Schroedinger Equation in a $\vec{B}$-field

$$\mathcal{E} = \frac{1}{2m}(\bar{P}\cdot\bar{P}) + V(\vec{r})$$

From Einstein-De Broglie relations, we get

$$\hbar\omega = \frac{\hbar^2}{2m}(\bar{k}\cdot\bar{k}) + V(\vec{r})$$

is NOT a dispersion relation.

$\Rightarrow$ Schroedinger's equation.

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

Steps for formulating the Schroedinger equation from a classical expression:

① Write the classical equation of motion in terms of the canonical momentum, $\bar{P}$, and generalized potential, V:

$$\frac{d\bar{P}}{dt} = -\bar{\nabla}V$$

② Use these quantities to write the energy of the system

$$\mathcal{E} = \frac{\bar{P}\cdot\bar{P}}{2m} + V(r)$$

③ Transform the classical expression into a quantum mechanical one by ~~applying~~ using the Einstein- De Broglie equations.

$$\mathcal{E} = \hbar\omega \Rightarrow i\hbar\frac{\partial}{\partial t}$$

$$p = \hbar k \Rightarrow -i\hbar\bar{\nabla}$$

$V(\vec{r})$ can be a function of time actually.

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r},t)\psi}$$

Schroedinger's Equation

$\boxed{\text{Probability Currents}}$

$\psi(r,t) \Rightarrow \qquad P(r,t) = |\psi(r,t)|^2 = \psi^*(r,t)\psi(r,t)$ Max Born.

$$\int d\vec{r}\, \psi^*(r,t)\psi(r,t) = 1$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

$(\times \psi^*) \Rightarrow \; i\hbar \psi^* \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + V\psi^*\psi$

Take complex conjugate

$$-i\hbar \psi \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + V\psi\psi^*$$

$$\rightarrow \quad i\hbar \frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

But $\forall\, f, \bar{C}$, we have $\quad \bar{\nabla}\cdot(f\bar{C}) = f\bar{\nabla}\cdot\bar{C} + \bar{C}\cdot\bar{\nabla} f$

$$\rightarrow \quad i\hbar \frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\left(\bar{\nabla}\cdot(\psi^*\bar{\nabla}\psi - \psi\bar{\nabla}\psi^*)\right)$$

we define the probability current density

$$\bar{J} = \frac{\hbar}{2mi}\left(\psi^*\bar{\nabla}\psi - \psi\bar{\nabla}\psi^*\right) = \mathrm{Re}\left\{\psi^*\frac{\hbar}{im}\bar{\nabla}\psi\right\}$$

$$\rightarrow \quad \boxed{\frac{\partial P}{\partial t} + \bar{\nabla}\cdot\bar{J} = 0}$$

$\bar{J}$ in an electromagnetic field?

Lorentz's law

$$m\frac{d\bar{v}}{dt} = q\left(\bar{E} + \bar{v}\times\bar{B}\right)$$

$$\downarrow$$

$$\boxed{\frac{d}{dt}\left(\begin{array}{c}\text{canonical}\\ \text{momentum}\end{array}\right) = -\bar{\nabla}\left(\begin{array}{c}\text{externally applied}\\ \text{potential}\end{array}\right)}$$

$\bar{B} = \bar{\nabla}\times\bar{A} \qquad$ since $\bar{\nabla}\cdot\bar{B} = 0$

$\rightarrow$ Faraday's law $\qquad \bar{\nabla}\times\left(\bar{E} + \frac{\partial \bar{A}}{\partial t}\right) = 0$

Since the curl of a gradient of any single-valued scalar field is zero,

$$\bar{E} = -\frac{\partial \bar{A}}{\partial t} - \bar{\nabla}\phi$$

$$m\frac{d\bar v}{dt} = -q\left(\bar\nabla\phi + \frac{\partial \bar A}{\partial t} - \bar v\times(\bar\nabla\times\bar A)\right)$$

$$\frac{d\bar A}{dt} = \frac{\partial \bar A}{\partial t} + (\bar v\cdot\bar\nabla)\bar A$$

$$\Rightarrow \frac{d}{dt}\Big(\underbrace{m\bar v + q\bar A}_{\bar P}\Big) = -q\left[\bar\nabla\phi - (\bar v\cdot\bar\nabla)\bar A - \bar v\times(\bar\nabla\times\bar A)\right]$$

$$\frac{d\bar P}{dt} = -q\bar\nabla\phi + \frac{q}{m}(\bar P\cdot\bar\nabla)\bar A - \frac{q^2}{m}(\bar A\cdot\bar\nabla)A + \frac{q}{m}\bar P\times(\bar\nabla\times\bar A) - \frac{q^2}{m}\bar A\times(\bar\nabla\times\bar A)$$

Use the vector identities

$$\bar C\times(\bar\nabla\times\bar D) = \bar\nabla(\bar C\cdot\bar D) - (\bar C\cdot\bar\nabla)\bar D - (\bar D\cdot\bar\nabla)\bar C - \bar D\times(\bar\nabla\times\bar C)$$

and $\bar C\times(\bar\nabla\times\bar C) = \frac{1}{2}\bar\nabla(\bar C\cdot\bar C) - (\bar C\cdot\bar\nabla)\bar C$

$$\rightarrow \frac{d\bar P}{dt} = -q\bar\nabla\phi + \frac{q}{m}\bar\nabla(\bar P\cdot\bar A) - \frac{q^2}{2m}\bar\nabla(\bar A\cdot\bar A) - \frac{q}{m}(\bar A\cdot\bar\nabla)\bar P - \frac{q}{m}\bar A\times(\bar\nabla\times\bar P)$$

$$\boxed{\frac{d\bar P}{dt} = -\bar\nabla\Big(\underbrace{q\phi - \frac{q}{m}\bar P\cdot\bar A + \frac{q^2}{2m}\bar A\cdot\bar A}_{V}\Big)}$$

$$\underbrace{\bar P}_{\text{Canonical momentum}} = \underbrace{m\bar v}_{\text{kinetic momentum}} + \underbrace{q\bar A}_{\text{Field momentum}}$$

$$\boxed{\mathcal{E} = \frac{P\cdot P}{2m} + \left(q\phi - \frac{q}{m}\bar P\cdot\bar A + \frac{q^2}{2m}\bar A\cdot\bar A\right)}$$

$$\mathcal{E} = \frac{1}{2m}\left(\bar{P} - q\bar{A}\right)\cdot\left(\bar{P} - q\bar{A}\right) + q\phi$$

$$\mathcal{E} \Rightarrow i\hbar\frac{\partial}{\partial t}$$

$$\bar{P} \Rightarrow -i\hbar\bar{\nabla}$$

⇒ Quantum form of Lorentz's law

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\frac{\hbar}{i}\bar{\nabla} - q\bar{A}\right)^2\psi + q\phi\psi}$$

⇒ Probability current of a charge quantum particle in an electromagnetic field

$$\bar{J} = \mathrm{Re}\left\{\psi^*\left(\frac{\hbar}{im}\bar{\nabla} - \frac{q}{m}\bar{A}\right)\psi\right\}$$

Problem 43: Choice of gauge $\vec{A}$, to describe magnetic field $\vec{B} =$ ~~$nablaX\vec{A}$~~ $\vec{\nabla}\times\vec{A}$

To describe electrons in the presence of an external magnetic field, the following Hamiltonian is used

$$H = \frac{(\vec{p} - q\vec{A})^2}{2m} + V(x,y,z), \tag{668}$$

For uniform magnetic field $\vec{B} =$ ~~$nablaX\vec{A}$~~ $\vec{\nabla}\times\vec{A}$ the gauge $\vec{A}$ is typically selected among three gauges:

$$\vec{A} = (-\frac{By}{2}, \frac{Bx}{2}, 0) \tag{669}$$

called the symmetric gauge,

$$\vec{A} = (0, Bx, 0) \tag{670}$$

called the asymmetric gauge, and

$$\vec{A} = (-By, 0, 0) \tag{671}$$

is the Landau gauge.

Each of the three gauges above describe a constant magnetic feild $\vec{B}$ along the z-direction.

Find a way to write a general gauge $\vec{A}$ such that any of the three gauges above can be generated by the approximate selection of a parameter.

Solution:

If we use

$$\vec{A} = [-(1-\xi)By, \xi Bx, 0] \tag{672}$$

for which it is easily shown that

$$\vec{\nabla} x \vec{A} = B\hat{k} \tag{673}$$

where $\hat{k}$ is the unit vector along the z-axis. $\vec{A}$ reduces to the symmetric, asymmetric, and Landau guage for the parameter ξ equal to $\frac{1}{2}$, 1, and 0, respectively.

Landau Levels.
From S. Datta, "Electronic Transport in Mesoscopic Systems" Cambridge (1995).

We consider a rectangular conductor that is uniform in the x-direction and has some transverse confining potential $U(y)$ (see Fig. 1.6.1). The motion of electrons in such a conductor is described by the effective mass equation (see Eq.(1.2.2))

$$\left[E_s + \frac{(i\hbar\nabla + e\mathbf{A})^2}{2m} + U(y)\right]\Psi(x,y) = E\Psi(x,y)$$

We assume a constant magnetic field B in the z-direction perpendicular to the plane of the conductor. This can be represented by a vector potential of the form

$$\mathbf{A} = \hat{x}By \quad \Rightarrow \quad A_x = By \quad \text{and} \quad A_y = 0$$

so that Eq.(1.2.2) can be rewritten as

$$\left[E_s + \frac{(p_x + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(y)\right]\Psi(x,y) = E\Psi(x,y) \tag{1.6.1}$$

where $\qquad p_x \equiv -i\hbar\dfrac{\partial}{\partial x} \quad \text{and} \quad p_y \equiv -i\hbar\dfrac{\partial}{\partial y}$

The solutions to Eq.(1.6.1) can be expressed in the form of plane waves (L: length of conductor over which the wavefunctions are normalized)

$$\Psi(x,y) = \frac{1}{\sqrt{L}}\exp[ikx]\chi(y) \tag{1.6.2}$$

where the transverse function $\chi(y)$ satisfies the equation

$$\left[E_s + \frac{(\hbar k + eBy)^2}{2m} + \frac{p_y^2}{2m} + U(y)\right]\chi(y) = E\chi(y) \tag{1.6.3}$$

Note that the choice of vector potential is not unique for the given magnetic field. For example we could choose $A_x = 0$ and $A_y = -Bx$. The solutions would then look very different though the physics of course must remain the same. It is only with our choice of gauge, that the solutions have the form of plane waves in the x-direction. We will use this gauge in all our discussions.

We are interested in the nature of the transverse eigenfunctions and the eigenenergies for different combinations of the confining potential U and the magnetic field B. In general for arbitrary confinement potentials $U(y)$

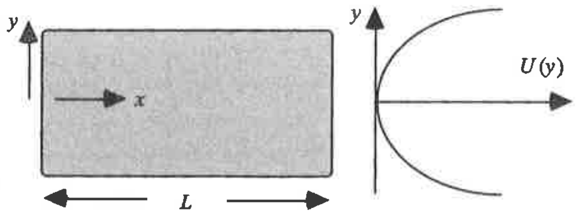

Fig. 1.6.1. A rectangular conductor assumed to be uniform in the x-direction and having some transverse confining potential $U(y)$.

there are no analytical solutions. However, for a parabolic potential (which is often a good description of the actual potential in many electron waveguides)

$$U(y) = \frac{1}{2} m\omega_0^2 y^2$$

analytical solutions can be written down and this is what we will discuss in this section. Later in Chapter 4 we will discuss an approximate solution that can be used at high magnetic fields for arbitrary confining potentials. An interesting discussion of the relation between the quantum mechanical solutions and the classical trajectories can be found in Section 12 of Ref.[1.1].

Confined electrons (U ≠ 0) in zero magnetic field (B = 0)

Consider first the case of zero magnetic field, so that Eq.(1.6.3) reduces to

$$\left[E_s + \frac{\hbar^2 k^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2} m\omega_0^2 y^2\right]\chi(y) = E\chi(y) \tag{1.6.4}$$

The eigenfunctions of Eq.(1.6.4) are well-known (see any quantum mechanics text such as L. I. Schiff (1968), *Quantum Mechanics*, Third Edition, (New York, McGraw–Hill) Section 13). The eigenenergies and eigenfunctions are given by

$$\chi_{n,k}(y) = u_n(q) \quad \text{where} \quad q = \sqrt{m\omega_0/\hbar}\, y \tag{1.6.5a}$$

$$E(n,k) = E_s + \frac{\hbar^2 k^2}{2m} + \left(n + \tfrac{1}{2}\right)\hbar\omega_0, \quad n = 0,1,2,\ldots \tag{1.6.5b}$$

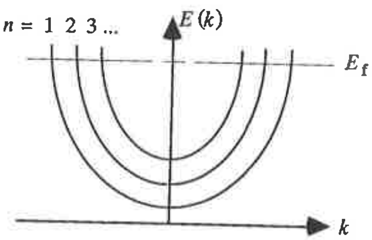

Fig. 1.6.2. Dispersion relation, $E(k)$ vs. k. for electric subbands arising from electrostatic confinement in zero magnetic field. Different subbands are indexed by n.

where
$$u_n(q) = \exp\left[-q^2/2\right]H_n(q)$$

$H_n(q)$ being the nth Hermite polynomial. The first three of these polynomials are

$$H_0(q) = \frac{1}{\pi^{1/4}}, \quad H_1(q) = \frac{\sqrt{2}q}{\pi^{1/4}} \quad \text{and} \quad H_2(q) = \frac{2q^2 - 1}{\sqrt{2}\pi^{1/4}}$$

The velocity is obtained from the slope of the dispersion curve:

$$v(n,k) = \frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k} = \frac{\hbar k}{m} \tag{1.6.5c}$$

The dispersion relation is sketched in Fig. 1.6.2. States with different index n are said to belong to different subbands just like the subbands that arise from the confinement in the z-direction (see Section 1.2). The spacing between two subbands is equal to $\hbar\omega_0$. The tighter the confinement, the larger ω_0 is, and the further apart the subbands are. Usually the confinement in the z-direction is very tight (~ 5–10 nm) so that the corresponding subband spacing is large (~ 100 meV) and only one or two subbands are customarily occupied. Indeed, in all our discussions we will assume that only one z-subband is occupied. But the y-confinement is relatively weak and the corresponding subband spacing is often quite small so that a number of these are occupied under normal operating conditions. The subbands are often referred to as *transverse modes* in analogy with the modes of an electromagnetic waveguide.

Unconfined electrons (U = 0) in non-zero magnetic field (B ≠ 0)

Next we consider unconfined electrons ($U = 0$) in a magnetic field. This is the case that we discussed qualitatively in the last section. In this case Eq.(1.6.1) reduces to

$$\left[E_s + \frac{p_y^2}{2m} + \frac{(eBy + \hbar k)^2}{2m}\right]\chi(y) = E\chi(y)$$

which can be rewritten in the form

$$\left[E_s + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2(y + y_k)^2\right]\chi(y) = E\chi(y) \qquad (1.6.6)$$

where $$y_k \equiv \frac{\hbar k}{eB} \quad \text{and} \quad \omega_c \equiv \frac{|e|B}{m} \qquad (1.6.7)$$

Eq.(1.6.6) is basically a one-dimensional Schrödinger equation with a parabolic potential just as we had before. The only difference is that the parabola is centered at $y = -y_k$ instead of $y = 0$. Thus the eigenenergies and eigenfunctions look very similar to the results for electric subbands (see Eqs.(1.6.5a,b,c)):

$$\chi_{n,k}(y) = u_n(q - q_k) \qquad (1.6.8a)$$

$$E(n,k) = E_s + (n + \tfrac{1}{2})\hbar\omega_c, \quad n = 0,1,2,\ldots \qquad (1.6.8b)$$

where $$q = \sqrt{m\omega_c/\hbar}\, y \quad \text{and} \quad q_k = \sqrt{m\omega_c/\hbar}\, y_k$$

The mathematics describing Landau levels (or magnetic subbands) indexed by n is thus very similar to the mathematics describing the electric subbands for a parabolic confining potential. However, despite the formal similarity the physical content is completely different. The difference is

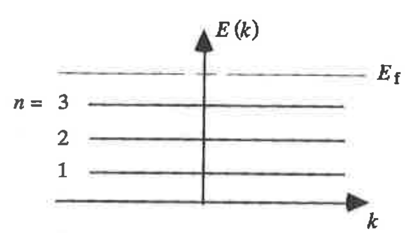

Fig. 1.6.3. Dispersion relation, $E(k)$ vs. k. for Landau levels (or magnetic subbands) in an unconfined system in non-zero magnetic field. Different Landau levels are indexed by n.

easily appreciated if we look at the velocity associated with these states which is obtained from the slope of the dispersion curve (sketched in Fig. 1.6.3):

$$v(n,k) = \frac{1}{\hbar}\frac{\partial E(n,k)}{\partial k} = 0! \tag{1.6.8c}$$

Although the eigenfunctions have the form of plane waves exp $[ikx]$, these waves have no group velocity because the energy E is independent of k. If we were to construct a wavepacket out of these states localized in x it would not move. This is in keeping with what we would expect from classical dynamics which predicts that an electron in a magnetic field will describe closed circular orbits in the x–y plane that do not move in any particular direction. The spatial extent of each wavefunction in the y-direction is approximately

$$\sqrt{\frac{\hbar}{m\omega_c}} = \frac{\sqrt{\hbar\omega_c/m}}{\omega_c} \to \frac{v}{\omega_c}$$

This is equal to the radius of the classical orbit that an electron would describe if it had an energy of $\hbar\omega_c/2$.

An important difference between the eigenfunctions corresponding to electric subbands (Eq.(1.6.5a)) and those corresponding to magnetic subbands (Eq.(1.6.8a)) is that in the latter case the wavefunctions shift along the transverse coordinate y as we change the wavevector k in the longitudinal direction. This is depicted in Fig. 1.6.4. One question that often comes up is the following: how many electrons can fit into one Landau level? In Section 1.5 we obtained the answer heuristically by arguing that this number, N, must equal the two-dimensional density of states multiplied by the energy spacing between two Landau levels:

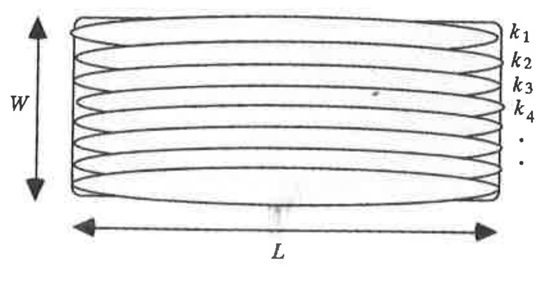

Fig. 1.6.4. Pictorial representation of the eigenfunctions (in a magnetic field) corresponding to a fixed index n but different values of k.

$$N = \frac{mS}{\pi\hbar^2} \times \hbar\omega_c = \frac{|e|BS}{\pi\hbar}$$

We can obtain this result more rigorously by noting that the allowed values of k are spaced by $2\pi/L$, which means that the corresponding wavefunctions are spaced by

$$\Delta y_k = \frac{\hbar\Delta k}{|e|B} = \frac{2\pi\hbar}{|e|BL}$$

along the y-coordinate. Hence the total number of states is given by

$$N = 2\,(\text{for spin}) \times \frac{W}{\Delta y_k} = \frac{|e|BS}{\pi\hbar}$$

in agreement with the heuristic result.

Confined electrons (U ≠ 0) in non-zero magnetic field (B ≠ 0)

Finally we consider the general case with a confining potential and a non-zero magnetic field. The eigenstates then form magneto-electric subbands which reduce to electric subbands when $B = 0$ and to magnetic subbands when $U = 0$. We start from Eq.(1.6.3) with a parabolic potential

$$\left[E_s + \frac{p_y^2}{2m} + \frac{(eBy + \hbar k)^2}{2m} + \frac{1}{2}m\omega_0^2 y^2\right]\chi(y) = E\chi(y)$$

and rewrite it in the form

$$\left(E_s + \frac{p_y^2}{2m} + \frac{1}{2}m\frac{\omega_0^2\omega_c^2}{\omega_{c0}^2}y_k^2 + \frac{1}{2}m\omega_{c0}^2\left[y - \frac{\omega_c^2}{\omega_{c0}^2}y_k\right]^2\right)\chi(y) = E\chi(y)$$

where $$\omega_{c0}^2 \equiv \omega_c^2 + \omega_0^2 \tag{1.6.9}$$

Once again, Eq.(1.6.9) is basically a one-dimensional Schrödinger equation with a parabolic potential and the eigenenergies and eigenfunctions look very similar to the results for electric subbands (Eqs.(1.6.5a,b,c)) and for magnetic subbands (Eqs.(1.6.8a,b,c)):

$$\chi_{n,k}(y) = u_n\left[q - \frac{\omega_c^2}{\omega_{c0}^2}q_k\right] \tag{1.6.10a}$$

where $q = \sqrt{m\omega_{c0}/\hbar}\, y$ and $q_k = \sqrt{m\omega_{c0}/\hbar}\, y_k$

$$E(n,k) = E_s + \frac{1}{2} m \frac{\omega_0^2 \omega_c^2}{\omega_{c0}^2} y_k^2 + \left(n + \tfrac{1}{2}\right)\hbar\omega_{c0}$$

$$= E_s + \left(n + \tfrac{1}{2}\right)\hbar\omega_{c0} + \frac{\hbar^2 k^2}{2m} \frac{\omega_0^2}{\omega_{c0}^2} \qquad (1.6.10b)$$

The velocity is given by

$$v(n,k) = \frac{1}{\hbar} \frac{\partial E(n,k)}{\partial k} = \frac{\hbar k}{m} \frac{\omega_0^2}{\omega_{c0}^2} \qquad (1.6.10c)$$

The dispersion relation and the velocity are sketched in Fig. 1.6.5. It would seem that the effect of the magnetic field is simply to increase the mass by a factor that depends on the relative magnitudes of the confinement parameter ω_0 and the cyclotron frequency ω_c:

$$m \to m\left[1 + \frac{\omega_c^2}{\omega_0^2}\right]$$

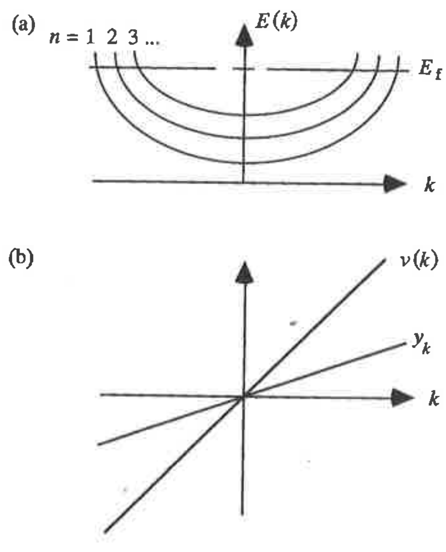

Fig. 1.6.5. Magneto-electric subbands in a parabolic potential: (*a*) Dispersion relation, $E(k)$ vs. k. for different subbands indexed by n. (*b*) Velocity, $v(k)$ vs. k and transverse location y_k vs. k for any subband n.

For zero magnetic field, the cyclotron frequency is zero and we recover the purely electric subbands discussed earlier. As the magnetic field is increased, the cyclotron frequency gets larger and the mass increases making the dispersion relations look nearly flat as expected from our discussion of magnetic subbands.

There is, however, a more profound change in the eigenstates due to the magnetic field, which is not apparent from this description. To see this, we have to look at the spatial location of the eigenstates as a function of k. We know that the wavefunction corresponding to a state (n,k) is centered around $y = y_k$ where

$$y_k = \hbar k/eB \quad \Rightarrow \quad y_k = v(n,k)\frac{\omega_0^2 + \omega_c^2}{\omega_c \omega_0^2}$$

as shown in Fig. 1.6.5b. The point is that the transverse location of the wavefunction is proportional to its velocity. As the magnetic field is increased, *states carrying current along +x shift to one side of the sample while states carrying current in the other direction shift to the other side of the sample.* This seems reasonable from a classical viewpoint since the Lorentz force $e\mathbf{v} \times \mathbf{B}$ is opposite for electrons moving in opposite directions. Increasing the magnetic field thus causes a reduction in the spatial overlap between the forward and backward propagating states, resulting in a suppression of the backscattering due to imperfections. The effect can be spectacular as we will see in Chapter 4.