9/27/07

Now charged particle motion in a uniform $\vec{B}$ field, a problem closely related to harmonic oscillators and important in applications. First, two remarks however.

First remark. The HO Hamiltonian for a mechanical H.O. is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$

This can be put into a more symmetrical form by the transformation,

$$p = \sqrt{m\omega}\; p'$$

$$x = \frac{1}{\sqrt{m\omega}}\, x'$$

which preserves the canonical commutation relations,

$$[x, p] = [x', p'] = i\hbar.$$

In terms of the new variables,

$$H = \frac{\omega}{2}\left(x'^2 + p'^2 \right).$$

The second remark concerns velocity operators. The Hamiltonian for a charged particle in an EM field is

Here we do <u>not</u> assume $\vec{B}$ is uniform or even static.

$$H = \frac{1}{2m}\left[\vec{p} - \frac{q}{c}\vec{A} \right]^2 + q\phi . \qquad q = \text{charge of particle.}$$

The first term is physically just the kinetic energy. We define the <u>velocity operator</u> (a vector of operators) by

$$\vec{v} = \frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A} \right).$$

This definition is borrowed from classical mechanics, or else we can make a purely quantum motivation by invoking the Heisenberg eqns of motion,

$$\vec{v} = \dot{\vec{x}} = \frac{1}{i\hbar}[\vec{x}, H] = \frac{1}{m}\left(\vec{p} - q/c\,\vec{A}\right).$$

The velocity operators do not commute, in general. Using $[x_i, p_j] = i\hbar\,\delta_{ij}$, we find

$$[v_i, v_j] = \frac{1}{m^2}\left[p_i - \frac{q}{c}A_i,\ p_j - \frac{q}{c}A_j\right]$$

$$= -\frac{q}{m^2 c}\Big(\,[p_i, A_j] + [A_i, p_j]\Big)$$

$$= +\frac{i\hbar q}{m^2 c}\left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right)$$

or,

$$\boxed{[v_i, v_j] = \frac{i\hbar q}{m^2 c}\,\varepsilon_{ijk}\,B_k}$$

The velocity components commute if $\vec{B} = 0$, otherwise not.

Also, we note the commutators,

$$\boxed{[x_i, v_j] = \frac{i\hbar}{m}\,\delta_{ij}}$$

In terms of the velocity operators, the Hamiltonian is

$$H = \frac{1}{2} m v^2 + q\phi,$$

which is more transparent than the usual expression (in terms of the canonical momentum $\vec{p}$).

Now let's set $\vec{E}=0$, $\vec{B}=B\hat{z}$ ($B=$ const), and $q=-e$ (where $e>0$, that is, a negative particle). First we solve the <u>classical problem</u>. The Newton-Lorentz eqns are

$$m\vec{a} = -e\,\frac{\vec{v}}{c}\times\vec{B} \qquad \left(\begin{array}{l}\vec{v}=\dot{\vec{x}}\\ \vec{a}=\ddot{\vec{x}}\end{array}\right)$$

or

$$\vec{B}=B\hat{z}$$

$$\vec{a} = \omega\,\hat{z}\times\vec{v}$$

where

$$\omega = \frac{eB}{mc} > 0 \qquad (\text{gyrofrequency}).$$

Integrating once, we get

$$\vec{v} = \omega\,\hat{z}\times\vec{x} + \vec{c},$$

where $\vec{c}$ is a constant vector. Writing out all 3 components, we have

$$\left.\begin{aligned} v_x &= -\omega y + c_x \\ v_y &= +\omega x + c_y \\ v_z &= c_z \end{aligned}\right\}$$

The particle velocity is constant in the z-direction, that is,

it is free-particle motion. We'll just write v_z for the z-velocity (not c_z), and remember that it is constant. As for the x and y components, let's set

$$c_x = \omega Y$$
$$c_y = -\omega X ,$$

where X and Y are constants that we use instead of c_x, c_y, so we have

$$\left.\begin{aligned} v_x &= -\omega(y-Y) \\ v_y &= \omega(x-X) \end{aligned}\right\} .$$

or

$$\left.\begin{aligned} X &= x - v_y/\omega \\ Y &= y + v_x/\omega \end{aligned}\right\} .$$

We interpret X, Y physically in a moment.

Now define

$$\begin{aligned} \xi &= x - X \\ \eta &= y - Y \end{aligned} \quad \text{so} \quad \begin{aligned} \dot{\xi} &= \dot{x} = v_x \\ \dot{\eta} &= \dot{y} = v_y \end{aligned}$$

then

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \end{pmatrix} = \omega \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} .$$

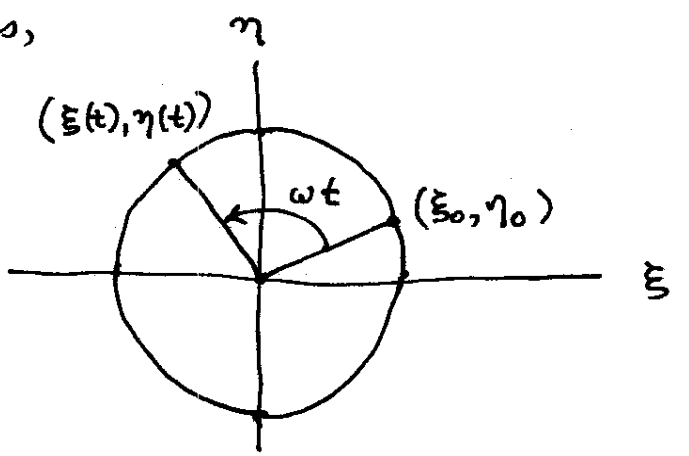
This can be solved by exponentiating the matrix,

$$\exp\left[\omega t\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\right] = \begin{pmatrix} \cos\omega t & -\sin\omega t \\ \sin\omega t & \cos\omega t \end{pmatrix},$$

which is a rotation matrix in the x-y plane in a positive (counterclockwise) direction. Thus the solution is

$$\begin{pmatrix} \xi(t) \\ \eta(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & -\sin\omega t \\ \sin\omega t & \cos\omega t \end{pmatrix}\begin{pmatrix} \xi_0 \\ \eta_0 \end{pmatrix},$$

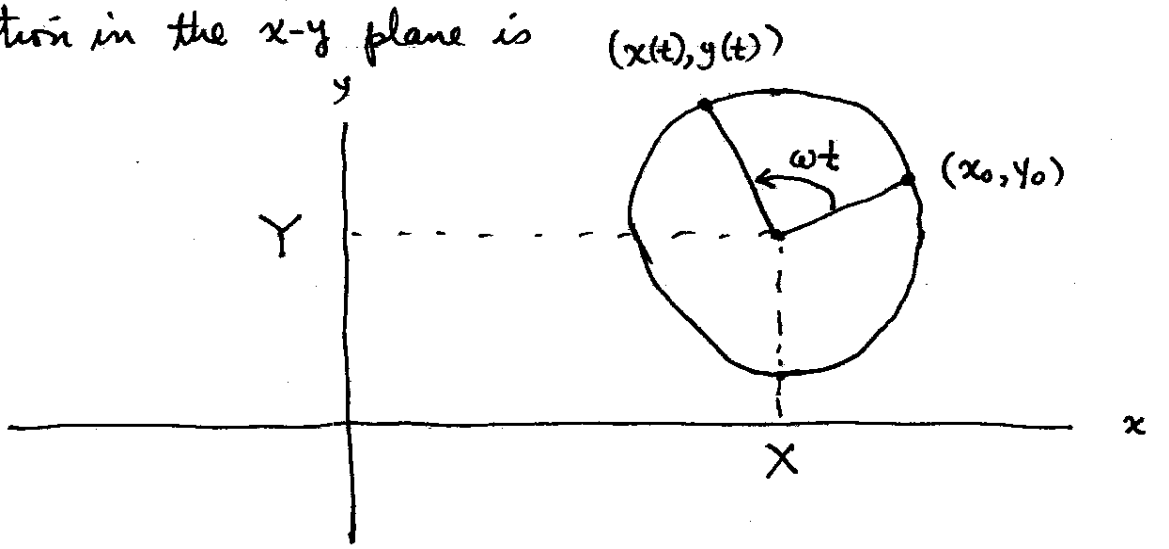
or in pictures,



Or, since

$$x = X + \xi$$
$$y = Y + \eta$$

the motion in the x-y plane is



Constants X and Y are the center of the circle, which is called the <u>guiding center</u> (or its projection onto the xy plane, if we include the z-motion). The ~~motion~~ orbit in 3d space is a helix.

Now we turn to the quantum problem. First we find the spectrum of H, (the eigenvalues) which is easier than finding the ~~wave~~ eigen-functions. The energy eigenvalues are gauge-invariant (they do not depend on the choice of vector potential), and we shall determine them by gauge-invariant means.

The Hamiltonian is (in terms of velocity operators)

$$H = \frac{1}{2} m v^2 = \frac{1}{2} m (v_x^2 + v_y^2) + \frac{1}{2} m v_z^2 = H_\perp + H_\parallel .$$

The energy is purely kinetic, and is broken into perpendicular (to $\vec{B}$) and parallel (to $\vec{B}$) parts. Since $\vec{B} = B\hat{z}$ and $q = -e$, the velocity commutators are

$$[v_x, v_y] = \frac{-i\hbar e B}{m^2 c} = \frac{-i\hbar\omega}{m}, \quad \left(\text{where } \omega = \frac{eB}{mc} = \text{freq. of classical motion}\right)$$

$$[v_x, v_z] = [v_y, v_z] = 0.$$

We see immediately that $[H_\perp, H_\parallel] = 0$, so they ($H_\perp$ and $H_\parallel$) possess simultaneous eigenstates.

Our strategy for analyzing H is to borrow definitions

of physically interesting operators from the classical solution and to explore their properties. The most interesting operators for the $\perp$ motion are X, Y and v_x, v_y, while for the $\parallel$ motion they are z, v_z. The definitions of X, Y (the guiding center operators) are

$$X = x - v_y/\omega$$
$$Y = y + v_x/\omega$$

exactly as in the classical case, but now interpreted as operator equations. Later we will have to distinguish between operators and c-numbers (classical values or eigenvalues), so we will write $\hat{X}, \hat{Y}$ etc vs. X, Y etc. when we want to make the distinction clear.

The commutator of X and Y is

$$[X, Y] = \left[x - \frac{v_y}{\omega}, y + \frac{v_x}{\omega}\right] = \frac{i\hbar}{m\omega}$$
$$= \frac{1}{\omega}[x, v_x] - \frac{1}{\omega}[v_y, y] + \frac{1}{\omega^2}[v_y, v_x]$$

Also, by similar calculations we find that X and Y commute with v_x, v_y. Including the z, v_z variables, we get an overall set of commutation relations,

$$[X, Y] = \frac{i\hbar}{m\omega}$$

$$[X, v_x] = [X, v_y] = [X, z] = [X, v_z]$$
$$= [Y, v_x] = [Y, v_y] = [Y, z] = [Y, v_z] = 0$$

$$[v_y, v_x] = \frac{i\hbar\omega}{m}$$

swapped order

$$[v_x, z] = [v_x, v_z] = [v_y, z] = [v_y, v_z] = 0$$

$$[z, v_z] = \frac{i\hbar}{m}.$$

We have 6 operators, X, Y, v_x, v_y, z, v_z with 3 nonvanishing commutators proportional to $i\hbar$, and all others zero. To within constant factors, it is a set of 3 pairs of conjugate variables. Let us therefore define:

$$\left.\begin{aligned} X &= \frac{1}{\sqrt{m\omega}} Q_1 \\ Y &= \frac{1}{\sqrt{m\omega}} P_1 \\ v_y &= \sqrt{\frac{\omega}{m}}\, Q_2 \\ v_x &= \sqrt{\frac{\omega}{m}}\, P_2 \\ z &= Q_3 \\ m v_z &= P_3 \end{aligned}\right]$$

then:

$$[Q_i, Q_j] = [P_i, P_j] = 0$$
$$[Q_i, P_j] = i\hbar\,\delta_{ij}.$$

By working with variables of obvious physical importance, we have found a "canonical transformation", $(x\, y\, z\, p_x\, p_y\, p_z) \to (Q_1\, Q_2\, Q_3\, P_1\, P_2\, P_3)$, i.e. one which preserves the canonical commutation relations.

Now we express H in terms of these new variables. We have

$$H = \underbrace{\frac{\omega}{2}\left(Q_2^2 + P_2^2\right)}_{H_\perp} + \underbrace{\frac{\hat{P}_3^2}{2m}}_{H_\parallel}.$$

The operator $H_\perp$ is a harmonic oscillator, with eigenvalues $(n+\frac{1}{2})\hbar\omega$. These are called <u>Landau levels</u> (quantized states of $\perp$ kinetic energy). Operator $H_\parallel$ is a 1d free particle Hamiltonian. The energies are

$$E = E_\perp + E_\parallel$$

$$= (n+\tfrac{1}{2})\hbar\omega + \frac{P_3^2}{2m}$$

eigenvalue of $\hat{P}_3$.

This Hamiltonian is unusual because it is independent of both Q_1 and P_1 (essentially the guiding center positions operators $\hat{X}, \hat{Y}$). This makes sense, since the classical energy is independent of X, Y (the circle can be centered anywhere in the x-y plane without changing the energy).