Quantum dynamics of an electric charge in an oscillating pulsed magnetic field

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We investigate the motion of a charged particle under the action of a time-dependent oscillating magnetic field. For one and two magnetic pulses we obtain analytical expressions for the *free current decay* and *current echo*, respectively, in agreement with a recently proposed classical description of the electrical current in fields **E** and **B**. In a continuous ac field the particle eigenstates are calculated. When the resonance condition is achieved, the axis of quantization is turned over by 90°. The results suggest a magnetic *pulsed resonant* method to separate charged particles in a beam. [S1063-651X(97)05502-5]

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The problem of an ensemble of paramagnetic moments in an oscillating magnetic field gained a great deal of interest from the middle 1940s with the work of Bloch, Hansen, and Packard [1] and Hahn [2]. The latter discovered the existence of spin echoes and demonstrated that they were solutions of the Bloch equations under pulsed magnetic fields. Spin echoes can also be easily deduced from a quantum-mechanical approach [3]. Hahn's discovery founded *pulsed nuclear magnetic resonance* (NMR), a technique which has spread over many areas of scientific research and technical applications.

On the other hand, the quantum dynamics of a charged particle in a homogeneous static magnetic field is of considerable practical and academic interest, and has been investigated by many authors [4–6]. The general problem is finding the solution for the Schrödinger equation

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t}=\mathcal{H}\psi=\frac{1}{2m}[\mathbf{P}-q\mathbf{A}]^2\psi, \tag{1}$$

where q is the particle charge, m its mass, and the magnetic field is obtained from $\mathbf{B}=\nabla\times\mathbf{A}$. If $\mathcal{H}$ is time independent, the general solution of Eq. (1) will be given by

$$\psi(t)=\exp[-(i/\hbar)\mathcal{H}t]\psi(0). \tag{2}$$

In this paper we shall consider the quantum dynamics of a charged particle under the action of an oscillating magnetic field given by

$$\mathbf{B}(t)=\mathbf{i}B_1\cos(\omega t)+\mathbf{j}B_1\sin(\omega t)+\mathbf{k}B_0. \tag{3}$$

In this case **B** can still be derived from a vector potential $\mathbf{A}(t)$ through the same relation $\mathbf{B}=\nabla\times\mathbf{A}$, but obviously solution (2) will no longer be valid. However, there is still a way to solve the problem, which is to consider the particle motion in a *rotating reference frame* where **B** is stationary [3]. It has been shown recently that a similar treatment for the classical equations of motion of the electrical current in the presence of fields **E** and **B** leads to interesting resonance phenomena similar to the free induction decay and spin echo in the magnetic case. These have been called *free current decay* and *current echo* [8].

The transformation of a magnetic field given by Eq. (3) to a rotating reference frame with angular frequency ω is a well known procedure [3]. The result is the *time-independent effective field*

$$\mathbf{B}_e=(\omega/\gamma-B_0)\mathbf{k}+B_1\mathbf{i}, \tag{4}$$

where $\gamma\equiv q/m$ is the analog of the gyromagnetic ratio in the usual NMR. Writing $\Delta B=\omega/\gamma-B_0$, the components of the corresponding vector potential in this system of coordinates will be

$$A_x=-\tfrac{1}{2}(\Delta B)Y,$$

$$A_y=\tfrac{1}{2}[(\Delta B)X-B_1Z],$$

$$A_z=\tfrac{1}{2}B_1Y.$$

We see from the above that the potential vector is given by $\mathbf{A}=-(1/2)\mathbf{R}\times\mathbf{B}_e$. We also see that **A** satisfies the Coulomb gauge: $\nabla\cdot\mathbf{A}=0$. Here we are not distinguishing operators in the rotating and laboratory frames. Wherever necessary, a clear distinction will be made.

Replacing the components of **A** in the Hamiltonian one finds

$$\mathcal{H}=\frac{P_x^2+P_y^2+P_z^2}{2m}+\frac{m\gamma^2(\Delta B)^2}{8}(X^2+Y^2)+\frac{m\gamma^2B_1^2}{8}(Y^2+Z^2)+\frac{\gamma(\Delta B)}{2}L_z+\frac{\gamma B_1}{2}L_x-\frac{m\gamma^2}{4}B_1(\Delta B)XZ. \tag{5}$$

Expression (2) and Hamiltonian (5) allow the calculation of the expected value of an observable $\hat{Q}$ at any instant of time t. In this paper we will apply these expressions to study the quantum dynamics of a charged particle in the magnetic field given by Eq. (3) in the cases where the field is applied as a sequence of one and two pulses, respectively, each one with the same duration τ. Then we briefly discuss the case where the field is applied continuously.

In what follows, we will suppose that we are close to the resonance frequency, that is, $\omega \approx \omega_c$. This means that when the pulse is ''on,'' $B_1 \gg \Delta B$. We see that under this assumption, the Hamiltonian (5) is diagonalized. It is also interesting to note that when the pulse is ''turned off'' ($B_1=0$) Eq. (5) is again diagonal. This is an important consideration to be taken into account when investigating the application of more than one pulse, as shown below.

Let us calculate $\langle \dot{Y} \rangle(\tau)$, the expected value for the particle speed at $t=\tau$. This will be given by [9]

$$i\hbar\langle \dot{Y}\rangle(\tau)=\langle[Y,\mathcal{H}]\rangle(\tau) =\frac{\langle P_y\rangle(\tau)}{m}+\frac{\Delta\omega}{2}\langle X\rangle(\tau)-\frac{\omega_1}{2}\langle Z\rangle(\tau). \qquad (6)$$

Since by hypothesis we are close to the resonance, the term in $\Delta\omega$ can be neglected. Now, according to Eq. (2), $\langle P_y\rangle(\tau)$ is given by

$$\langle P_y\rangle(\tau)=\int \psi^*(0)e^{(i/\hbar)\mathcal{H}\tau}P_y e^{-(i/\hbar)\mathcal{H}\tau}\psi(0)d^3r. \qquad (7)$$

We will write $\mathcal{H}=\mathcal{H}_\parallel+\mathcal{H}_\perp$, where

$$\mathcal{H}_\parallel=P_x^2/2m$$

$$\mathcal{H}_\perp=\mathcal{H}_{yz}+\omega_1 L_x/2,$$

with $\omega_1=\gamma B_1$ and

$$\mathcal{H}_{yz}=(P_y^2+P_z^2)/2m+m\omega_1^2(Y^2+Z^2)|8.$$

It is easy to verify that $[\mathcal{H}_\parallel,L_x]=[\mathcal{H}_\parallel,\mathcal{H}_{yz}]=[L_x,\mathcal{H}_{yz}]=0$, so we can factorize the exponential operator in Eq. (7) into a product of three terms which commute among themselves [9].

We begin by calculating the operator

$$e^{(i/\hbar)\mathcal{H}_{yz}\tau}P_y e^{-(i/\hbar)\mathcal{H}_{yz}\tau}.$$

The Hamiltonian $\mathcal{H}_{yz}$ is a complicated function of Y, Z, P_y, and P_z. Since the z components commute with the y components, this operator can be further factorized, leaving only

$$e^{(i/2m\hbar)\tau P_y^2+(im\gamma^2B_1^2/8\hbar)\tau Y^2}P_y e^{-(i/2m\hbar)\tau P_y^2-(im\gamma^2B_1^2/8\hbar)\tau Y^2}.$$

In order to find a closed form for this operator, consider the expression [10]

$$e^{\hat{O}}P_y e^{-\hat{O}}=P_y+[\hat{O},P_y]+\frac{1}{2!}[\hat{O},[\hat{O},P_y]] +\frac{1}{3!}[\hat{O},[\hat{O},[\hat{O},P_y]]]+\cdots.$$

Replacing $\hat{O}=(i/2m\hbar)\tau P_y^2+(im\gamma^2B_1^2/8\hbar)\tau Y^2$ in the above series and using the expression $[AB,C]=A[B,C]+[A,C]B$, one finds

$$e^{\hat{O}}P_y e^{-\hat{O}}=\left[1-\frac{1}{2!}\left(\frac{\omega_1\tau}{2}\right)^2+\frac{1}{4!}\left(\frac{\omega_1\tau}{2}\right)^4-\cdots\right]P_y -\frac{m\omega_1^2\tau}{4}\left[1-\frac{1}{3!}\left(\frac{\omega_1\tau}{2}\right)^2+\frac{1}{5!}\left(\frac{\omega_1\tau}{2}\right)^4-\cdots\right]Y. \qquad (8)$$

The terms between brackets are well known series [11]

$$\sum_{n=0}^{\infty}(-1)^n\frac{x^{2n}}{(2n)!}=\cos(x),$$

$$\sum_{n=0}^{\infty}(-1)^n\frac{x^{2n}}{(2n+1)!}=x^{-1}\sin(x),$$

with $x=\omega_1\tau/2$. The final result is

$$e^{\hat{O}}P_y e^{-\hat{O}}=\cos\left(\frac{\omega_1\tau}{2}\right)P_y-\frac{m\omega_1}{2}\sin\left(\frac{\omega_1\tau}{2}\right)Y.$$

Then, the next operators to be calculated are

$$e^{(i\omega_1\tau/2\hbar)L_x}\left[\cos\left(\frac{\omega_1\tau}{2}\right)P_y-\frac{m\omega_1}{2}\sin\left(\frac{\omega_1\tau}{2}\right)Y\right]e^{(-i\omega_1\tau/2\hbar)L_x},$$

which represents a rotation of Y and P_y about the x axis by an angle $\omega_1\tau/2=\gamma B_1\tau/2$. Using the relations [9]

$$e^{(i/\hbar)\phi L_x}Ye^{(-i/\hbar)\phi L_x}=Y\cos\phi-Z\sin\phi,$$

$$e^{(i/\hbar)\phi L_x}P_y e^{(-i/\hbar)\phi L_x}=P_y\cos\phi-P_z\sin\phi,$$

one finds

$$\langle P_y\rangle(\tau)=p_{y0}\cos^2\left(\frac{\gamma B_1\tau}{2}\right)-\frac{p_{0z}}{2}\sin(\gamma B_1\tau) -\frac{m\omega_1}{2}\left[\frac{y_0}{2}\sin(\gamma B_1\tau)-z_0\sin^2\left(\frac{\gamma B_1\tau}{2}\right)\right], \qquad (9)$$

where $q_0=\int\psi^*(0)\hat{Q}\psi(0)d^3r$ stands for the expected value of an observable $\hat{Q}$ at $t=0$. (Note that the last operator to be applied on Eq. (7), $\exp[(i/2m\hbar)P_x^2]$, does not act either on Y or P_y.)

Now it remains for us to calculate $\langle Z\rangle(\tau)$. It is easy to verify that

$$e^{(i/\hbar)\mathcal{H}_{yz}\tau}Ze^{-(i/\hbar)\mathcal{H}_{yz}\tau}=\cos\left(\frac{\omega_1\tau}{2}\right)Z+\frac{2}{m\omega_1}\sin\left(\frac{\omega_1\tau}{2}\right)P_z.$$

From this, one finds

$$\langle Z\rangle(\tau)=z_0\cos^2\left(\frac{\gamma B_1\tau}{2}\right)+\frac{y_0}{2}\sin(\gamma B_1\tau) +\frac{2}{m\omega_1}\left[\frac{p_{0z}}{2}\sin(\gamma B_1\tau)+p_{0y}\sin^2\left(\frac{\gamma B_1\tau}{2}\right)\right]. \qquad (10)$$

Gathering all the terms in Eq. (6), we finally have

$$m\langle\dot{Y}\rangle(\tau)=p_{0y}\cos(\gamma B_1\tau)-p_{0z}\sin(\gamma B_1\tau)$$
$$-\frac{m\gamma B_1}{2}[z_0\cos(\gamma B_1\tau)+y_0\sin(\gamma B_1\tau)]. \tag{11}$$

With simplifying initial conditions $x_0=y_0=z_0=0$; $p_{x0}=p_{y0}=0$, and $p_{z0}=p_0$, we arrive at

$$m\langle\dot{Y}\rangle(\tau)=-p_0\sin(\gamma B_1\tau).$$

Repeating the above procedure for the x and z components one finds

$$m\langle\dot{Z}\rangle(\tau)=+p_0\cos(\gamma B_1\tau),$$

$$m\langle\dot{X}\rangle(\tau)=0.$$

Other quantities of interest can be calculated in the same way. For instance,

$$\langle Y\rangle(\tau)=-\sin^2(\gamma B_1\tau/2)2p_0/m\omega_1.$$

We can correlate the above result for $m\langle\dot{Y}\rangle(\tau)$ with the semiclassical expression for the electrical current density

$$J_y(\tau)=-nq\langle\dot{Y}\rangle(\tau)=J_0\sin(\gamma B_1\tau), \tag{12}$$

where $J_0=nqp_0/m$ and n is the particle density. This is the same expression as that obtained classically for the *free current decay* in Ref. [8]. Note that we could have taken into account the *initial direction* of p_o by adding an arbitrary phase δ onto the expression for $m\langle\dot{Y}\rangle(\tau)$. For instance,

$$m\langle\dot{Y}\rangle(\tau)=-2p_0\sin\left(\frac{\gamma B_1\tau}{2}+\delta\right)\cos\left(\frac{\gamma B_1\tau}{2}+\delta\right)$$
$$=-p_0\sin(\gamma B_1\tau+2\delta),$$

where $\delta=0$ represents a particle initially moving in the direction $+z$, whereas if $\delta=\pi/2$ we will simply have a change in the sign of $\langle P_y\rangle$, corresponding to an inversion in the direction of p_0.

In order to calculate $m\langle\dot{Y}\rangle$ for a sequence of two pulses we must remember that during the time the pulses are ''on,'' the dynamics of the particle will develop under the Hamiltonian

$$\mathcal{H}=\frac{P_x^2+P_y^2+P_z^2}{2m}+\frac{m\omega_1^2}{8}(Y^2+Z^2)+\frac{\omega_1}{2}L_x$$

and during the intervals when they are ''off,'' $B_1=0$, and $\mathcal{H}$ becomes

$$\mathcal{H}=\frac{P_x^2+P_y^2+P_z^2}{2m}+\frac{m\Delta\omega^2}{8}(X^2+Y^2)+\frac{\Delta\omega}{2}L_z.$$

The calculation is rather tedious because of the various terms appearing in the above Hamiltonians, but it can be carried out in a way similar to that of Ref. [3] for the calculation of the spin echo in the magnetic case, and using the results of the previous paragraphs. At the resonance ($\Delta\omega=0$), one finds for the *current echo* amplitude

$$m\langle\dot{Y}\rangle(2\tau)=p_0\sin^2(\gamma B_1\tau/2)\sin(\gamma B_1\tau). \tag{13}$$

This expression agrees with the classical result [8]. The other two terms add to it in the general result. They are associated to the *free current decays* after the first and second pulses as shown by Bloom for the magnetic case [12].

At this point it may be worth remembering that the above results are valid for *any* charged particle. The only difference will be on the ''gyromagnetic factor,'' $\gamma=q/m$, the ratio between the particle charge and mass. The sign of γ determines the sense of the particle rotation in the field, whereas its magnitude defines its cyclotron frequency. For the *muon*, for instance, whose mass is about 200 times bigger than the electron mass, the resonance frequency will be correspondingly lower. The same is true for ''heavy electrons'' in the intermetallic compounds known as *heavy fermions*, or still for ions in an ion beam. As an example, take a triply ionized atom of ^{157}Gd which has $q/m\approx0.18$ MHz kG^{-1}. In a field $B_1=1$ kG, the particle frequency on the rotating frame at the resonance will be $\nu_1=\omega_1/2\pi\approx0.3$ MHz. If the initial energy of the particle is 1 keV, the maximum distance reached on the y axis will be approximately 40 cm.

Finally, we shall mention that Hamiltonian (5) can also be easily diagonalized in the situation where the ac field is applied continuously. All we have to do is to ''rotate'' the z axis by an angle $\theta=\arctan(B_1/\Delta B)$ to a new reference system where $B_e=(B_1^2+\Delta B^2)^{1/2}$ is axial. The Hamiltonian then becomes the standard one for an electron in a ''static'' field, with cyclotron frequency $\omega_c'=\gamma B_e$, and eigenvalues given by [9]

$$E_n'(p_z')=\left(n'+\frac{1}{2}\right)\hbar\omega_c'+p_z'^2/2m, \tag{14}$$

where $\omega_c'=qB_e/m$ is the particle *cyclotron frequency about the effective field in the rotating frame*.

The above result has some interesting consequences. We note that if ω is far from the resonance frequency, that is, $\Delta\omega\gg\omega_1$ (or $\Delta B\gg B_1$), the Landau levels will be quantized on the x-y plane [9]. But at the resonance, $\Delta\omega=0$, these levels are turned over and the quantization will take place on the z-y plane with energies given by

$$E_n(p_x)=(n+\tfrac{1}{2})\hbar\omega_1+p_x^2/2m. \tag{15}$$

Consequently, the quantization axis can be rotated continuously from z to x by sweeping ω over the resonance frequency.

Summarizing, we have investigated the quantum-dynamical behavior of a charged particle in an oscillating magnetic field. We analyzed two distinct cases: (i) the oscillating field is applied as a sequence of pulses and (ii) it is applied continuously. In both cases there exists an exact analytical solution, irrespective of the relative magnitudes of the static and oscillating fields. The main conclusions are as follows: (i) expressions for the free current decay and current echoes at the resonance can be derived; these expressions agree with those obtained from a classical approach in Ref.

[8]; (ii) on the second case, the eigenstates of the particle are obtained. The so-called *Landau tubes* are turned over the direction of the field as the resonance frequency is approached. This effect may be of practical importance, for instance, in the de Haas–van Alphen effect, where the intersection between the Landau tubes and the Fermi surface in metals gives rise to oscillations in various physical properties with the field amplitude, such as the magnetic susceptibility, etc. [7]. We have not considered the particle spin on this paper, but its inclusion is straightforward if spin-orbit coupling is neglected.

From the above it is clear that these effects are not restricted to systems where a *relaxation time* exists, as discussed in Ref. [8]. They can, in principle, be observed even in isolated free particles in vacuum, as for instance, in an ion beam. This may be of relevance for the development of a magnetic pulse technique for charged particle spectroscopy. In solid state physics it may find useful applications in the investigation of transport properties in conducting media, through the study of the electron cyclotron resonance, electron-electron, and electron-lattice scattering rates.

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