Dynamics of Bloch electrons

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1. Introduction

The dynamics of the Bloch electrons are determined by simple relations

$$\hbar \dot{\boldsymbol{k}} = \boldsymbol{F} = -e(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}),$$

where $\boldsymbol{F}$ is the Lorentz force, $\boldsymbol{E}$ and $\boldsymbol{B}$ are the electric field and the magnetic field. The velocity v is given by

$$\boldsymbol{v} = \dot{\boldsymbol{r}} = \boldsymbol{v}_k = \frac{1}{\hbar}\nabla_k \varepsilon_k$$

where $\mathbf{v}_\mathbf{k}$ is the group velocity. The wavevector $\boldsymbol{k}$ is the quantum number which describes a Bloch state.

It is surprising that these results are so simple and elegant, in spite of the fact that the wavefunction of the Bloch electrons is given by

$$\psi_k(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_k(\boldsymbol{r}).$$

We can use the above equations for the discussion of the motion of Bloch electrons. Nevertheless, here we discuss the validity of such a simple equation, under the basis of the quantum mechanics.

2. Derivation of group velocity I

For free electrons, we have

$$m\boldsymbol{v} = \hbar \boldsymbol{k}.$$

This relation is not valid for the Bloch electrons. The electron experiences a large and rapidly fluctuating force as it moves through the periodic potential, so that its instantaneous velocity and momentum likewise fluctuate rapidly. However, its mean velocity, averaged over a unit cell, is well-defined, and is given by

$$\langle \boldsymbol{v} \rangle = \int \psi^* \frac{\boldsymbol{p}}{m} \psi d^3 \boldsymbol{r}$$
$$= \frac{i}{\hbar} \int \psi^* [H, \boldsymbol{r}] \psi d^3 \boldsymbol{r}$$

Here we use the commutation relation of the quantum mechanics,

$$[\boldsymbol{r}, H] = \frac{i\hbar}{m} \boldsymbol{p}\,, \qquad \frac{\boldsymbol{p}}{m} = \frac{i}{\hbar} [H, \boldsymbol{r}]$$

where H is the Hamiltonian and is defined by

$$H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})\,.$$

When the wavefunction of the Bloch electron is given by

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r})$$

we get

$$\langle \boldsymbol{v} \rangle = \frac{i}{\hbar} \int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}{}^*(\boldsymbol{r}) [H, \boldsymbol{r}] e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r}) d^3 \boldsymbol{r}$$

Here we note that

(i) the property (I)

$$\nabla_k [e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}}] = -ie^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{r} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + ie^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H \boldsymbol{r} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$
$$= ie^{-i\boldsymbol{k}\cdot\boldsymbol{r}} [H, \boldsymbol{r}] e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

and

(ii) the property (II)

$$H(\boldsymbol{p},\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}H(\boldsymbol{p}+\boldsymbol{k},\boldsymbol{r})$$

which is derived from the relation

$$\boldsymbol{p}[e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\phi(\boldsymbol{r})] = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\boldsymbol{p}+\boldsymbol{k})\phi(\boldsymbol{r})$$

for any $\phi(\mathbf{r})$. Then the velocity can be rewritten as

$$\begin{aligned}
\langle \boldsymbol{v} \rangle &= \frac{i}{\hbar}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}[H,\boldsymbol{r}]e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} \\
&= \frac{1}{\hbar}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})\nabla_{k}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}He^{i\boldsymbol{k}\cdot\boldsymbol{r}}]u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} \\
&= \frac{1}{\hbar}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})\nabla_{k}[e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}H(\boldsymbol{p}+\boldsymbol{k},\boldsymbol{r})]u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} \\
&= \frac{1}{\hbar}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})\nabla_{k}[H(\boldsymbol{p}+\boldsymbol{k},\boldsymbol{r})]u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r}
\end{aligned}$$

Here we use the Feynman theorem

$$\frac{\partial}{\partial\lambda}\int \phi_{\lambda}^{*}(\boldsymbol{r})H(\lambda)\phi_{\lambda}(\boldsymbol{r})d\boldsymbol{r} = \int \phi_{\lambda}^{*}(\boldsymbol{r})\frac{\partial H(\lambda)}{\partial\lambda}\phi_{\lambda}(\boldsymbol{r})d\boldsymbol{r}$$

Then we have

$$\begin{aligned}
\langle \boldsymbol{v} \rangle &= \frac{1}{\hbar}\nabla_{k}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})H(\boldsymbol{p}+\boldsymbol{k},\boldsymbol{r})u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} \\
&= \frac{1}{\hbar}\nabla_{k}\int u_{\boldsymbol{k}}^{*}(\boldsymbol{r})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}He^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} \\
&= \frac{1}{\hbar}\nabla_{k}\int \psi_{\boldsymbol{k}}^{*}(\boldsymbol{r})H\psi_{\boldsymbol{k}}(\boldsymbol{r})d^{3}\boldsymbol{r} = \frac{1}{\hbar}\nabla_{k}\varepsilon_{\boldsymbol{k}}
\end{aligned}$$

This expression leads to a surprisingly simple result;

$$\langle \boldsymbol{v} \rangle = v_{n}(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{k}\varepsilon_{n}(\boldsymbol{k}).$$

This velocity is called the group velocity. Since

$$d\varepsilon = v_n(\boldsymbol{k}) \cdot d\boldsymbol{k},$$

the wavevector d$\boldsymbol{k}$ on the constant energy surface (dε = 0) is perpendicular to the group velocity;

$$d\varepsilon = v_n(\boldsymbol{k}) \cdot d\boldsymbol{k} = 0.$$

In other words, the group velocity is normal to the surface of $\varepsilon_{\mathbf{k}}$ = constant.

3. Derivation of the group velocity II

We start with the Schrodinger equation for the Bloch electron,

$$H\psi_k(\boldsymbol{r}) = [-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})]\psi_k(\boldsymbol{r}) = \varepsilon_k \psi_k(\boldsymbol{r}),$$

where

$$\psi_k(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_k(\boldsymbol{r}),$$

$V(\boldsymbol{r})$ is a periodic potential. We note that

$$\begin{aligned}\nabla^2\psi_k(\boldsymbol{r}) &= \nabla^2[e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_k(\boldsymbol{r})] \\ &= e^{i\boldsymbol{k}\cdot\boldsymbol{r}}[-k^2 u_k(\boldsymbol{r}) + \nabla^2 u_k(\boldsymbol{r}) + 2i\boldsymbol{k}\cdot\nabla u_k(\boldsymbol{r})]\end{aligned}$$

$$(\nabla + i\boldsymbol{k})^2 u_k(\boldsymbol{r}) = [-k^2 u_k(\boldsymbol{r}) + \nabla^2 u_k(\boldsymbol{r}) + 2i\boldsymbol{k}\cdot\nabla u_k(\boldsymbol{r})]$$

and

$$\nabla^2\psi_k(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\nabla + i\boldsymbol{k})^2 u_k(\boldsymbol{r})$$

Then we get the Schrödinger equation for $u_{\mathbf{k}}(\mathbf{r})$,

$$[-\frac{\hbar^2}{2m}\nabla^2 + V(r)]\psi_k(r) = [-\frac{\hbar^2}{2m}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\nabla + i\boldsymbol{k})^2 u_{\boldsymbol{k}}(\boldsymbol{r}) + V(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_k(\boldsymbol{r})]$$
$$= \varepsilon_k e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_k(\boldsymbol{r})$$

or

$$[-\frac{\hbar^2}{2m}(\nabla + i\boldsymbol{k})^2 + V(\boldsymbol{r})]u_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r})$$

or simply,

$$H_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_k u_k(\boldsymbol{r}) \qquad (1)$$

with

$$H_k = -\frac{\hbar^2}{2m}(\nabla + i\boldsymbol{k})^2 + V(\boldsymbol{r})$$

We take an derivative Eq.(1) with respect to $\boldsymbol{k}$.

$$(H_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}})\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r}) = -[\nabla_k(H_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}})]u_{\boldsymbol{k}}(\boldsymbol{r})$$
$$= [\frac{i\hbar^2}{m}(\nabla + i\boldsymbol{k}) + \nabla_k\varepsilon_{\boldsymbol{k}}]u_{\boldsymbol{k}}(\boldsymbol{r})$$

The velocity $\boldsymbol{v}_{\mathrm{k}}$ is evaluated as

$$\langle \boldsymbol{v} \rangle = \boldsymbol{v}_k = \frac{\hbar}{im}\int e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}^{\ *}(\boldsymbol{r})\nabla[e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r})]d^3\boldsymbol{r}\,.$$

Since

$$\nabla e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}(\nabla + i\boldsymbol{k})u_{\boldsymbol{k}}(\boldsymbol{r})$$

we have

$$\hbar \boldsymbol{v}_k = -\frac{i\hbar^2}{m}\int u_{\boldsymbol{k}}{}^*(\boldsymbol{r})(\nabla + i\boldsymbol{k})u_{\boldsymbol{k}}(\boldsymbol{r})d^3\boldsymbol{r}$$

or

$$\begin{aligned}\hbar \boldsymbol{v}_k &= -\int u_{\boldsymbol{k}}{}^*(\boldsymbol{r})\frac{i\hbar^2}{m}(\nabla + i\boldsymbol{k})u_{\boldsymbol{k}}(\boldsymbol{r})d^3\boldsymbol{r} \\ &= -\int u_{\boldsymbol{k}}{}^*(\boldsymbol{r})[(H_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}})\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r}) - (\nabla_k \varepsilon_{\boldsymbol{k}})u_{\boldsymbol{k}}(\boldsymbol{r})]d^3\boldsymbol{r} \\ &= \nabla_k \varepsilon_{\boldsymbol{k}}\int u_{\boldsymbol{k}}{}^*(\boldsymbol{r})u_{\boldsymbol{k}}(\boldsymbol{r})d^3\boldsymbol{r} - \int u_{\boldsymbol{k}}{}^*(\boldsymbol{r})[(H_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}})\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r})d^3\boldsymbol{r} \\ &= \nabla_k \varepsilon_{\boldsymbol{k}}\end{aligned}$$

using the relation

$$\frac{i\hbar^2}{m}(\nabla + i\boldsymbol{k})u_{\boldsymbol{k}}(\boldsymbol{r}) = (H_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}})\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}(\boldsymbol{r}) - (\nabla_k \varepsilon_{\boldsymbol{k}})u_{\boldsymbol{k}}(\boldsymbol{r})$$

Note that the integral vanishes because of the Hermitian nature of $H_{\mathbf{k}}$.

4. **Mathematica**

```
Clear["Global`*"]; Needs["VectorAnalysis`"];
SetCoordinates[Cartesian[x, y, z]]; K = {kx, ky, kz};
R = {x, y, z}; ψ[x_, y_, z_] := Exp[i (K.R)] u[x, y, z];
eq11 = Laplacian[ψ[x, y, z]] // Simplify;

eq12 = Grad[ψ[x, y, z]] // Simplify
```

$$\left\{e^{i\,(kx\,x+ky\,y+kz\,z)}\left(i\,kx\,u[x,\,y,\,z]+u^{(1,0,0)}[x,\,y,\,z]\right),\right.$$
$$e^{i\,(kx\,x+ky\,y+kz\,z)}\left(i\,ky\,u[x,\,y,\,z]+u^{(0,1,0)}[x,\,y,\,z]\right),$$
$$\left.e^{i\,(kx\,x+ky\,y+kz\,z)}\left(i\,kz\,u[x,\,y,\,z]+u^{(0,0,1)}[x,\,y,\,z]\right)\right\}$$

```
L1 := (Grad[#] + i K #) &; L1x := (D[#, x] + i kx #) &;
L1y := (D[#, y] + i ky #) &; L1z := (D[#, z] + i kz #) &;
A1 = L1[u[x, y, z]] // Simplify;
eq2 = L1x[A1[[1]]] + L1y[A1[[2]]] + L1z[A1[[3]]] //
  Simplify
```

$$-\left(kx^2+ky^2+kz^2\right)u[x,\,y,\,z]+$$
$$2\,i\,kz\,u^{(0,0,1)}[x,\,y,\,z]+u^{(0,0,2)}[x,\,y,\,z]+$$
$$2\,i\,ky\,u^{(0,1,0)}[x,\,y,\,z]+u^{(0,2,0)}[x,\,y,\,z]+$$
$$2\,i\,kx\,u^{(1,0,0)}[x,\,y,\,z]+u^{(2,0,0)}[x,\,y,\,z]$$

```
eq3 = eq11 - e^(i (K.R)) eq2 // Simplify
```

0

5. Derivation of acceleration theorem (I)

The work done on the electron (-*e*) by the electric field $\boldsymbol{E}$ in the interval Δt is

$$\Delta W = (-e)\boldsymbol{E}\cdot\Delta\boldsymbol{r} = (-e)\boldsymbol{E}\cdot\boldsymbol{v}_g\Delta t\,.$$

The change of the kinetic energy in the electron is

$$\Delta K = \hbar\boldsymbol{v}_g\cdot\Delta\boldsymbol{k}\,.$$

Using the work-energy theorem ($\Delta K = \Delta W$), we have

$$\hbar\boldsymbol{v}_g\cdot\Delta\boldsymbol{k} = (-e)\boldsymbol{E}\cdot\boldsymbol{v}_g\Delta t$$

or

$$\frac{d\boldsymbol{k}}{dt} = \boldsymbol{F} = (-e)\boldsymbol{E}$$

which is the same relation as for free electrons. We may write this equation for the motion of an electron in the presence of an electric field $\boldsymbol{E}$ and a magnetic field $\boldsymbol{B}$. According to the Newton's second law, we get

$$\frac{d\boldsymbol{p}}{dt} = \hbar\frac{d\boldsymbol{k}}{dt} = \boldsymbol{F} = -e(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v}_k \times \boldsymbol{B})$$

where $\boldsymbol{F}$ is the Lorentz force, (-e) is the charge of electron and $\mathbf{v}_k$ is the group velocity of the electron.

6. Derivation of acceleration theorem (II)

We consider the Hamiltonian of an electron on a loop of wire with the distance L, is given by

$$H = \frac{1}{2m}(p + \frac{e}{c}A)^2 + V(x)$$

where A is a vector potential. The Schrodinger equation of the system is given by

$$H\psi(x) = [\frac{1}{2m}(p + \frac{e}{c}A)^2 + V(x)]\psi(x) = \varepsilon\psi(x)$$

$$\psi(x + L) = \psi(x)$$

Where $\psi(x)$ is the wavefunction. We introduce a new wave function defined by

$$\psi(x) = \exp(-\frac{ieAx}{\hbar c})\phi(x)$$

The substitution of this new wavefunction into the original Schrodinger equation leads to

$$[\frac{1}{2m}p^2 + V(x)]\phi(x) = \varepsilon\phi(x)$$

The wavefunction $\phi(x)$ is actually the Bloch wave function,

$$\phi(x) = e^{ikx} u_k(x)$$

where $u_k(x)$ satisfies the periodic boundary condition. Since

$$\psi(x)\exp(\frac{ieAx}{\hbar c}) = \phi(x) = e^{ikx} u_k(x)$$

and

$$\psi(x+L) = \psi(x)$$

we have

$$\psi(x+L)\exp(\frac{ieA(x+L)}{\hbar c}) = \phi(x+L) = e^{ik(x+L)} u_k(x+L)$$

$$\psi(x)\exp(\frac{ieAx}{\hbar c}) = \phi(x) = e^{ik(x)} u_k(x)$$

From these, we obtain the relation

$$e^{ikL} = \exp(\frac{ieAL}{\hbar c}),$$

or

$$kL = \frac{eAL}{\hbar c} + 2\pi l,$$

or

$$k = \frac{eA}{\hbar c} + \frac{2\pi l}{L}.$$

Since

$$A = -cEt$$

$$k = -\frac{eEt}{\hbar} + \frac{2\pi l}{L}$$

$$\hbar\dot{k} = -eE \qquad \textbf{(Acceleration theorem)}$$

7. Derivation of the acceleration theorem (III)

In the presence of an electric field, the Hamiltonian is given by

$$H = H_0 + e\mathbf{E}\cdot\mathbf{r}$$

where H_0 is the Hamiltonian of the crystal in zero field. We consider any function, which is given by

$$\psi_k(\mathbf{r}) = e^{ik\cdot r}\phi_k(\mathbf{r})$$

where this function is not always the Bloch function. Note that

$$\nabla_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r}) + i\mathbf{r}\psi_{\mathbf{k}}(\mathbf{r}),$$

or

$$\mathbf{r}\psi_{\mathbf{k}}(\mathbf{r}) = -i\nabla_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r}) + ie^{i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r}),$$

Then we have

$$\begin{aligned} H\psi_{\mathbf{k}}(\mathbf{r}) &= H_0\psi_{\mathbf{k}}(\mathbf{r}) + (e\mathbf{E}\cdot\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) \\ &= H_0\psi_{\mathbf{k}}(\mathbf{r}) + e\mathbf{E}\cdot[-i\nabla_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r}) + ie^{i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r})] \\ &= (H_0 + ie^{i\mathbf{k}\cdot\mathbf{r}}e\mathbf{E}\cdot\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}} - ie\mathbf{E}\cdot\nabla_{\mathbf{k}})\psi_{\mathbf{k}}(\mathbf{r}) \\ &= (H_F - ie\mathbf{E}\cdot\nabla_{\mathbf{k}})\psi_{\mathbf{k}}(\mathbf{r}) \end{aligned}$$

Since $\psi_{\mathbf{k}}(\mathbf{r})$ is an arbitrary function, we find that the Hamiltonian can be described by

$$H = H_0 + H_1 - ie\mathbf{E}\cdot\nabla_{\mathbf{k}} = H_F + H_2$$

with

$$H_1 = ie^{i\mathbf{k}\cdot\mathbf{r}}e\mathbf{E}\cdot\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}},$$

$$H_2 = -ie\mathbf{E}\cdot\nabla_{\mathbf{k}}$$

and

$$H_F = H_0 + H_1$$

We consider the eigenvalue problem,

$$H_0\varphi_{\mathbf{k}\gamma} = \varepsilon_k{}^0\varphi_{\mathbf{k}\gamma}$$

where γ denotes the specific band number. From the symmetry of the translation of H_0, $\varphi_{k\gamma}$ can be expressed by the Bloch wave function,

$$\varphi_{\mathbf{k}\gamma}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{k\gamma}(\mathbf{r})$$

Now we calculate the matrix element of H_1

$$H_1\left|\varphi_{\mathbf{k}\gamma}\right\rangle = i\sum_{k'}\left|\varphi_{\mathbf{k}'\delta}\right\rangle\left\langle\varphi_{\mathbf{k}'\delta}\left|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{E}\cdot\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}\right|\varphi_{\mathbf{k}\gamma}\right\rangle$$

With

$$\begin{aligned} i\left\langle\varphi_{\mathbf{k}'\delta}\left|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{E}\cdot\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}\right|\varphi_{\mathbf{k}\gamma}\right\rangle &= i\mathbf{E}\cdot\int d\mathbf{r}u_{\mathbf{k}'\delta}{}^{*}(\mathbf{r})e^{-i\mathbf{k}'\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}}\nabla_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}\gamma}(\mathbf{r}) \\ &= i\mathbf{E}\cdot\int d\mathbf{r}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}u_{\mathbf{k}'\delta}{}^{*}(\mathbf{r})\nabla_{\mathbf{k}}u_{\mathbf{k}\gamma}(\mathbf{r}) \end{aligned}$$

We note that the vector defined by

$$u_{\mathbf{k}'\delta}^{*}(\mathbf{r})\nabla_{\mathbf{k}}u_{\mathbf{k}\gamma}(\mathbf{r})$$

has the full periodicity of the lattice;

$$u_{\mathbf{k}'\delta}^{*}(\mathbf{r})\nabla_{\mathbf{k}}u_{\mathbf{k}\gamma}(\mathbf{r}) = \mathbf{f}(\mathbf{r})$$

with

$$\mathbf{f}(\mathbf{r}+\mathbf{R}) = \mathbf{f}(\mathbf{r})$$

Using the reciprocal lattice vector $\boldsymbol{G}$, the function $\boldsymbol{f}(\boldsymbol{r})$ can be expressed as

$$\boldsymbol{f}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} \boldsymbol{f}_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} \ .$$

Then

$$\begin{aligned}\int d\boldsymbol{r} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}[u_{\boldsymbol{k}'\delta}^{*}(\boldsymbol{r})\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}\gamma}(\boldsymbol{r})] &= \int d\boldsymbol{r} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \sum_{\boldsymbol{G}} \boldsymbol{f}_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} \\ &= \sum_{\boldsymbol{G}} \boldsymbol{f}_{\boldsymbol{G}} \int d\boldsymbol{r} e^{i(\boldsymbol{k}-\boldsymbol{k}'+\boldsymbol{G})\cdot\boldsymbol{r}}\end{aligned}$$

This integral is not zero only when

$$\boldsymbol{k}'-\boldsymbol{k} = \boldsymbol{G}$$

If we choose to work $\boldsymbol{k}$, $\boldsymbol{k}'$ in the first Brillouin zone, we must have

$$\boldsymbol{k}-\boldsymbol{k}' = 0$$

This means that

$$\left\langle \varphi_{\boldsymbol{k}'\delta} \middle| e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{E}\cdot\nabla_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \middle| \varphi_{\boldsymbol{k}\gamma} \right\rangle = 0$$

for

$$\boldsymbol{k}-\boldsymbol{k}' \neq 0$$

It follows that H_F gives inter band mixing between γ and δ. While H_F can cause no change of $\boldsymbol{k}$, the term $-ie\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}$ can cause a change of $\boldsymbol{k}$.

Here we define a set of functions $\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r})$ as the eigenfunctions of

$$H_F\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r})=\varepsilon_{\boldsymbol{k}\gamma}\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r}),$$

where γ denotes the specific band number. Since H_F is invariant under the translation of lattice, $\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r})$ satisfies the Bloch condition; $\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r})$ is in general different from $e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}\gamma}(\mathbf{r})$. The Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\chi(\boldsymbol{r},t)=(H_F-ie\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}})\chi(\boldsymbol{r},t). \qquad (1)$$

We try a solution with

$$\chi(\boldsymbol{r},t)=e^{-i\frac{\varepsilon_{\boldsymbol{k}\gamma}t}{\hbar}}\chi_{\boldsymbol{k}\gamma}(\boldsymbol{r}),$$

where no interband transition is assumed (i.e., within the same band γ). The derivative is

$$i\hbar\frac{\partial}{\partial t}\chi(\boldsymbol{r},t)=(\varepsilon_{\boldsymbol{k}\gamma}+i\hbar\frac{d\boldsymbol{k}}{dt}\cdot\nabla_{k})\chi(\boldsymbol{r},t). \qquad (2)$$

by taking into account of the time dependence of $\boldsymbol{k}$ (k is not a constant of the motion). The comparison between Eqs.(1) and (2) yields

$$\frac{d\mathbf{k}}{dt}=-e\mathbf{E}$$

8. The motion of electron in the presence of $\boldsymbol{B}$

In the absence of $\boldsymbol{E}$ = 0, we have

$$\hbar\frac{d\boldsymbol{k}}{dt}=-\frac{e}{c}\boldsymbol{v}_k\times\boldsymbol{B}.$$

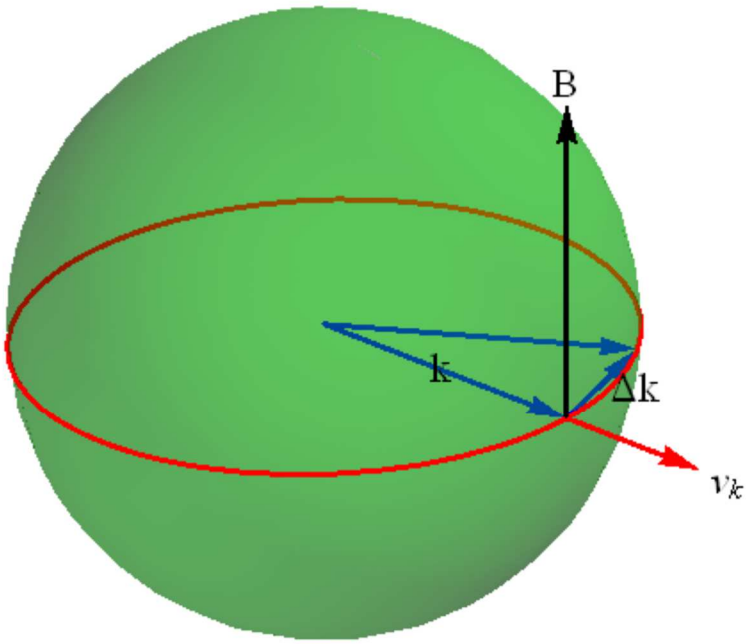
Suppose that $\boldsymbol{B}$ is directed along the z axis. Then we get

$$\hbar \frac{dk_z}{dt} = 0,$$

or

$$k_z = k_{\mathbf{B}} = \text{constant}.$$

where $k_{\mathbf{B}}$ is the component of $\boldsymbol{k}$ parallel to $\boldsymbol{B}$. The motion in the $\boldsymbol{k}$ space is on a plane normal to the direction of $\boldsymbol{B}$, and the orbit is defined by the intersection of this plane with a surface of constant energy, as shown in the figure below.


B
k
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v_k

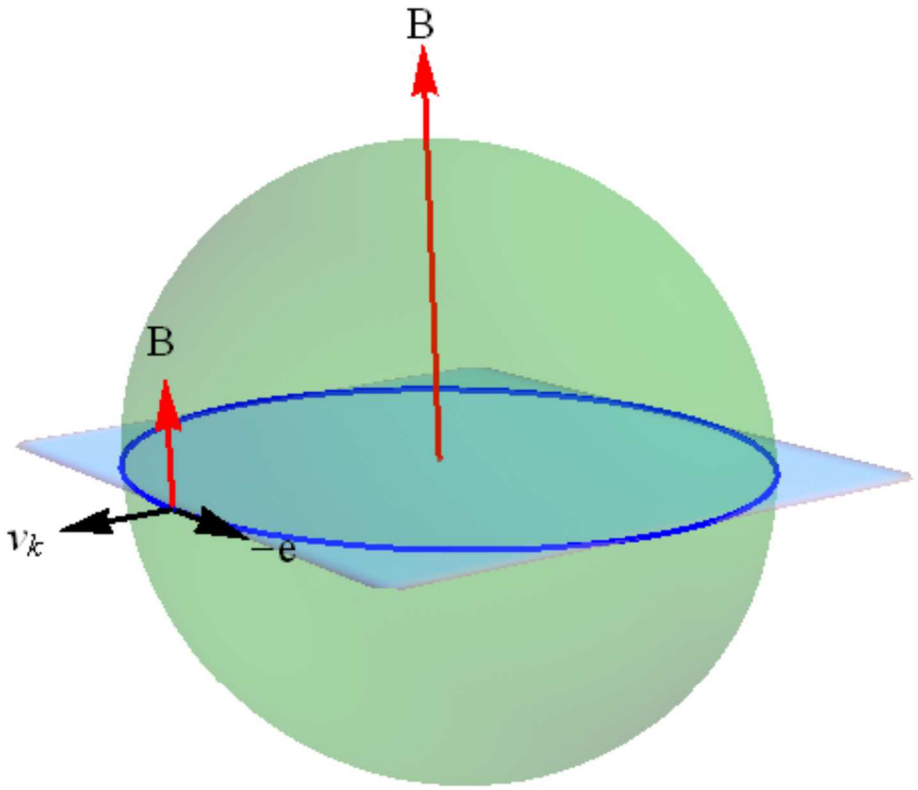


Fig. Motion of electron in the ***k***-space in the presence of the magnetic field (along the *z* axis). We assume the Fermi sphere for the simplicity. The Fermi sphere is filled with electrons. The energy increases toward the exterior. The group velocity is normal to the Fermi surface. When the magnetic field is applied along the *z* axis, the motion of the lectron in the ***k*** space is on a plane normal to the direction of ***B***, and the orbit is defined by the intersection of this plane with a surface of constant energy.

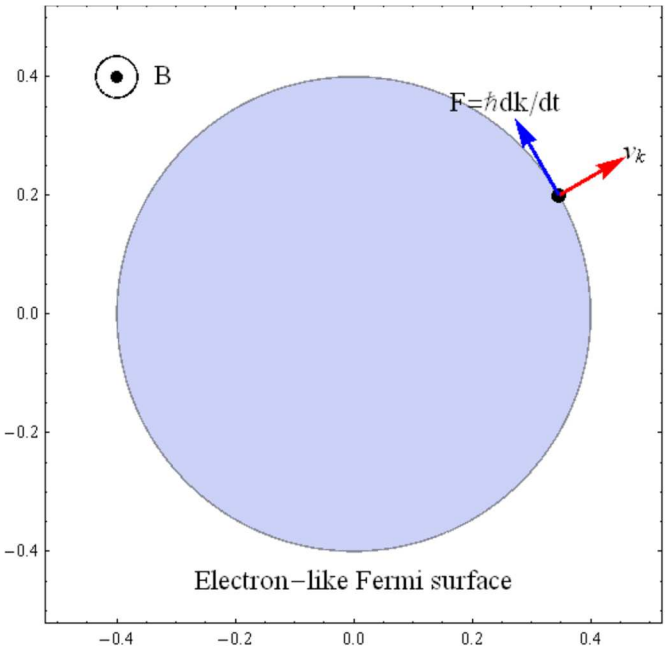


Fig. Top view. Electron-like Fermi surface (the shape of the Fermi surface is sphere). The magnetic field ***B*** is out of the page. The group velocity is normal to the Fermi surface in this figure. The electron rotates counterclockwise in the orbit.

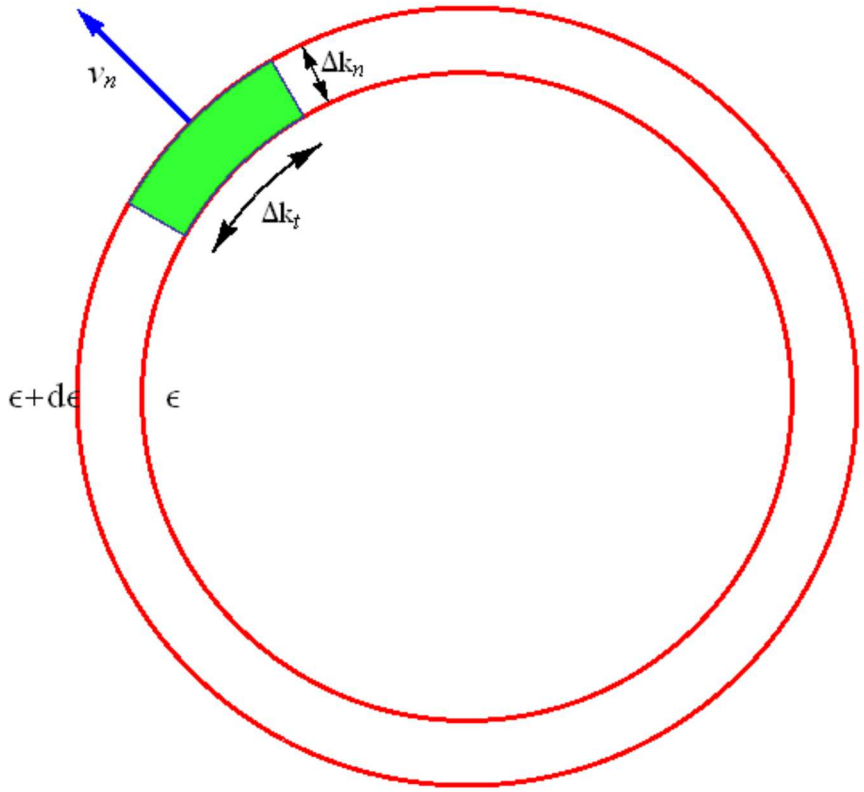


Fig. The area ΔA enclosed between two adjacent orbits on a given slice-plane is given by $\Delta A = \oint \Delta k_n dk_t$. The magnetic field $\boldsymbol{B}$ is applied in a direction (out of the page). $A(\varepsilon, k_B)$ is the area of the orbit which is determined by the energy ε and k_B (the component of $\boldsymbol{k}$ parallel to $\boldsymbol{B}$.

From the above equation, we get

$$c\hbar \Delta k_t = e v_n B \Delta t \,,$$

where k_t is measured around the orbit and v_n is the component of velocity $\boldsymbol{v}_\mathrm{k}$ normal to $\boldsymbol{B}$. The component v_n is defined as

$$v_n = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k_n},$$

where k_n is measured normal to the orbit. Here we define the period T_c, which is the time taken for the electron to travel once around the orbit,

$$\int dt = T_c = \oint \frac{c\hbar dk_t}{eBv_n} = \frac{c\hbar}{eB}\oint \frac{dk_t}{v_n} = \frac{c\hbar^2}{eB}\frac{\partial A(\varepsilon, k_B)}{\partial \varepsilon}.$$

The area ΔA enclosed between two adjacent orbits on a given slice-plane is given by

$$\Delta A = \oint \Delta k_n dk_t .$$

or

$$\frac{\partial A(\varepsilon, k_B)}{\partial \varepsilon} = \oint \frac{\partial k_n}{\partial \varepsilon} dk_t = \oint \frac{dk_t}{\frac{\partial \varepsilon}{\partial k_n}} = \frac{1}{\hbar}\oint \frac{dk_t}{v_n} .$$

The period T is also defined as

$$T = \frac{2\pi}{\omega_c},$$

using the cyclotron (angular) frequency ω_c, defined by

$$\omega_c = \frac{eB}{m^* c} .$$

The effective mass m^* is thus defined as

$$m^* = \frac{\hbar}{2\pi}\oint \frac{dk_t}{v_n} = \frac{\hbar^2}{2\pi}\frac{\partial A(\varepsilon, k_B)}{\partial \varepsilon}$$

For the electron-like Fermi surface, $m^*>0$ and for the hole-like Fermi surface, $m^*<0$. Using the relation

$$\Delta A(\varepsilon) = \hbar\omega_c \frac{\partial A(\varepsilon, k_B)}{\partial \varepsilon} = \frac{2\pi eB}{\hbar c}$$

we can evaluate the degeneracy for the Landau level (we will discuss in the de Haas van Alphen effect)

$$\Delta A(\varepsilon)\frac{L^2}{(2\pi)^2}=\frac{2\pi eB}{\hbar c}\frac{L^2}{(2\pi)^2}=\frac{eBL^2}{2\pi\hbar c}.$$

where L^2 is the area of the system.

((**Note**)) The cyclotron frequency of free electron (classical electricity and magnetism)

$$m\frac{v^2}{r}=\frac{1}{c}evB, \qquad \text{or} \qquad \frac{v}{r}=\frac{eB}{mc}$$

Then the cyclotron frequency is

$$\omega_c=\frac{2\pi}{T}=\frac{v}{r}=\frac{eB}{mc}.$$

9. The motion of Bloch electron in the real space.

As the electron traverses its orbit in ***k***-space, it will at the same time purse a corresponding path through the real space. Since

$$\frac{d\mathbf{r}}{dt}=\mathbf{v}_{\mathbf{k}}$$

we have

$$\frac{d\mathbf{k}}{dt}=-\frac{e}{c\hbar}\frac{d\mathbf{r}}{dt}\times\mathbf{B}$$

so that

$$\mathbf{k}-\mathbf{k}_B=-\frac{e}{c\hbar}(\mathbf{r}-\mathbf{r}_0)\times\mathbf{B}$$

If we choose the direction of B as the z axis, we get

$$x - x_0 = \frac{\hbar c}{eB} k_y , \qquad y - y_0 = -\frac{\hbar c}{eB} k_x$$

or

$$(x - x_0) + i(y - y_0) = \frac{\hbar c}{eB} e^{-i\pi/2} (k_x + ik_y)$$

The orbit in the ***k*** -space is similar to that in the ***r*** - space. The orbit of the real space can be obtained from the rotation of the orbit in the ***k***-space [scaled by the factor ($\hbar c/eB = 1/l^2$)] by $-\pi/2$.

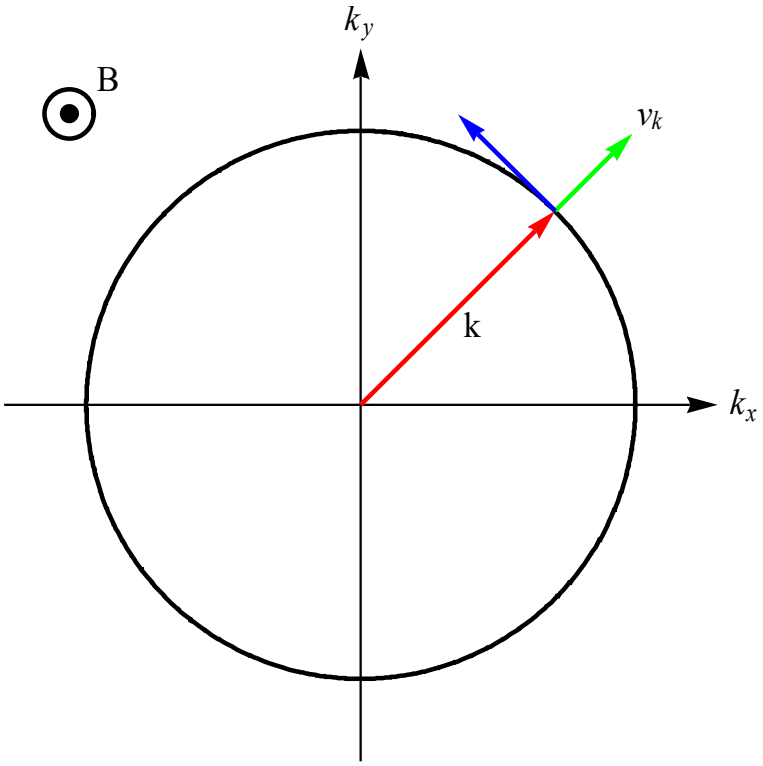


Fig. The motion of Bloch electron in the ***k*** space in the presence of a magnetic field ***B*** which is directed in the direction (out of page)

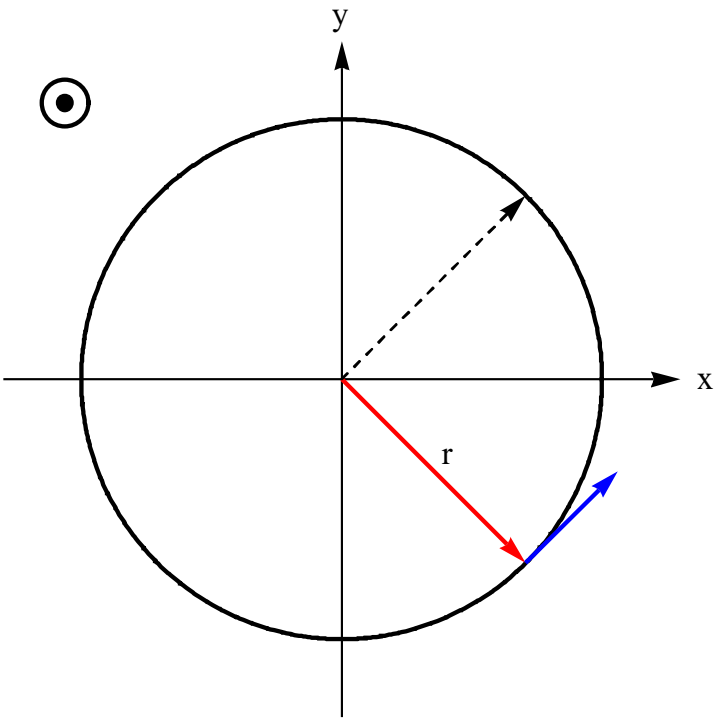


Fig. The motion of Bloch electron in the ***r*** space in the presence of a magnetic field ***B*** which is directed in the direction (out of page)

10 Motion of the hole in the hole-like Fermi surface

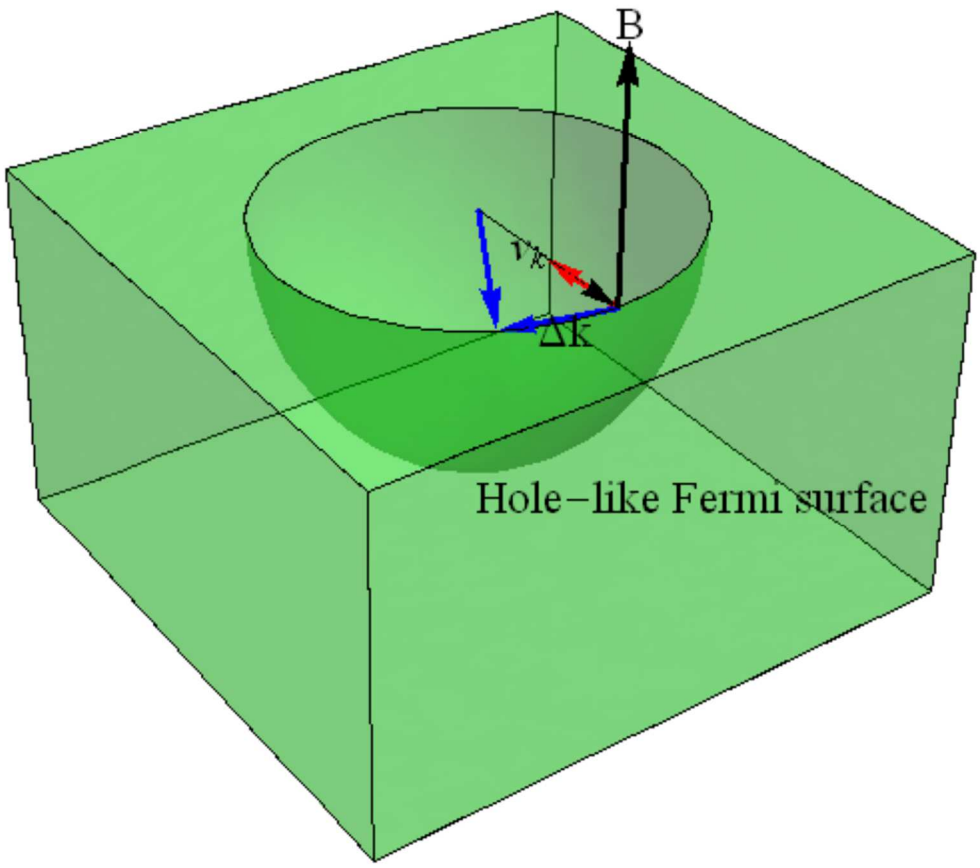


Fig. Cross sectional view of the hole-like Fermi surface (in this case, spherical). The shaded area is filled with electrons. The energy increases toward the exterior. The group velocity is normal to the Fermi surface. In this case, the velocity is directed in a direction from the Fermi surface to the center. When the magnetic field is applied along the z axis, the motion of the lectron in the $\boldsymbol{k}$ space is on a plane normal to the direction of $\boldsymbol{B}$, and the orbit is defined by the intersection of this plane with a surface of constant energy.

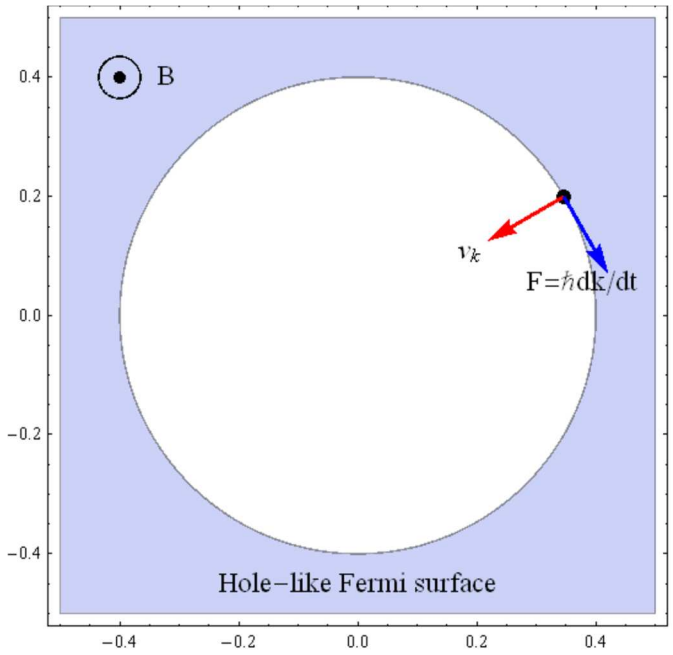


Fig. Hole-like Fermi surface. The magnetic field ***B*** is out of the page.

11. Bloch oscillations

The acceleration theorem. In the presence of a uniform electric field ***E*** the momentum of the wave packet obeys

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F} = (-e)\mathbf{E}\,.$$

The group velocity is

$$\mathbf{v} = \frac{1}{\hbar}\nabla_k \varepsilon_n(\mathbf{k})\,.$$

For the tight binding approximation for the 1D system,

$$\varepsilon_n(\mathbf{k}) = \varepsilon_0 - 2t_0 \cos(ak)\,,$$

where t_0 is in the unites of energy. We use the relation

$$\mathbf{v} = \frac{d\mathbf{r}}{dt}.$$

Then we get

$$k(t) - k(0) = -\frac{eEt}{\hbar}.$$

When $k(0) = 0$, we have

$$k = k(t) = -\frac{eEt}{\hbar}.$$

Since the group velocity is equal to d$\boldsymbol{r}$/dt,

$$v = \frac{dx}{dt} = \frac{1}{\hbar}\frac{\partial \varepsilon(k)}{\partial k} = \frac{2t_0 a}{\hbar}\sin(ak) = -\frac{2t_0 a}{\hbar}\sin(\frac{eaEt}{\hbar})$$

Then the location of the electron oscillates in time as

$$x = \frac{2t_0}{eE}\cos(\frac{eaEt}{\hbar}).$$

The position x oscillates with time.

$$\omega = \frac{eaE}{\hbar}.$$

In order to observe these oscillations, the period of one Bloch oscillation should be less than the relaxation time; $\tau = 10^{-14}$ s at room temperature. For $\omega\tau > 1$, the electric field E should satisfies the condition that

$$E > \frac{\hbar}{\tau ea}$$

For a = 1 Å, $\tau = 10^{-14}$ s, e = 1.602176487 x 10^{-19} C, and $\hbar$ = 1.05457162853 x 10^{-34} J s, E should be larger than 6.6 x 10^{6} V/cm. Thus it is very difficult to observe the Bloch

oscillation in metals. Note that the Bloch oscillations have been detected in a cesium atoms trapped in an optical lattice.

12. Effect of relaxation time

We consider the effect of the relaxation time in the Bloch oscillation.

$$\hbar\frac{dk}{dt} = -eE - \frac{mv}{\tau}$$

and

$$v = \frac{2t_0 a}{\hbar}\sin(ak)\,.$$

We define the dimensionless variables.

$$q = ak\,,$$

$$\frac{dq}{dt} = -\frac{eaE\tau}{\hbar} - \frac{2mt_0 a^2}{\hbar^2}\sin(q) = -\alpha - \beta\sin q\,,$$

where

$$\alpha = \frac{eaE\tau}{\hbar}\,, \qquad \beta = \frac{2mt_0 a^2}{\hbar^2}\,.$$

This equation can be further simplified as

$$\frac{dq}{dt'} = -1 - \frac{\beta}{\alpha}\sin q = -1 - k\sin q\,,$$

where

$$t' = \alpha t = \frac{eaE\tau}{\hbar}t\,.$$

11. Mathematica

We solve the differential equation

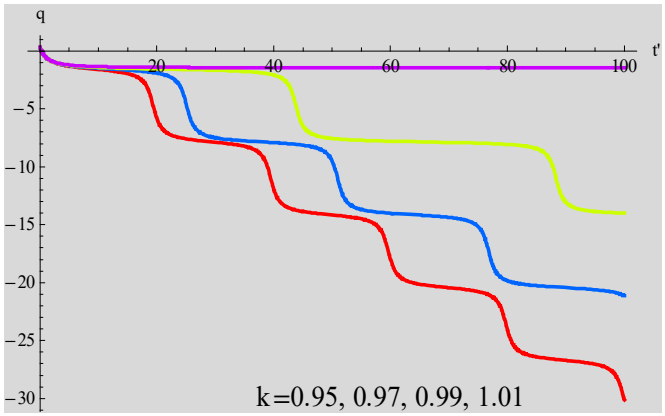
$$\frac{dq}{dt'} = -1 - \frac{\beta}{\alpha}\sin q = -1 - k\sin q\,.$$

with the initial condition $q(t'=0) = q_0$, by using the NDSolve of Mathematica. The choice of the initial condition is almost independent of the time dependence of $q(t')$ and velocity,

$$v(t') = \frac{2t_0 a}{\hbar}\sin(ak) = \frac{2t_0 a}{\hbar}\sin[q(t')]\,.$$

However, the time dependence of $q(t')$ and $v(t')$ is strongly dependent on the choice of the parameter k; k = -1.01 – 1.01 (in the present case).

(1) k = 1.01, 0.99, 0.87, and 0.95.



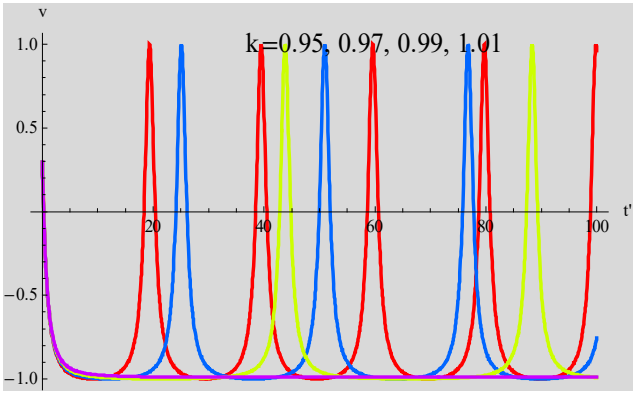


Fig. Time (t') dependence of $q(t')$ and $v(t')$. k = 0.95 (red), 0.97 (blue), 0.99 (yellow), 1.01 (purple). When k is positive and k approaches 1 from the small value of k, the period of the oscillation tends to increases. For k>1.0, no oscillation in $v(t')$ occurs.

(2) $k = 0.8$

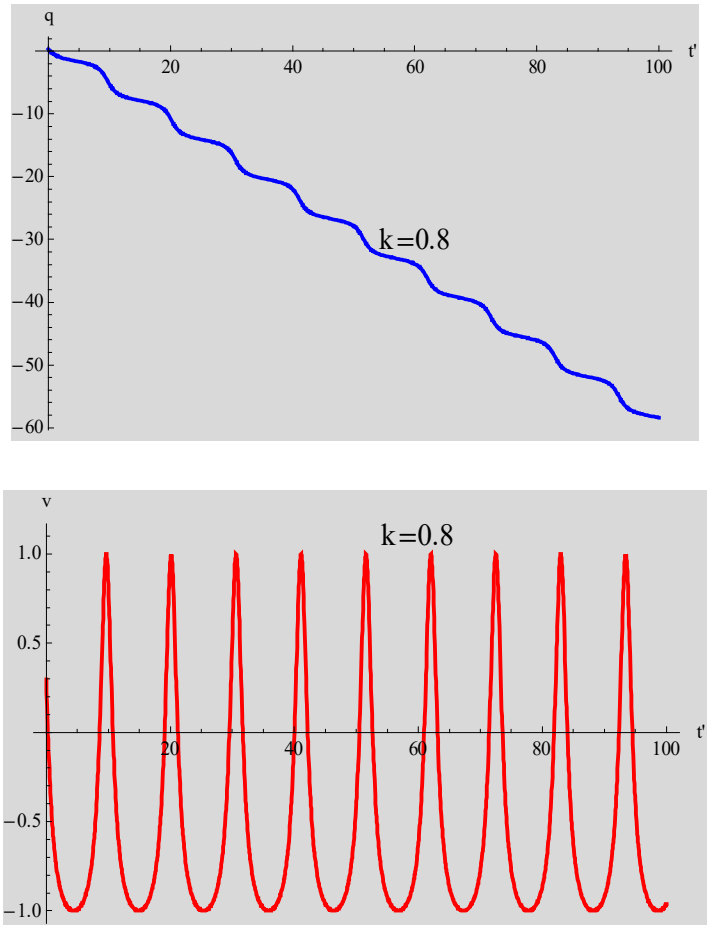


Fig. Time (t') dependence of $q(t')$ and $v(t')$. k = 0.8.

(3) $k = 0$

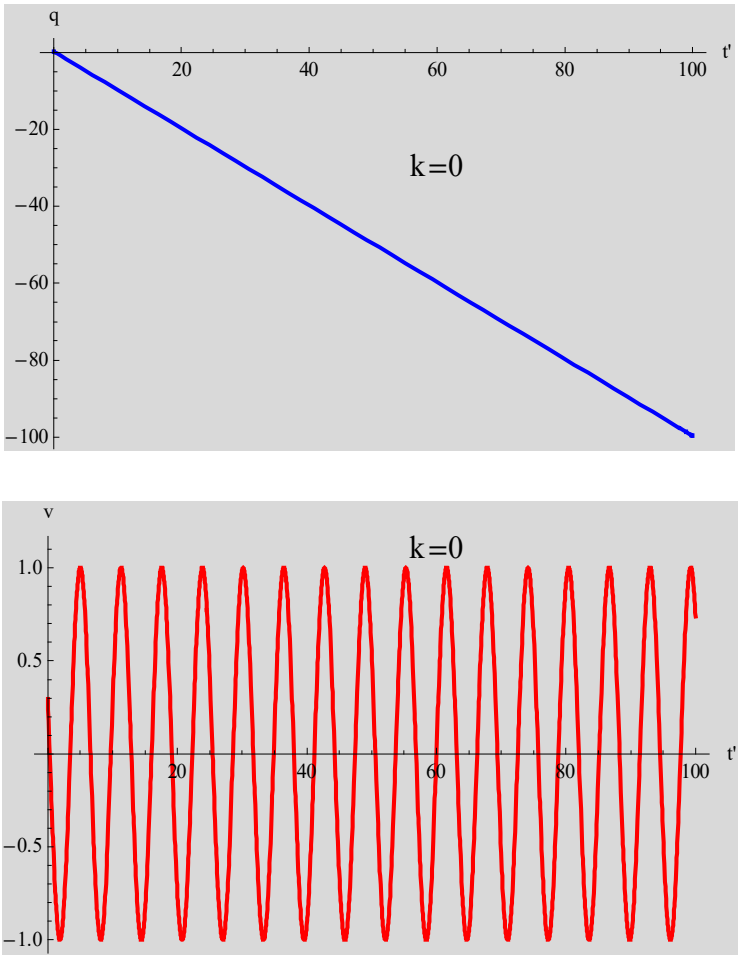
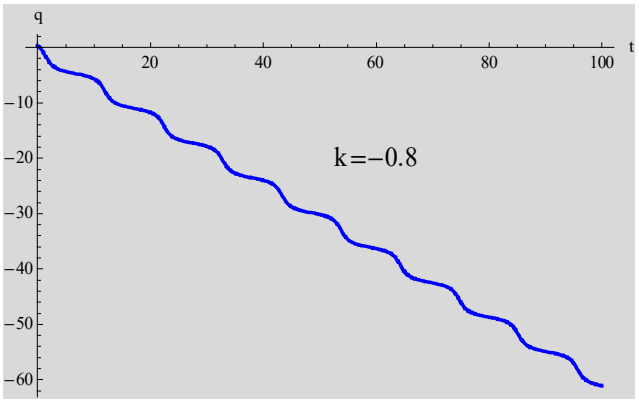


Fig. Time (t') dependence of $q(t')$ and $v(t')$. $k = 0$. $q(t')$ is completely proportional to t'. The oscillation of $v(t')$ is ideally sinusoidal.

(4) $k = -0.8$



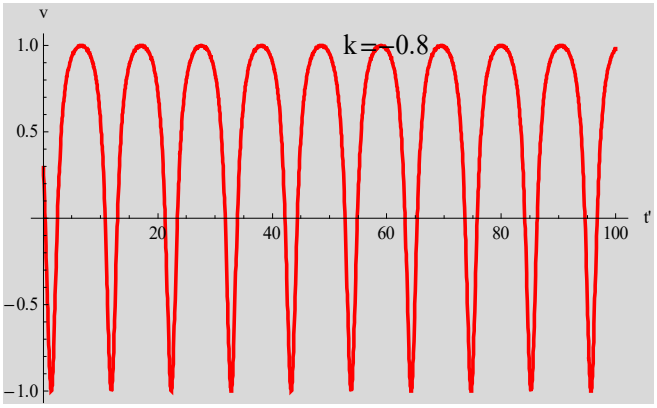
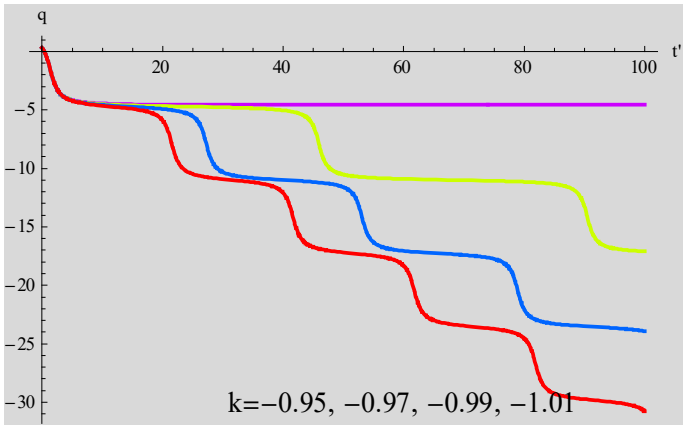


Fig. Time (t') dependence of $q(t')$ and $v(t')$. k = -0.8. $q(t')$ periodically undergoes a step-like change with time t'. The oscillation of $v(t')$ is distorted from the sinusoidal oscillation.

(5) k = -0.95, -0.97, -0.99, and -1.01



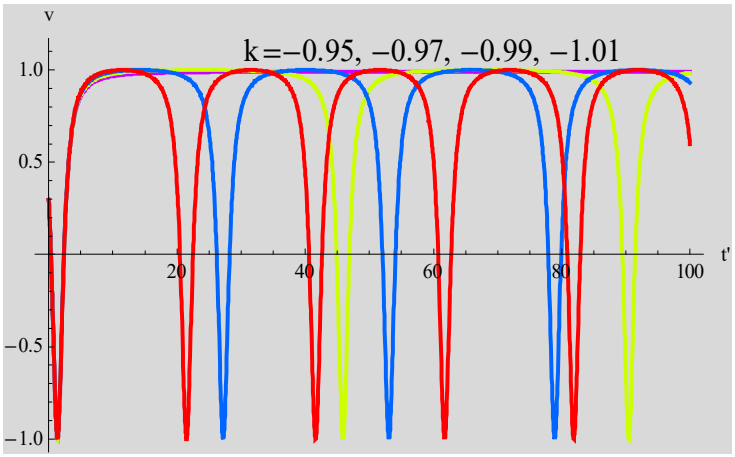
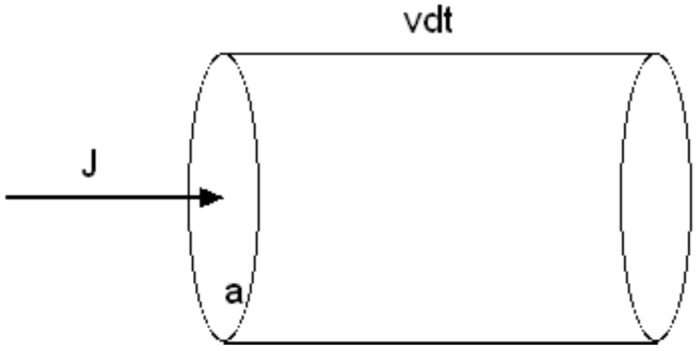


Fig. Time (t') dependence of $q(t')$ and $v(t')$. k = 0.95 (red), 0.97 (blue), 0.99 (yellow), 1.01 (purple). When k is negative and $|k|$ approaches 1 from the small value of $|k|$, the period tends to increases. For $|k|>1.0$, no oscillation in $v(t')$ occurs.

APPENDIX

1. Quantum mechanics: probability current density



First we consider the particles number flowing per unit area per unit time, ***J***:

$$Jadt = |\psi(\mathbf{r},t)|^2 avdt$$

where v is the velocity of each particle and a is the area of cross section. The probability density is

$$\rho(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 ,$$

where $\psi(\mathbf{r},t)$ is the wavefunction. The integral

$$\int \rho(r,t)d^3\mathbf{r} = \int |\psi(\mathbf{r},t)|^2 d^3\mathbf{r},$$

taken over some finite volume Ω, is the probability of finding the particle in this volume. Let us calculate the derivative of the probability with respect to time t.

$$\begin{aligned}\frac{\partial}{\partial t}\int |\psi(\mathbf{r},t)|^2 d^3\mathbf{r} &= \int (\frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t})d^3\mathbf{r} \\ &= -\frac{1}{i\hbar}\int [(H^*\psi^*)\psi - \psi^*(H\psi)]d^3\mathbf{r}\end{aligned}$$

Here the Schrodinger equation is given by

$$i\hbar\frac{\partial \psi}{\partial t} = H\psi .$$

The complex conjugate of this equation is

$$-i\hbar\frac{\partial \psi^*}{\partial t} = H^*\psi^* = H\psi^* .$$

Since

$$H^* = H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$$

we get

$$\begin{aligned}(H^*\psi^*)\psi - \psi^*(H\psi) &= (H\psi^*)\psi - \psi^*(H\psi) \\ &= \{[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})]\psi^*\}\psi - \psi^*\{[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})]\psi\}\end{aligned}$$

or

$$(H^*\psi^*)\psi - \psi^*(H\psi) = -\frac{\hbar^2}{2m}[(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)].$$

Then we have

$$\frac{\partial}{\partial t}\int |\psi(\mathbf{r},t)|^2 d^3\mathbf{r} = \frac{\hbar}{2mi}\int [(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)]d^3\mathbf{r}$$

Note that

$$(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi) = \nabla\cdot(\psi\nabla\psi^* - \psi^*\nabla\psi)$$

((**Proof**))

We use the formula of vector analysis.

$$\nabla\cdot(\phi\mathbf{a}) = \nabla\phi\cdot\mathbf{a} + \phi\nabla\cdot\mathbf{a}$$

$$\nabla\cdot(\psi\nabla\psi^*) = \nabla\psi\cdot\nabla\psi^* + \psi\nabla^2\psi^*$$

The complex conjugate of the above equation

$$\nabla\cdot(\psi^*\nabla\psi) = \nabla\psi^*\cdot\nabla\psi + \psi^*\nabla^2\psi$$

Thus

$$(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi) = \nabla\cdot(\psi\nabla\psi^* - \psi^*\nabla\psi)$$

Then

$$\frac{\partial}{\partial t}\int |\psi(\mathbf{r},t)|^2 d^3\mathbf{r} == -\frac{1}{i\hbar}\int [(H^*\psi^*)\psi - \psi^*(H\psi)]d^3\mathbf{r}$$
$$= \frac{\hbar}{2mi}\int \nabla\cdot(\psi\nabla\psi^* - \psi^*\nabla\psi)d^3\mathbf{r}$$

We note that

$$\int \frac{\partial}{\partial t}\rho d\mathbf{r} = -\int \nabla \cdot \mathbf{J} d\mathbf{r} = -\int \mathbf{J} \cdot d\mathbf{a} \qquad \text{(Gauss's theorem)}$$

or

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \mathbf{J} = 0 \qquad \text{(Equation of continuity)}$$

Then the probability current density can be defined as

$$\mathbf{J} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*) = \frac{1}{m}\mathrm{Re}[\langle \psi | \mathbf{p} | \psi \rangle]$$

since

$$\begin{aligned}\mathbf{J} &= \frac{1}{m}\mathrm{Re}[\langle \psi | \mathbf{p} | \psi \rangle] \\ &= \frac{1}{2m}(\psi^* \frac{\hbar}{i}\nabla \psi - \psi \frac{\hbar}{i}\nabla \psi^*) \\ &= \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*) = -\frac{i\hbar}{2m}(\psi^* \nabla \psi - \psi \nabla \psi^*)\end{aligned}$$

Suppose that the wavefunction is given by the Bloch wavefunction. Then

$$\begin{aligned}\psi^* \nabla \psi &= e^{-i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}{}^*(\mathbf{r}) \nabla [e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})] \\ &= e^{-i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}{}^*(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} (\nabla + i\mathbf{k}) u_{\mathbf{k}}(\mathbf{r}) \\ &= u_{\mathbf{k}}{}^*(\mathbf{r})(\nabla + i\mathbf{k}) u_{\mathbf{k}}(\mathbf{r})\end{aligned}$$

$$\begin{aligned}\psi \nabla \psi^* &= e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) \nabla [e^{-i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}{}^*(\mathbf{r})] \\ &= e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} (\nabla - i\mathbf{k}) u_{\mathbf{k}}{}^*(\mathbf{r}) \\ &= u_{\mathbf{k}}(\mathbf{r})(\nabla - i\mathbf{k}) u_{\mathbf{k}}{}^*(\mathbf{r})\end{aligned}$$

The probability current density ***J*** is

$$\mathbf{J} = -\frac{i\hbar}{2m}[u_{\mathbf{k}}^{*}(\mathbf{r})(\nabla + i\mathbf{k})u_{\mathbf{k}}(\mathbf{r}) - u_{\mathbf{k}}(\mathbf{r})(\nabla - i\mathbf{k})u_{\mathbf{k}}^{*}(\mathbf{r})]$$
$$= -\frac{i\hbar}{2m}[u_{\mathbf{k}}^{*}(\mathbf{r})(\nabla + i\mathbf{k})u_{\mathbf{k}}(\mathbf{r}) - u_{\mathbf{k}}(\mathbf{r})(\nabla - i\mathbf{k})u_{\mathbf{k}}^{*}(\mathbf{r})]$$

We note that

$$u_{\mathbf{k}}^{*}(\mathbf{r})(\nabla + i\mathbf{k})u_{\mathbf{k}}(\mathbf{r}) = \frac{m}{i\hbar^2}[u_{\mathbf{k}}^{*}(\mathbf{r})(H_{\mathbf{k}} - \varepsilon_{\mathbf{k}})\nabla_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}) - u_{\mathbf{k}}^{*}(\mathbf{r})(\nabla_k\varepsilon_{\mathbf{k}})u_{\mathbf{k}}(\mathbf{r})]$$

$$-u_{\mathbf{k}}(\mathbf{r})(\nabla - i\mathbf{k})u_{\mathbf{k}}^{*}(\mathbf{r}) = \frac{m}{i\hbar^2}[u_{\mathbf{k}}(\mathbf{r})(H_{\mathbf{k}} - \varepsilon_{\mathbf{k}})\nabla_{\mathbf{k}}u_{\mathbf{k}}^{*}(\mathbf{r}) - u_{\mathbf{k}}(\mathbf{r})(\nabla_k\varepsilon_{\mathbf{k}})u_{\mathbf{k}}^{*}(\mathbf{r})]$$

Then we get

$$u_{\mathbf{k}}^{*}(\mathbf{r})(\nabla + i\mathbf{k})u_{\mathbf{k}}(\mathbf{r}) - u_{\mathbf{k}}(\mathbf{r})(\nabla - i\mathbf{k})u_{\mathbf{k}}^{*}(\mathbf{r}) = \frac{m}{i\hbar^2}[u_{\mathbf{k}}^{*}(\mathbf{r})(H_{\mathbf{k}} - \varepsilon_{\mathbf{k}})\nabla_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r})$$
$$+ u_{\mathbf{k}}(\mathbf{r})(H_{\mathbf{k}} - \varepsilon_{\mathbf{k}})\nabla_{\mathbf{k}}u_{\mathbf{k}}^{*}(\mathbf{r}) - 2(\nabla_k\varepsilon_{\mathbf{k}})u_{\mathbf{k}}^{*}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})]$$

Using the relation

$$H_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r}) = \varepsilon_k u_k(\mathbf{r})$$

$$\langle \mathbf{v} \rangle = \int d\mathbf{r}\mathbf{J}(\mathbf{r})$$
$$= (-\frac{i\hbar}{2m})(-\frac{2m}{i\hbar^2})\int d\mathbf{r}(\nabla_k\varepsilon_{\mathbf{k}})u_{\mathbf{k}}^{*}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})]$$
$$= \frac{1}{\hbar}\nabla_k\varepsilon_{\mathbf{k}}\int d\mathbf{r}u_{\mathbf{k}}^{*}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\hbar}\nabla_k\varepsilon_{\mathbf{k}}$$

APPENDIX-II

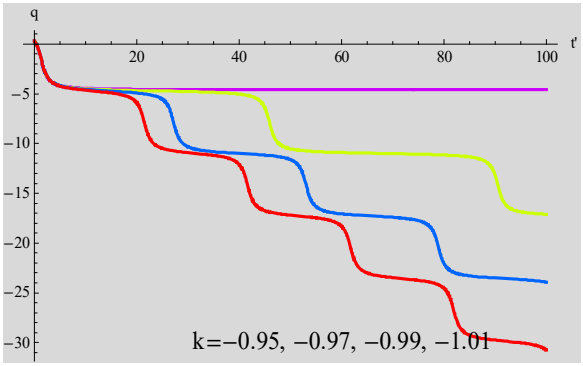
Mathematica program for the Bloch oscillation with finite relaxation time

Bloch oscillations

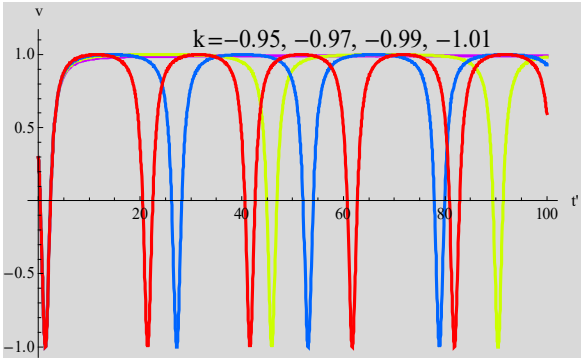
```
Clear["Global`*"];

Blochv[q0_, a1_, tmax_, opts__] :=
 Module[{numsol, numgraph},
  numsol = NDSolve[{ q'[t] == -1 - a1 Sin[q[t]], q[0] == q0}, q[t], {t, 0, tmax}] // Flatten;
  v[t_] := Sin[q[t]] /. numsol;
  numgraph = Plot[Evaluate[v[t]], {t, 0, tmax}, opts, DisplayFunction → Identity]]

Blochq[q0_, a1_, tmax_, opts__] :=
 Module[{numsol, numgraph},
  numsol = NDSolve[{ q'[t] == -1 - a1 Sin[q[t]], q[0] == q0}, q[t], {t, 0, tmax}] // Flatten;
  numgraph = Plot[Evaluate[q[t] /. numsol], {t, 0, tmax}, opts, DisplayFunction → Identity]]
 Gblochq1 =
  Blochq[0.3, #, 100, PlotStyle → {Thick, Hue[30 (-0.95 - #)]}, AxesLabel → {"t'", "q"},
     Background → LightGray, PlotRange → All, DisplayFunction → Identity] & /@ Range[-1.01, -0.95, 0.02];
 g1 = Graphics[{Text[Style["k=-0.95, -0.97, -0.99, -1.01", Black, 15], {60, -30}]}];
 Show[Gblochq1, g1, DisplayFunction → $DisplayFunction]
```




```
 Gblochv1 =
  Blochv[0.3, #, 100, PlotStyle → {Thick, Hue[30 (-0.95 - #)]}, AxesLabel → {"t'", "v"},
     Background → LightGray, PlotRange → All, DisplayFunction → Identity] & /@ Range[-1.01, -0.95, 0.02];
 g1 = Graphics[{Text[Style["k=-0.95, -0.97, -0.99, -1.01", Black, 15], {60, 1.1}]}];
 Show[Gblochv1, g1, DisplayFunction → $DisplayFunction]
```



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