Ex1329: Periodic lattice in uniform field, Bloch oscillations

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The problem:

Consider a particle in a 1D periodic lattice. The lattice constant is a and the hopping frequency is c . There is an applied electric field f.
(1) Write the Hamiltonian $\mathcal{H}(p,x)$ with f that is derived from a scalar potential $V(x)$.
(2) Derive the classical equations of motion and solve them. What is the period of the oscillation? What is the spatial amplitude of the oscillation?
(3) Write the Hamiltonian $\widetilde{\mathcal{H}}(p,t)$ with f that is derived from a vector potential A. What is the gauge transformation of the basis that relates the two Hamiltonians?
(4) Find an explicit expression in terms of Bessel function for the evolving probability distribution $\rho(x,t)$.
(5) What is the solution $\rho(x,t)$ in the zero field limit? Plot or describe in words how the spreading profile looks like in this case.
(6) Verify that for finite field the amplitude of the Bloch oscillations is in agreement with the classical result.

The solution:

(1) We look at an N-site, periodic lattice. For an electric field in the positive direction the scalar potential will be:

$$\hat{V}(x) = -ef\hat{x}$$

In the site basis the position operator will be:

$$\hat{x}\left|n\right\rangle = an\left|n\right\rangle$$

We start by describing the Hamiltonian of a discrete N-site system:

$$\mathcal{H} = \begin{pmatrix} 0 & c & 0 & \cdots & \cdots & c \\ c & 0 & c & \cdots & \cdots & 0 \\ \vdots & c & 0 & c & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ c & \vdots & \vdots & \vdots & c & 0 \end{pmatrix} - aef \begin{pmatrix} 1 & 0 & \cdots & \cdots & \cdots & \cdots \\ 0 & 2 & 0 & \cdots & \cdots & \cdots \\ \vdots & \ddots & 3 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots & N \end{pmatrix}$$

Translated into operator form:

$$\hat{\mathcal{H}} = c(\hat{D} + \hat{D}^{\dagger}) - ef\hat{x} = 2c\cos(a\hat{p}) - ef\hat{x}$$

The last transition used the known relation:

$$\hat{D} = e^{-ia\hat{p}}$$

(2) Using Hamilton EOM:

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial x} = ef \;\; ; \;\; \dot{x} = \frac{\partial \mathcal{H}}{\partial p} = -2ca\sin(ap)$$

Solving for the momentum:

$$p = p_0 + eft$$

And for the position:

$$x = x_0 + \frac{2c}{ef}\cos(eaft + ap_o)$$

Thereby, deducing that the classical frequency is:

$$\omega_{classical} = eaf$$

and the spatial amplitude of oscillations is $\frac{2c}{ef}$.

(3) The general form (in $c = 1$ units) for Hamiltonian in a site problem is

$$h(\hat{x}, \hat{p}, \hat{A}, \hat{V}) = 2c\, cos(a(\hat{p} - e\hat{A})) + \hat{V}$$

We now write a new Hamiltonian with the electric field f derived from the EM vector potential $\frac{A(t)}{e}$ as opposed to the EM scalar potential $\frac{V(x)}{e}$. We wish to transform to a frame where there is no scalar potential, i.e:

$$\tilde{V} = 0$$

where the former scalar potential is $V(x) = -ef\hat{x}$. As a direct result we are forced to introduce a vector potenial $\tilde{A}$ with geometric phase same as the former dynamic phase:

$$\tilde{A}(t) = A + \frac{\partial \Lambda(x,t)}{\partial x} = \left\{\textbf{Defining the gauge phase } \Lambda(x,t) = V(x)t\right\} = -eft$$

Defining a new position state:

$$|\tilde{x}\rangle = e^{i\Lambda(x,t)}\,|x\rangle$$

The new hamiltonian will then be:

$$\tilde{\mathcal{H}} = 2c\cos(a(\hat{p} - e\tilde{A}(t)) + \tilde{V}(x) = 2c\cos(a(\hat{p} + eft))$$

By solving the classical EOM we obtain the same result as for the former Hamiltonian.

(4) We shall work with the new Hamiltonian, $\tilde{\mathcal{H}} = \mathcal{H}$, and use the fact that the eigenstates are the momentum states ψ_k. Writing Schrodinger equation:

$$\frac{\partial \psi_k}{\partial t} = -i\mathcal{H}\psi_k$$

$$\frac{\partial \psi_k}{\partial t} = -i2c\cos(a(\hat{p} + eft))\psi_k$$

$$\frac{\partial \psi_k}{\partial t} = -i2c\cos(a(k + eft))\psi_k$$

$$\frac{\partial \psi_k}{\psi_k} = -i2c\cos(a(k + eft))\partial t$$

$$\psi_k(t) = \psi_{k,0} \times \mathrm{e}^{-i2c\int_0^t \cos(a(k+eft'))\,\mathrm{d}t'}$$

and consequently:

$$\tilde{\psi}(k,t) = \tilde{\psi}(k,0) \times \mathrm{e}^{-i2c\int\limits_0^t cos(a(k+eft'))\,\mathrm{d}t'}$$

Let us define $\epsilon = aef$, writing:

$$\int\limits_0^t \cos(ak + \epsilon t')\,\mathrm{d}t' = \frac{1}{\epsilon}(\sin(ak + \epsilon t) - \sin(ak)) = \frac{2}{\epsilon}\sin(\frac{\epsilon t}{2})\cos(ak + \frac{\epsilon t}{2})$$

the last equation is achieved using trigonometric identity for difference of sines.
The position wavefunction is merely the inverse Fourier transform of the momentum wavefunction:

$$\psi(x,t) = 2\pi \int\limits_0^{2\pi/a} \mathrm{e}^{ikx}\tilde{\psi}(k,0) \times \mathrm{e}^{-i\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2})\cos(ak+\frac{\epsilon t}{2})}\mathrm{d}k$$

To find $\tilde{\psi}(k,0)$ we can assume that at $t = 0$ the particle is set at $x = 0$, and use $\psi(x,0) = \sqrt{a}\delta(x)$**.
We see that this is in fact the inverse Fourier transform, so $\tilde{\psi}(k,0) = \frac{\sqrt{a}}{2\pi}$.

Introducing the BesselJ integral:

$$J_n(z) = \frac{1}{2\pi i^n}\int\limits_0^{2\pi} \mathrm{e}^{in\Phi}\mathrm{e}^{iz\cos(\Phi)}\mathrm{d}\Phi$$

Defining:

$$\Phi = ka + \frac{\epsilon t}{2}$$

$$\mathrm{d}k = \frac{\mathrm{d}\Phi}{a}$$

$$z = -\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2})$$

Reffering to $x = na$, we can now rewrite the integral as:

$$\psi(x,t) = \frac{\sqrt{a}}{a}\mathrm{e}^{-i\frac{\epsilon tn}{2}} \int\limits_{\epsilon t/2}^{2\pi+\epsilon t/2} \mathrm{e}^{in\Phi}\mathrm{e}^{z\cos(\Phi)}\mathrm{d}\Phi = \frac{1}{\sqrt{a}}J_n(-\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2})) \times \mathrm{e}^{-i\frac{\epsilon tn}{2}}$$

The integrand is a periodic function, therefore only the limits' difference matters and we get the Bessel function.

Using **:

$$\psi_n(t) = \sqrt{a}\psi(x,t) = J_n(-\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2})) \times \mathrm{e}^{-i\frac{\epsilon tn}{2}}$$

Noting that $c < 0$.

$$\rho_n(t) = |\psi_n(t)|^2 = |J_n(-\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2}))|^2$$

$$\rho(x,t) = |\psi(x,t)|^2 = \frac{1}{a}|J_{x/a}(-\frac{4c}{\epsilon}\sin(\frac{\epsilon t}{2}))|^2$$

For a more general result, one can change $n = n - n_0$ where n_0 is the original site at $t = 0$.

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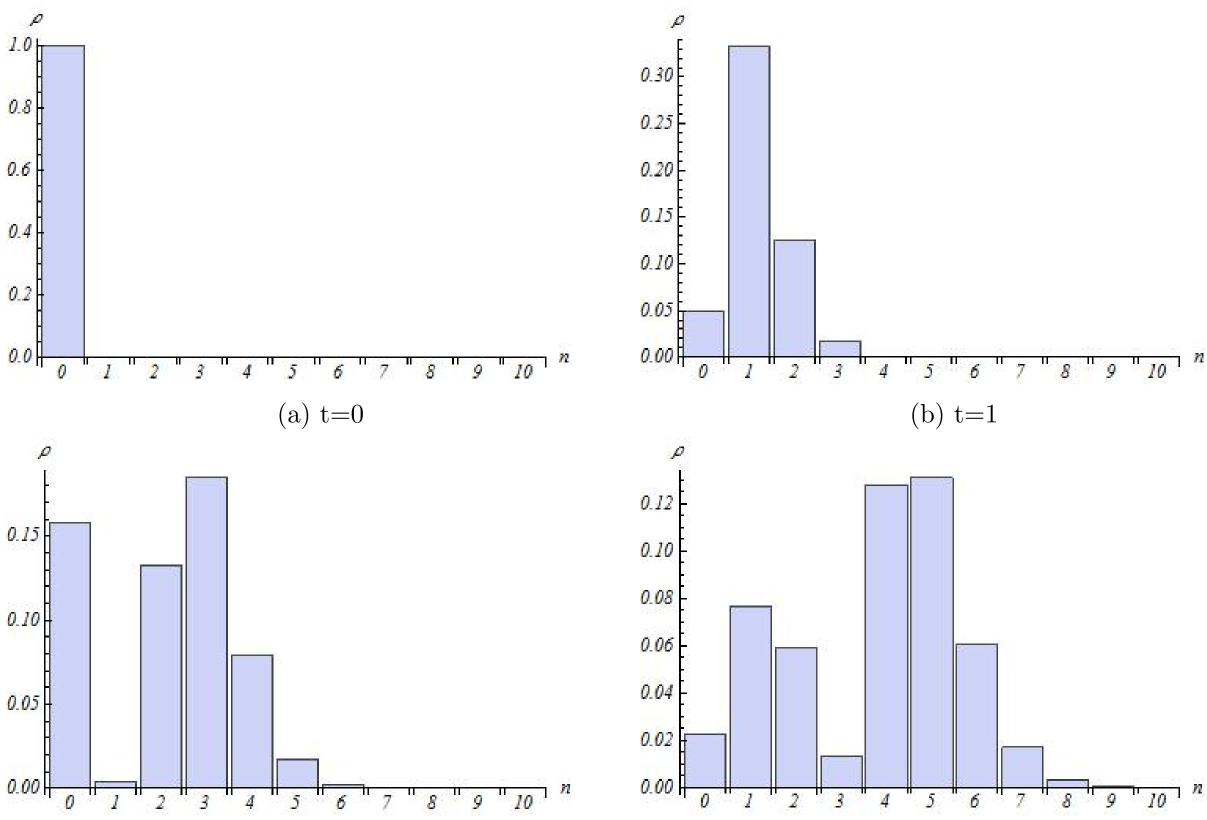
$$\psi(x,0) = \frac{1}{\sqrt{a}}\psi_x(0) = \frac{1}{\sqrt{a}}\delta_{x,0} = \frac{1}{\sqrt{a}}\delta(x)a$$

(5) The Solution for $\rho(x,t)$ in the zero field limit will be:

$$\lim_{\epsilon\to 0}\rho(x,t) = \lim_{\epsilon\to 0}\frac{1}{a}|J_{x/a}(-2ct\,\mathrm{sinc}(\epsilon t))|^2 = \frac{1}{a}|J_{x/a}(-2ct)|^2$$

Taking $a = -c = 1$ we plot the probability distribution in eleven sites (0 to 10) in 4 different times 0 to 3:



(a) t=0

(b) t=1

(c) t=2

(d) t=3

Figure 1: Spreading profile of the probability distribution in the zero field limit

It is noticeable that for $t = 0$ the particle is situated at $n = 0$ as expected, and as time progresses the probability for the particle to be in other sites exists. The further the site is from the initial position, the lower the probability to find the particle in that site, again as expected. If we concentrate on the "position" of the particle (taken as the highest column) it looks as if it will oscillate between the sites. Alternatively, we may concentrate on the lowest column which is trailing the leading column, traveling at more or less constant speed through the sites. It acts like a string node, given enough time, the particle gains probabilities of appearing before or after it.

(6) Bessel functions can be characterized into two regimes, the first is where the argument is smaller then the index of the specific Bessel function, there the amplitude is stable and corresponds to the relation between them. The second is where the argument is larger than the index, there the amplitude decreases exponentially. We recognize the effective spatial amplitude of the probability oscillation in the sites with the former, where $|J_n(z)|^2$ is the functional dependence of ρ on site and time. This produces the following condition:

$$\frac{4c}{\epsilon} > \frac{x}{a}$$

Deriving the result:

$$x < \frac{4ac}{\epsilon}$$

Which is in agreement (up to a factor of 2) with the classical spatial amplitude $\frac{2ac}{\epsilon}$.