}{4} XZ - \frac{\gamma\Delta B}{2} L_z - \frac{\gamma B_1}{2} L_x \end{aligned} \tag{25}$$

where $\Delta B \equiv B_0 + 2\omega/\gamma$. By adding and subtracting the quantity

$$\frac{m\gamma^2}{8}\left(\frac{4\omega^2}{\gamma^2} + \frac{4\omega B_0}{\gamma}\right)(X^2+Y^2) - \frac{m\gamma B_1}{4} 2\omega XZ$$

[1] For the quantum treatment we keep capitals throughout the section.

the effective hamiltonian can be re-written as:

$$\mathcal{H}'_{eff} = \frac{P^2}{2m} + \frac{m\gamma^2 \Delta B^2}{8}(X^2+Y^2) + \frac{m\gamma^2 B_1^2}{8}(Y^2+Z^2)$$
$$-\frac{m\gamma^2 \Delta B B_1}{4} XZ - \frac{\gamma \Delta B}{2} L_z - \frac{\gamma B_1}{2} L_x + q\frac{\omega}{2}\left[B_1 XZ - \left(\frac{\omega}{\gamma}+B_0\right)(X^2+Y^2)\right] \quad (26)$$

which, in turn, has the general form:

$$\mathcal{H}'_{eff} = \frac{1}{2m}(\mathbf{P} - q\mathbf{A}_{eff})^2 + q\phi_{eff} \quad (27)$$

where the *effective scalar potential* is again given by

$$\phi_{eff} = \frac{\omega}{2}\left[B_1 XZ - \left(\frac{\omega}{\gamma}+B_0\right)(X^2+Y^2)\right] \quad (28)$$

$\mathbf{A}_{eff}$ being the *effective vector potential*. The components of $\mathbf{A}_{eff}$ can be obtained by commuting X, Y and Z with $\mathcal{H}'_{eff}$, and comparing the result with the definition of the canonical momentum $\mathbf{P} = m\dot{\mathbf{R}} + q\mathbf{A}$. For instance:

$$i\hbar\dot{X} = [X, \mathcal{H}'_{eff}] = \frac{1}{2m} 2i\hbar P_x + \frac{\gamma\Delta B}{2} i\hbar Y$$

$$P_x = m\dot{X} - q\frac{\Delta B}{2} Y$$

Consequently,

$$A_{eff,x} = -\frac{\Delta B}{2} Y$$

Repeating the procedure for the other components, one obtains:

$$A_{eff,y} = -\frac{B_1}{2} Z + \frac{\Delta B}{2} X$$

$$A_{eff,z} = \frac{B_1}{2} Y$$

These results are the *same* as those obtained in ref. [6], the only difference being a factor '2' in the definition of ΔB.

Written in the form of Eq. (26), the hamiltonian exhibits the effects of the electric field. Contrary to what happens when this is neglected [6], it shows two resonance frequencies. At the Larmor frequency, $\Delta B = 0$, and the hamiltonian becomes:

$$\mathcal{H}'_{eff} = \frac{P^2}{2m} + \frac{m\gamma^2 B_1^2}{8}(Y^2+Z^2) + \frac{\gamma B_1}{2} L_x - \frac{m\gamma^2 B_0 B_1}{4} XZ + \frac{m\gamma^2 B_0^2}{4}(X^2+Y^2) \quad (29)$$

which represents a particle in a static magnetic field along the x direction, plus an electric field potential. The eigenstates of the particle in this case cannot be easily found. On the other hand, at the cyclotron frequency, the second term of ϕ_{eff} in Eq. (28) vanishes, and the hamiltonian becomes:

$$\mathcal{H}'_{eff} = \frac{P^2}{2m} + \frac{m\gamma^2 B_0^2}{8}(X^2+Y^2) + \frac{m\gamma^2 B_1^2}{8}(Y^2+Z^2)$$
$$-\frac{m\gamma^2 B_0 B_1}{4} XZ - \frac{\gamma B_0}{2} L_z + \frac{\gamma B_1}{2} L_x \quad (30)$$

which represents a particle moving in a *static magnetic* field $\mathbf{B}_{eff} = B_0\mathbf{k} - B_1\mathbf{i}$. This hamiltonian can easily written in a diagonal form by defining the angle

$$\theta = tg^{-1}\left(\frac{B_1}{B_0}\right)$$

between the z-axis and $\mathbf{B}_{eff}$, and writing the operators of $\mathcal{H}'_{eff}$ in (30) in terms of the new coordinates, X', Y' and Z', where the effective field is axial.

The particle's eigenenergies are given in this case by:

$$E_n = \frac{P_z'}{2m} + \left(n + \frac{1}{2}\right) \hbar\omega_c' \tag{31}$$

where $\omega_c' = \gamma B_{eff} = \gamma\sqrt{B_0^2 + B_1^2}$ is the cyclotron frequency about the effective field in the rotating system. From this one sees that the quantization axis can be rotated continuously by changing the angle θ through the change in the ratio B_1/B_0.

IV Conclusions

In this paper we have studied the classical and the quantum dynamics of a charged particle in oscillating magnetic and electric fields which are related through the Faraday law. The equations of motion show two resonance frequencies, one at the Larmor frequency (ω_L) and another at the cyclotron frequency (ω_c). When the field frequency equals ω_c, the particle is confined to a simple closed trajectory, but when $\omega = \omega_L$, it drifts away, the same happening to off resonance particles whose frequencies are very close to ω_c. The use of a "rotating coordinate system" such as used in conventional nuclear magnetic resonance allows the derivation of analytical solutions for the equations of motion.

By using the corresponding quantum-mechanical transformation, one finds the exact wavefunction of the particle in the laboratory system. When $\omega = \omega_c$, the effective hamiltonian corresponds to that of a charged particle in an static magnetic field. In this case the particle eigenenergies are derived in the rotating coordinate system, and it is shown that the direction of the axis of quantization can be continuously rotated by changing the ratio between the intensities of the fields. On the other hand, when $\omega = \omega_L$, the hamiltonian is a mixture of effective magnetic and electric fields, and the eigenenergies cannot be easily derived.

The Hamiltonian (30) predicts the existence of "current echoes", and therefore is in accordance with the results of references [6] and [7]. There is, however, one important difference which appears in the present case where the electric field is considered. Contrary to what happens in [6], the static field term does not vanish at resonance. Thus, in order to describe properly the formation of a current echo in the present situation, one must consider $B_1 \gg B_0$ when the pulse is "on", and obviously $B_1 = 0$ when it is off. Having this in mind, the calculation for the current echo amplitude can be carried out in the same way as described in [6].

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