1. Probability conservation (based on a problem in Schwabl). Recall that the Hamiltonian for a charged particle (charge e) of mass m in an electromagnetic field described by the potentials $\phi(\boldsymbol{x}, t)$ and $\boldsymbol{A}(\boldsymbol{x}, t)$ is,

$$H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\phi\,.$$

Show that a wave function ψ which is a solution of Schroedinger's equation with this Hamiltonian, satisfies the probability continuity condition,

$$\frac{\partial}{\partial t}(\psi^*\psi) + \nabla\cdot\boldsymbol{j} = 0\,,$$

with $\boldsymbol{j}$ defined as

$$\begin{aligned}\boldsymbol{j} &= \frac{\hbar}{2mi}\left(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi - \frac{2ie}{\hbar c}\boldsymbol{A}\psi^*\psi\right)\\ &= \frac{1}{2m}\left(\psi^*\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\boldsymbol{A}\right)\psi + \psi\left(\frac{\hbar}{-i}\nabla - \frac{e}{c}\boldsymbol{A}\right)\psi^*\right)\,.\end{aligned}$$

Note that $\boldsymbol{A}$ is assumed to be real.

Solution

To start with, calculate $-\nabla\cdot\boldsymbol{j}$ using the $\boldsymbol{j}$ given above.

$$\begin{aligned}-\nabla\cdot\boldsymbol{j} = \frac{-1}{2m}\Bigg[&\left(\frac{\hbar}{i}(\nabla\psi^*)\cdot(\nabla\psi) + \frac{\hbar}{-i}(\nabla\psi)\cdot(\nabla\psi^*)\right)\\ &+\left(-\frac{e}{c}\,\boldsymbol{A}\cdot(\nabla\psi^*)\,\psi - \frac{e}{c}\,\boldsymbol{A}\cdot(\nabla\psi)\,\psi^*\right)\\ &+\left(\frac{\hbar}{i}\psi^*\nabla^2\psi + \frac{\hbar}{-i}\psi\nabla^2\psi^*\right)\\ &+\left(-\frac{e}{c}\,\psi^*(\nabla\cdot\boldsymbol{A})\psi - \frac{e}{c}\,\psi(\nabla\cdot\boldsymbol{A})\psi^*\right)\\ &+\left(-\frac{e}{c}\,\psi^*(\boldsymbol{A}\cdot\nabla)\psi - \frac{e}{c}\,\psi(\boldsymbol{A}\cdot\nabla)\psi^*\right)\Bigg]\,.\end{aligned}$$

Only the terms in the first line cancel! It's tempting to get rid of the $\nabla\cdot\boldsymbol{A}$ terms, but we're not necessarily in a static situation or the Coulomb gauge. Simplifying slightly,

$$\begin{aligned}-\nabla\cdot\boldsymbol{j} = \frac{1}{2m}\Bigg[&\frac{\hbar}{i}\left(-\psi^*\nabla^2\psi + \psi\nabla^2\psi^*\right)\\ &+2\frac{e}{c}\,\left(\psi^*(\boldsymbol{A}\cdot\nabla)\psi + \psi(\boldsymbol{A}\cdot\nabla)\psi^* + \psi^*\psi(\nabla\cdot\boldsymbol{A})\right)\Bigg]\,.\end{aligned}$$

The Schroedinger equation is

$$H\psi = i\hbar\frac{\partial\psi}{\partial t} \,. \tag{1}$$

For it's complex conjugate, we might be tempted to write

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

but this only works when $H = p^2/2m + V$. In this case, we need to be careful.

$$(H\psi)^* = \left(\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\boldsymbol{A}\right)^2 + e\phi\right)^* \psi^* = \left(\frac{1}{2m}\left(\frac{\hbar}{-i}\nabla - \frac{e}{c}\boldsymbol{A}\right)^2 + e\phi\right)\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t} \,. \tag{2}$$

Multiply the first equation by ψ^*, the second by ψ, and subtract.

$$\begin{aligned}
\frac{\partial}{\partial t}(\psi^*\psi) &= \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t} \\
&= \frac{-i}{\hbar}\left(\psi^* H\psi - \psi H^*\psi^*\right) \\
&= \frac{-i}{\hbar}\left(\frac{1}{2m}\psi^*\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\boldsymbol{A}\right)^2\psi - \frac{1}{2m}\psi\left(\frac{\hbar}{-i}\nabla - \frac{e}{c}\boldsymbol{A}\right)^2\psi^* + \psi^* e\phi\psi - \psi e\phi\psi^*\right) \\
&= \frac{1}{2m}\Bigg[\left(-\frac{\hbar}{i}\psi^*\nabla^2\psi + \frac{\hbar}{i}\psi\nabla^2\psi^*\right) \\
&\qquad + \left(\frac{e}{c}\,\psi^*(\nabla\cdot\boldsymbol{A})\psi + \frac{e}{c}\,\psi(\nabla\cdot\boldsymbol{A})\psi^*\right) \\
&\qquad + \left(\frac{e}{c}\,\psi^*(\boldsymbol{A}\cdot\nabla\psi) + \frac{e}{c}\,\psi(\boldsymbol{A}\cdot\nabla\psi^*)\right) \\
&\qquad + \left(\frac{e}{c}\,\psi^*(\boldsymbol{A}\cdot\nabla\psi) + \frac{e}{c}\,\psi(\boldsymbol{A}\cdot\nabla\psi^*)\right) \\
&\qquad + \left(-\frac{ie^2}{\hbar c^2}\,\psi^* A^2\psi + \frac{ie^2}{\hbar c^2}\,\psi A^2\psi^*\right)\Bigg] \,,
\end{aligned}$$

which simplifies slightly to

$$\begin{aligned}
\frac{\partial}{\partial t}(\psi^*\psi) = \frac{1}{2m}\Bigg[&\frac{\hbar}{i}\left(-\psi^*\nabla^2\psi + \psi\nabla^2\psi^*\right) \\
&+ 2\frac{e}{c}\,\left(\psi^*(\boldsymbol{A}\cdot\nabla)\psi + \psi(\boldsymbol{A}\cdot\nabla)\psi^* + \psi^*\psi(\nabla\cdot\boldsymbol{A})\right)\Bigg] \,,
\end{aligned}$$

which is the same as we previously obtained for $-\nabla\cdot\boldsymbol{j}$.

Some comments. $\boldsymbol{p} - e\boldsymbol{A}/c = m\boldsymbol{v}$ is the kinetic momentum operator. The extra terms with $\boldsymbol{A}$ in the current come about because we need to correct the canonical momentum to get the kinetic momentum.

$\psi^*\psi$ and $\boldsymbol{j}$ as defined above are the matter probability density and the matter probability current. How would you write the charge probability density and charge probability current? (Answer: multiply them by e.)

——— End Solution ———

2. Crossed $\boldsymbol{E}$ and $\boldsymbol{B}$ fields (based on a problem in Schwabl). Consider a particle with mass m and charge e moving in uniform $\boldsymbol{B} = B\boldsymbol{e}_z$ and $\boldsymbol{E} = E\boldsymbol{e}_x$ fields with $E < B$. Use the gauge $\boldsymbol{A} = Bx\boldsymbol{e}_y$. The Hamiltonian is

$$H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 - eEx \, .$$

Find the eigenfunctions and eigenvalues for this Hamiltonian. Note that if you should find that the eigenfunctions involve standard functions which we already know about, you don't have to write out each one explicitly. For example, if you should find (you won't) that the eigenfunctions involve the Legendre polynomials $P_l(y)$, you can just leave $P_l(y)$ in your result rather than explicitly write out what $P_l(y)$ is. Of course, you have to say that P_l stands for a Legendre polynomial of order l.

Hint: you might start by reminding yourself what the classical motion looks like.

——— Solution ———

To start with the classical motion, there is no force in the z direction, so the z-component of velocity is constant. Note that if the particle has $v_y = -cE/B$, then the magnetic force exactly cancels the electric force and the particle moves at constant velocity in the negative y direction. If the particle has v_y different from above or a non-vanishing v_x, then the motion is circular motion in the xy-plane (clockwise as viewed from the positive z-direction) with a velocity in the $-y$-direction at $v_y = -cE/B$. (Often called $\boldsymbol{E} \times \boldsymbol{B}$ drift.) So, we are looking for eigenfunctions which have a constant v_z (or p_z) along with circular and linear motion in the xy-plane.

Writing out the Hamiltonian, we have

$$H = \frac{p_x^2}{2m} + \frac{1}{2m}\left(p_y - \frac{e}{c}Bx\right)^2 + \frac{1}{2m}p_z^2 - eEx \, .$$

We see that p_y and p_z commute with the Hamiltonian, so our eigenfunctions can be eigenfunctions of p_y, p_z, and H, simultaneously. Let $p_z\psi = \hbar k_z\psi$ and $p_y\psi = \hbar k_y\psi$. Then the eigenvalue equation becomes

$$\left(\frac{1}{2m}p_x^2 + \frac{1}{2m}\left(\hbar k_y - \frac{e}{c}Bx\right)^2 - eEx\right)\psi = \left(\mathcal{E} - \frac{\hbar^2 k_z^2}{2m}\right)\psi = \mathcal{E}'\psi \, ,$$

where we have used $\mathcal{E}$ to stand for the energy eigenvalue to distinguish it from E and $\mathcal{E}'$ for the energy eigenvalue with the energy due to the z motion removed.

Define $\omega = eB/mc$ and $v_0 = cE/B$. Then the time independent Schroedinger equation becomes

$$\left(\frac{1}{2m}p_x^2 + \frac{1}{2m}\left(\hbar k_y - m\omega x\right)^2 - m\omega v_0 x\right)\psi = \mathcal{E}'\psi ,$$

Let's work on the terms above involving x.

$$\frac{1}{2m}\left(\hbar k_y - m\omega x\right)^2 - m\omega v_0 x = \frac{m\omega^2}{2}\left(x^2 - 2\left(\frac{\hbar k_y}{m\omega} + \frac{v_0}{\omega}\right)x + \frac{\hbar^2 k_y^2}{m^2\omega^2}\right) .$$

Define

$$x_0 = \frac{\hbar k_y}{m\omega} + \frac{v_0}{\omega} .$$

Then

$$\begin{aligned}\frac{1}{2m}\left(\hbar k_y - m\omega x\right)^2 - m\omega v_0 x &= \frac{m\omega^2}{2}\left((x - x_0)^2 + \frac{\hbar^2 k_y^2}{m^2\omega^2} - x_0^2\right) \\ &= \frac{m\omega^2}{2}(x - x_0)^2 - \frac{1}{2}mv_0^2 - \hbar k_y v_0 .\end{aligned}$$

We can clean up the last two terms by adding and subtracting eEx_0,

$$\begin{aligned}-\frac{1}{2}mv_0^2 - \hbar k_y v_0 + eEx_0 - eEx_0 &= -\frac{1}{2}mv_0^2 - \hbar k_y v_0 + m\omega v_0\left(\frac{\hbar k_y}{m\omega} + \frac{v_0}{\omega}\right) - eEx_0 \\ &= \frac{1}{2}mv_0^2 - eEx_0 .\end{aligned}$$

Returning to the time independent Schroedinger equation, we have

$$\left(\frac{1}{2m}p_x^2 + \frac{m\omega^2}{2}(x - x_0)^2 + \frac{1}{2}mv_0^2 - eEx_0\right)\psi = \left(\mathcal{E} - \frac{\hbar^2 k_z^2}{2m}\right)\psi ,$$

So we see that the x motion is that of a harmonic oscillator centered at x_0 with frequency ω. The energy eigenvalues are

$$\mathcal{E}_{n,k_y,k_z} = (n + 1/2)\hbar\omega + \frac{\hbar^2 k_z^2}{2m} + \frac{1}{2}mv_0^2 - eEx_0 ,$$

with $\hbar k_y = m\omega x_0 - mv_0$ and (unnormalized) eigenfunction

$$\psi_{n,k_y,k_z} = \psi_n(x - x_0)e^{ik_y y}e^{ik_z z} ,$$

where ψ_n is the harmonic oscillator eigenfunction with frequency ω and quantum number n.

So, the motion has an energy corresponding to whatever kinetic energy we want in the z-direction, the kinetic energy due to the drift velocity in the y-direction and the kinetic energy due a harmonic oscillator at frequency ω in the x-direction. Since the center of oscillation is x_0, there is also an electric potential energy $-eEx_0$. Classically, the kinetic energy due to the motion in the xy plane looks like $mv_x^2/2 + m(v_y - v_0)^2/2$ where v_x and v_y are the velocity components of the circular motion relative to the center of the circle which is moving with velocity $-v_0\boldsymbol{e}_y$. Averaging over a period gives $mr^2\omega^2/2 + mv_0^2/2$ where r is the radius of the circular orbit. The cross term in the y-velocity averages to zero as does the variation in the electric potential energy as the particle oscillates in x. In the quantum case, the oscillator energy corresponds to $mr^2\omega^2/2$.

You might wonder where the drift velocity went in all this. Let $\hbar\Omega = \mathcal{E}_{n,k_y,k_z}$, so Ω is the oscillation frequency of the wave function. Then the group velocity component in the y-direction is $d\Omega/dk_y$. The only place k_y appears in the energy is in x_0. Carrying out the differentiation, we find $v_g = -cE/B = -v_0$, exactly the classical drift velocity.

——— End Solution ———

3. Magnetic barrier. This problem appeared on the May, 2002 prelims. The Θ functions used below are defined so that $\Theta(x) = 0$ if $x < 0$, $\Theta(x) = 1$ if $x > 0$ and $\Theta(0) = 1/2$. In other words, Θ is the unit step function and $\Theta(x) = \int_{-\infty}^{x} \delta(x')\,dx'$. Also you may find problem 1 in this assignment to be useful.

Consider a charged particle moving in the xy-plane subject to a magnetic field $B_z = B\Theta(x)\Theta(d-x)$. The magnetic field is constant in a strip of width d and zero everywhere else. We will study the problem of scattering of plane waves from this "magnetic barrier."

(a) Write down the Schroedinger Hamiltonian for this problem. You have to choose a gauge for the vector potential—choose the gauge $A_x = A_z = 0$, and also choose $A_y = 0$ for $x < 0$.

——— Solution ———

The vector potential is $\nabla \times \boldsymbol{A} = \boldsymbol{B}$. We take $A_y = 0$ for $x < 0$, $A_y = Bx$ for $0 \le x \le d$ and $A_y = Bd$ for $d < x$. Then the only non-zero B is within the strip and $B_z = \partial A_y/\partial x = B$. We assume the charge is $-e$, so the Hamiltonian (ignoring the z-direction as suggested by the problem) is

$$H = \frac{1}{2m}\left(p_x^2 + \left(p_y + \frac{e}{c}A_y\right)^2\right) ,$$

where A_y is defined above. A_y contains an x, so p_x does not commute with the Hamiltonian. However, there is no y in the Hamiltonian, p_y commutes with H, and p_y can be diagonalized with H. Since we are dealing with incident waves in the x-direction, $p_y = 0$.

The time independent Schroedinger equation takes the following forms:

$$\frac{p_x^2}{2m}\psi = E\psi , \qquad x < 0 .$$

$$\left(\frac{p_x^2}{2m} + \frac{e^2B^2x^2}{2mc^2}\right)\psi = E\psi\,, \qquad 0 < x < d\,.$$

$$\left(\frac{p_x^2}{2m} + \frac{e^2B^2d^2}{2mc^2}\right)\psi = E\psi\,, \qquad d < x\,.$$

End Solution

Consider the scattering problem for an electron incident from $x < 0$ and moving perpendicular to the barrier. For an incident wave $\exp(ikx)$ there will, in general be a transmitted wave $T\exp(ik_tx)$ and a reflected wave $R\exp(-ikx)$.

(b) The transmitted wave vector k_t is determined by simple kinematics in terms of k and Bd. What is that relation?

Solution

Using the Schroedinger equation for $x < 0$, we find $E = \hbar^2k^2/2m$. Using the Schroedinger equation for $d < x$, we find

$$E = \frac{\hbar^2k_t^2}{2m} + \frac{e^2B^2d^2}{2mc^2}\,,$$

so

$$k_t = \sqrt{k^2 - \frac{e^2B^2d^2}{\hbar^2c^2}} = \sqrt{k^2 - \frac{m^2\omega^2d^2}{\hbar^2}}\,,$$

where $\omega = eB/mc$ is the cyclotron frequency for the field B.

End Solution

(c) For a given barrier, you will find that, below a certain critical energy E_0, k_t is imaginary. What does this mean? Give a classical argument that leads to the same critical energy.

Solution

k_t is imaginary when $\hbar k < m\omega d$. This means that the wave is exponentially killed off moving to the right of the strip which means it is completely reflected. Classically, the particle enters the strip and starts moving on a circle. If the strip is greater than the radius of the circle, the particle will complete a semi-circle and leave the strip in the direction opposite to which it entered. This will occur if $mv = m\omega d$. Since mv corresponds to $\hbar k$, this happens at the same energy classically as quantum mechanically.

End Solution

(d) What is the direction of the transmitted probability flux? It is **not** along the x-axis!

Solution

Here we use the expression for $\boldsymbol{j}$ from problem 1. That expression is pretty tough to remember as it stands, but a good way to remember might be as follows. First of all the probability density is $\psi^*\psi$. When we have a density and we want a current, we need to multiply by the velocity. With quantum mechanics, we have to replace v by p/m and when we throw in an $\boldsymbol{A}$, it's $(p - eA/c)/m$ and finally we need to take the average with the operator operating on ψ and its complex conjugate operating on ψ^*. In any case,

$$\boldsymbol{j} = \frac{1}{2m}\left(\psi^*\left(\frac{\hbar}{i}\nabla + \frac{e}{c}\boldsymbol{A}\right)\psi + \psi\left(\frac{\hbar}{-i}\nabla + \frac{e}{c}\boldsymbol{A}\right)\psi^*\right) .$$

For $x > d$, the wave function is $T\exp(ik_t x)$ and the T is irrelevant for this discussion.

$$j_x = \frac{1}{2m}\left(\psi^* p_x \psi + \psi p_x^\dagger \psi^*\right) = \frac{\hbar k_t}{m} .$$

$$j_y = \frac{1}{2m}\left(\psi^*\frac{eBd}{c}\psi + \psi\frac{eBd}{c}\psi^*\right) = \omega d .$$

If ϕ is the angle the flux makes with the x-axis, then

$$\tan\phi = \frac{m\omega d}{\hbar k_t} = \frac{m\omega d}{\sqrt{\hbar^2 k^2 - m^2\omega^2 d^2}} .$$

It is interesting to note that at the critical energy found in the previous part, the transmitted probability current density is parallel to the y-axis.

End Solution

(e) Find the reflection and transmission coefficients in the limit $d \to 0$ with Bd fixed.

Solution

In this case, the vector potential is a step function at $x = 0$. It's 0 for $x < 0$ and Bd for $x > 0$. Since it's a step, ψ and its derivatives must be continuous at $x = 0$. These conditions give

$$1 + R = T ,$$

and

$$ik - ikR = ik_t T .$$

These can be solved to give

$$R = \frac{k - k_t}{k + k_t} , \qquad T = \frac{2k}{k + k_t} .$$

In terms of probability flux, the reflection and transmission coefficents are

$$r = k|R|^2/k = \left(\frac{k - k_t}{k + k_t}\right)^2 , \qquad t = k_t|T|^2/k = \frac{4kk_t}{(k + k_t)^2} ,$$

and of course, we use the k_t determined in part (b).

End Solution

4. In lecture, we worked out the generating function for Legendre polynomials,

$$F(x,\mu) = \sum_{l=0}^{\infty} x^l P_l(\mu) = \frac{1}{\sqrt{1-2x\mu+x^2}} \; .$$

(a) Use the generating function to demonstrate the following recursion relation among the polynomials,

$$(l+1)P_{l+1}(\mu) - (2l+1)\mu P_l(\mu) + lP_{l-1}(\mu) = 0 \; .$$

Hint: what happens if you differentiate the generating function and the series with respect to x?

Solution

$$\frac{\partial}{\partial x}\frac{1}{\sqrt{1-2x\mu+x^2}} = \frac{\mu - x}{(1-2x\mu+x^2)^{3/2}} = \frac{\mu-x}{(1-2x\mu+x^2)}F(x,\mu) \; .$$

Or

$$(1-2x\mu+x^2)\frac{\partial F}{\partial x} = (\mu - x)F \; .$$

Or

$$(1-2x\mu+x^2)\sum_{l=0}^{\infty} l x^{l-1} P_l(\mu) = (\mu - x)\sum_{l=0}^{\infty} x^l P_l(\mu) \; .$$

Now equate coefficients of x^l on both sides. This gives

$$(l+1)P_{l+1} - 2l\mu P_l(\mu) + (l-1)P_{l-1}(\mu) = \mu P_l(\mu) - P_{l-1}(\mu) \; ,$$

which, after rearrangement, becomes

$$(l+1)P_{l+1}(\mu) - (2l+1)\mu P_l(\mu) + lP_{l-1}(\mu) = 0 \; .$$

End Solution

(b) Demonstrate the following recursion relation among the polynomials

$$P'_{l+1}(\mu) - 2\mu P'_l(\mu) + P'_{l-1}(\mu) = P_l(\mu) \; .$$

Hint: what else can you differentiate with respect to?

Solution

Differentiate the generating function with respect to μ.

$$\frac{\partial F}{\partial \mu} = \frac{x}{1 - 2x\mu + x^2} F \, .$$

Or

$$(1 - 2x\mu + x^2) \sum_{l=0}^{\infty} x^l P_l'(\mu) = x \sum_{l=0}^{\infty} x^l P_l(\mu) \, .$$

Now equate the coefficients of x^{l+1},

$$P_{l+1}'(\mu) - 2\mu P_l'(\mu) + P_{l-1}'(\mu) = P_l(\mu) \, .$$

Note that with the recursion relations of parts (a) and (b) you can generate many others!

End Solution

(c) Use the generating function to obtain an expression for $P_l(0)$.

Solution

$$\begin{aligned} \sum_{l=0}^{\infty} x^l P_l(0) &= (1 + x^2)^{(-1/2)} \\ &= 1 + \left(\frac{-1}{2}\right) \frac{x^2}{1!} + \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right) \frac{x^4}{2!} + \left(\frac{-1}{2}\right)\left(\frac{-3}{2}\right)\left(\frac{-5}{2}\right) \frac{x^6}{3!} + \cdots \, , \end{aligned}$$

From this we can tell immediately that all the odd l polynomials vanish at $\mu = 0$. (We knew that anyway since they're odd functions of μ.) For even l,

$$P_l(0) = (-1)^{l/2} \frac{(l-1)!!}{2^{l/2}(l/2)!} = (-1)^{l/2} \frac{(l-1)!!}{l!!} \, ,$$

where !! means double factorial—a factorial where we leave out every other factor.

End Solution