Extension: 24 hours

21. Demonstrate our claim in the long solenoid discussion that the solution to the Schrödinger equation when there is a flux Φ in the solenoid is:

$$\psi(\mathbf{x},t) = \psi_L(\mathbf{x},t)e^{\underbrace{iqg_L(\mathbf{x})}_{\equiv \alpha_L}} + \psi_R(\mathbf{x},t)e^{\underbrace{iqg_R(\mathbf{x})}_{\equiv \alpha_R}}, \tag{1}$$

where

$$g_L(\mathbf{x}) \equiv \int_{\mathbf{x}_0}^{\mathbf{x}} d\mathbf{x}' \cdot \mathbf{A}(\mathbf{x}) \qquad \text{along a left path} \tag{2}$$

$$g_R(\mathbf{x}) \equiv \int_{\mathbf{x}_0}^{\mathbf{x}} d\mathbf{x}' \cdot \mathbf{A}(\mathbf{x}) \qquad \text{along a right path} \tag{3}$$

and $\psi_{L,R}(\mathbf{x},t)$ satisfy the Schrödinger equation when $\Phi = 0$.

We will show $\psi(\vec{x},t)$ satisfies the S.E. with

$$H = \frac{1}{2m}\left(-i\nabla - q\vec{A}(\vec{x},t)\right)^2$$

First notice that

$$H\,\psi e^{\alpha_L} = \frac{1}{2m}\Big(-\nabla^2\left(\psi_L e^{\alpha_L}\right) + iq\vec{A}\cdot\vec{\nabla}\left(\psi_L e^{\alpha_L}\right) + iq\,\vec{\nabla}\cdot\left(\vec{A}\psi_L e^{\alpha_L}\right) + q^2\vec{A}\cdot\vec{A}\left(\psi_L e^{\alpha_L}\right)$$

and

$$i\partial_t\left(\psi e^{\alpha_L}\right) = i(\partial_t\psi)\cdot e^{\alpha_L}.$$

Notice

$$\vec{\nabla}\left(\psi_L e^{\alpha_L}\right) = \left(\nabla\psi_L\right)e^{\alpha_L} + \psi_L\,\alpha_L'(x)\,e^{\alpha_L}$$

Moreover, Notice

$$\nabla \alpha_L(x) = iq\, g_L'(x) = iq\, \vec{A}_L(x)$$

along Left path.

$$(\vec{\nabla} g_L(x) = \vec{A}_L(x) \quad \text{since}$$

$$g_L(x) - g_L(x_0) = \int_{x_0}^{x} \vec{A}_L(x) \cdot d\vec{x}$$

Likewise,

$$\alpha_R'(x) = iq\, \vec{A}_R(x)$$

To make the calculations simpler, we choose $\vec{A}(\vec{x},t)$ so that $\vec{\nabla} \cdot \vec{A}(\vec{x},t) = 0$. (we can do this by letting $\vec{A}(\vec{x},t) \to \vec{A}(\vec{x},t) + \nabla X$ and picking X so that $\nabla^2 X = \vec{\nabla} \cdot -\vec{A}(\vec{x},t)$). Therefore,

$$\vec{\nabla} \cdot (\psi \vec{A}) = (\nabla \psi) \cdot \vec{A} + \psi \cancel{(\nabla \cdot \vec{A})}^{0}$$

$$= (\nabla \psi) \cdot \vec{A}$$

for any wavefunction ψ, including $\psi = \psi_L e^{\alpha_L}$.

We also see that

$$\nabla^2 (\psi_L e^{\alpha_L}) = \nabla\left(\nabla \psi_L e^{\alpha_L} + \psi_L \nabla \alpha_L e^{\alpha_L}\right)$$

$$= \nabla^2 \psi_L e^{\alpha_L} + 2 \nabla \psi_L \nabla \alpha_L e^{\alpha_L}$$

$$+ \psi_L \left(\nabla^2 \alpha_L e^{\alpha_L} + (\nabla \alpha_L)^2 e^{\alpha_L}\right)$$

$$= e^{\alpha_L}\left(\nabla^2 \psi_L + 2 \nabla \psi_L \cdot \nabla \alpha_L + \psi_L \left(\cancel{\nabla^2 \alpha_L}^{0} + (\nabla \alpha_L)^2\right)\right)$$

$$= e^{\alpha_L}\left(\nabla^2\psi_L + 2\nabla\psi_L\cdot\nabla\alpha_L + \psi_L\left(\cancel{\nabla^2\alpha_L} + (\nabla\alpha_L)^2\right)\right)$$

$$= e^{\alpha_L}\left(\nabla^2\psi_L + 2\nabla\psi_L\cdot\nabla\alpha_L + \psi_L(\nabla\alpha_L)^2\right)$$

Because

$$\nabla^2\alpha_L = \nabla\cdot\nabla\alpha_L \propto \vec{\nabla}\cdot\vec{A} = 0.$$

Thus,

$$H\left(\psi_L(x,t)\,e^{\alpha_L(x)}\right) = \frac{1}{2m}e^{\alpha_L}\Big(-\nabla^2\psi_L - 2\nabla\psi_L\cdot\nabla\alpha_L$$
$$- \psi_L(\nabla\alpha_L)^2 + 2\,\underbrace{iq\vec{A}}_{\vec{\nabla}\alpha_L}\cdot\left(\vec{\nabla}\psi_L + \psi_L\cdot iq\vec{A}\right)$$
$$+ q^2A^2\psi_L\Big)$$

We know

$$(\nabla\alpha_L)^2 = \left(iq\vec{A}(x)\right)^2 = -q^2A^2$$

and

$$\nabla\alpha_L = iq\vec{A}$$

Thus,

$$H\psi_L e^{\alpha_L} = \frac{e^{\alpha_L}}{2m}\Big(-\nabla^2\psi_L - \cancel{2\vec{\nabla}\alpha_L\cdot\vec{\nabla}\psi} + \cancel{q^2A^2\psi_L}$$
$$- \cancel{2q^2A^2\psi_L} + \cancel{2\vec{\nabla}\alpha_L\cdot\vec{\nabla}\psi} + \cancel{q^2A^2\psi_L}\Big)$$

$$= \frac{e^{\alpha_L}}{\ldots}\nabla^2\psi \ldots = e^{\alpha_L}(H\psi_L)$$

$$= -\frac{e^{\alpha_L}}{2m} \nabla^2 \psi_L = e^{\alpha_L}(H\psi_L)\big|_{\Phi=0}$$

$$= e^{\alpha_L}(i\partial_t \psi_L) = -i\partial_t(\psi_L e^{i\alpha_L})$$

Thus $\psi_L e^{i\alpha_L}$ satisfies the S.E. when $\Phi \neq 0$.

By symmetry, so does $\psi_R(x,t) e^{iq\varphi_R(x)}$.

By superposition,

$$\psi(x,t) = \psi_L e^{\alpha_L} + \psi_R e^{\alpha_R}$$

is therefore a solution. $\square$

22. Prove the theorem (essentially exercise 18.4.4 in text):

Theorem: Let the Hamiltonian for a charged particle interacting with an electromagnetic field be H:

$$H = \frac{1}{2m}\left[\mathbf{p} - q\mathbf{A}(\mathbf{x},t)\right]^2 + q\Phi(\mathbf{x},t) + U(\mathbf{x},t), \tag{4}$$

Let H' be the Hamiltonian obtained from H by a gauge transformation:

$$\mathbf{A}(\mathbf{x},t) \rightarrow \mathbf{A}'(\mathbf{x},t) = \mathbf{A}(\mathbf{x},t) + \nabla\chi(\mathbf{x},t) \tag{5}$$

$$\Phi(\mathbf{x},t) \rightarrow \Phi'(\mathbf{x},t) = \Phi(\mathbf{x},t) - \partial_t\chi(\mathbf{x},t), \tag{6}$$

If $i\partial_t\psi = H\psi$ and $i\partial_t\psi' = H'\psi'$, then

$$\psi'(\mathbf{x},t) = e^{iq\chi(\mathbf{x},t)}\psi(\mathbf{x},t). \tag{7}$$

Using physical intuition, we recognize that the primed wavefunction should be the same as the unprimed wavefunction up to a phase factor, since the probability distribution should be unaffected by the geometric freedoms of the vector potential and the electric potential. Therefore, we guess that ψ' has the form

$$\psi'(\vec{x}, t) = e^{iy(\vec{x},t)}\psi(\vec{x},t)$$

where $y(\vec{x}, t)$ is some phase factor dependent on position and time.

We know these things:

- $i\partial_t \psi' = H'\psi'$
- $i\partial_t \psi' = (i\partial_t \psi + i^2\partial_t y \psi)e^{iy}$
  $= (H\psi - \partial_t y \cdot \psi)e^{iy}$

$$\Rightarrow -\partial_t y \cdot \psi = e^{-iy}(H'\psi') - H\psi$$

We must therefore find a function of y that satisfies this equation. To make the calculations simpler, we choose $\vec{A}(\vec{x}, t)$ so that $\vec{\nabla} \cdot \vec{A}(\vec{x}, t) = 0$. (we can do this by picking X so that $\nabla^2 X = \vec{\nabla} \cdot \vec{A}'(\vec{x}, t)$).

First, we find H' in terms of H. This can be done by simply adding the extra terms introduce under the gauge transformation:

$$H' = H + \frac{1}{2m}\Big(-q\underbrace{\vec{p}}_{-i\vec{\nabla}}\vec{\nabla}X - q\vec{\nabla}X\underbrace{\vec{p}}_{-i\vec{\nabla}} + q^2 2\vec{A}\cdot\vec{\nabla}X + q^2(\nabla X)^2\Big) - q\,\partial_t X$$

Next, using Mathematica, we evaluate the expression below (all code at the end of the work for this problem):

$$(H'\psi')e^{-iy} - H\psi =$$

$$i\, m \left(q X^{(1,0)}[x,t] - y^{(1,0)}[x,t]\right) \psi^{(1,0)}[x,t] +$$
$$\frac{1}{2}\psi[x,t]\left(-2X^{(0,1)}[x,t] + m\left(q^2 X^{(1,0)}[x,t]^2 + 2qA[x]\left(qX^{(1,0)}[x,t] - y^{(1,0)}[x,t]\right) -\right.\right.$$
$$\left.\left.-\psi[x,t]\, X^{(0,1)}[x,t]\ [x,t]\, y^{(1,0)}[x,t] + y^{(1,0)}[x,t]^2 + i\, q X^{(2,0)}[x,t] - i\, y^{(2,0)}[x,t]\right)\right)$$

$$\left(\psi^{(1,0)} = \vec{\nabla}\psi\ ;\ X^{(0,1)} = \partial_t X,\ \text{etc}\right).$$

Since
$$(-\partial_t y)\cdot\psi = (H'\psi')e^{-iy} - H\psi,$$
we must have no factors of $\vec{\nabla}\psi$ on the RHS in order for this equation to hold for arbitrary ψ. Thus, we must have

$$qX^{(1,0)} - y^{(1,0)} = 0$$

$$\rightarrow q\vec{\nabla}X - \vec{\nabla}y = 0$$

$$\rightarrow y(x,t) = X(x,t) + c_1$$

where c_1 is a constant

Indeed, when we substitute this into Mathematica we get

$$(H'\psi')e^{-iy} - H\psi = -\psi[x,t]\, X^{(0,1)}[x,t]$$

Any other value of $y(x,t)$ will not result in the two sides of the equation being equal for all positions and times. Therefore, if $i\partial_t\psi = H\psi$ and $i\partial_t\psi' = H\psi'$, we must have $\psi'(x,t) = e^{iqX(x,t)}\psi(x,t)$ (up to some arbitrary constant phase factor e^{ic_1} obviously).

Here is the mathematica code below:

$(H_{00}(\psi) = H\psi, \quad H_{01}(\psi) = H\psi',$

$H_{10}(\psi) = H'\psi, \quad H_{11}(\psi) = H'\psi')$

```
Clear["Global`*"]
Print["Problem 2"]

(*Uncomment to see that subsituting this value for y does give the right result
*)
y[x, t] = q*X[x, t] + c1;

(*Original Hamiltonian of original wavefunction
*)
H00[f_] = 1/2m*(-D[f[x, t], {x, 2}] + q*I*(A[x]*D[f[x, t], x] + D[A[x]*f[x, t], x]) +
      q^2*(A[x])^2*f[x, t]) + (q*Φ[x] + U[x, t])*f[x, t];

(*Original Hamiltonian of new wavefunction
*)
H01[f_] = 1/2m*(-D[f[x, t]*Exp[I*y[x, t]], {x, 2}] + q*I*
        (A[x]*D[f[x, t]*Exp[I*y[x, t]], x] + D[A[x]*f[x, t]*Exp[I*y[x, t]], x]) +
      q^2*(A[x])^2*f[x, t]*Exp[I*y[x, t]]) +
   (q*Φ[x] + U[x, t])*f[x, t]*Exp[I*y[x, t]];

(*New Hamiltonian of Original wavefunction
*)
H10[f_] = H00[f] + 1/2m*
     (I*q*(D[X[x, t], x]*D[f[x, t], x] + D[f[x, t]*D[X[x, t], x], x]) + 2q^2*A[x]*
        D[X[x, t], x]*f[x, t] + q^2*D[X[x, t], x]^2*f[x, t]) - D[X[x, t], t]*f[x, t];

(*New Hamiltonian of New wavefunction
*)
H11[f_] =
  H01[f] + 1/2m*(I*q*(D[X[x, t], x]*D[f[x, t]*Exp[I*y[x, t]], x] + D[f[x, t]*
            Exp[I*y[x, t]]*D[X[x, t], x], x]) + 2q^2*A[x]*D[X[x, t], x]*f[x, t]*
        Exp[I*y[x, t]] + q^2*D[X[x, t], x]^2*f[x, t]*Exp[I*y[x, t]]) -
   D[X[x, t], t]*f[x, t]*Exp[I*y[x, t]];

Simplify[Simplify[Expand[H11[ψ]]*Exp[-I*y[x, t]]] - H00[ψ]]
```

```
Problem 2

Out[615]= -ψ[x, t] X^(0,1)[x, t]
```

*Exercise 18.5.2.** (1) Estimate the photoelectric cross section when the ejected electron has a kinetic energy of 10 Ry. Compare it to the atom's geometric cross section $\simeq \pi a_0^2$.

(2) Show that if we consider photoemission from the 1s state of a charge Z atom, $\sigma \propto Z^5$, in the limit $p_f a_0 / Z\hbar \gg 1$.

a) We know that the final KE of the ejected

a) We know that the final KE of the ejected electron is

$$E_f = 10 R_y = \frac{p_f^2}{2m}$$

Thus, the final momentum is

$$p_f = \sqrt{2mE_f} = 6.3\cdot10^{-24}\,kg\,m\,s^{-1}$$

Plugging this into 18.5.30 in Shankar, we have

$$\boxed{\sigma_{pe} = 1.315\cdot10^{-34}\,m^2}$$

The atom's geometric cross section is approximately

$$\sigma_{atom} \approx \pi a_0^2 = 8.8\cdot10^{-21}\,m^2$$

which is *much, much* larger than the photoelectric effect cross section of the electron.

b.) Notice that the only thing that has any dependence on the nuclear charge, Z, is the Bohr radius. As we have demonstrated in Ch 1a and Ph 125a, we know that the adjusted Bohr radius of the 1s orbital is proportional to 1/Z:

$a_0' \propto Z^{-1}$

Moreover, we know that $\frac{p_f a_0}{(Z\hbar)} \gg 1$. Therefore, from equation 18.5.31, we have

$$\sigma \approx \frac{128 a_0'^3 \pi e^2 p_f^3}{3m\hbar^3 \omega c\,(p_f^2 a_0'^2/\hbar^2)^4} \propto \frac{a_0'^3}{a_0'^8} = (a_0')^{-5}$$

$$\propto Z^5$$

as desired. $\square$

24. The text discusses the photoelectric effect using the "dipole approximation". While an electron is ejected from the atom in the photoelectric effect, this approximation is useful for lower energy interactions as well. We thus investigate induction of an atomic dipole moment due to an external electromagnetic field. We'll set up some things in this problem, and continue the discussion in the next problem set. As we have discussed, the Hamiltonian for an atomic electron in an external electromagnetic field may be written, in the Coulomb gauge:

$$H = H_0 + H_1, \tag{8}$$

where

$$H_0 = \frac{P^2}{2m} + V(R) \tag{9}$$

and

$$H_1 = -\frac{q}{m}\mathbf{P}\cdot\mathbf{A}(\mathbf{x},t) + \frac{q^2}{2m}\mathbf{A}(\mathbf{x},t)^2 - \frac{q}{m}\mathbf{S}\cdot\mathbf{B}(\mathbf{x},t). \tag{10}$$

We have included here the possibility of an interaction of the spin magnetic moment with the magnetic field.

We could discuss the relative strength of the different terms in a given situation, but here we'll assume that the $\mathbf{P}\cdot\mathbf{A}(\mathbf{x},t)$ term dominates.

(a) With this assumption, and also assuming that the wave is traveling in the y direction and the polarization is in the z direction, write H_1 in terms of the wavenumber k mode of the plane wave expansion for the field.

(b) The dipole approximation consists in assuming that the external field varies slowly over the relevant distance scale of the problem. Thus, the $e^{\pm i\mathbf{k}\cdot\mathbf{x}}$ factors are expanded in Taylor series and only the first term kept. In this approximation, write $H_D = H_1$ in terms of the strength $E_0 = |\mathbf{E}|$ of the electric field, where the D subscript indicates the dipole approximation. To simplify the algebra, make a choice of phase of pure imaginary for the relevant expansion coefficient of the vector potential.

a.) The wave has the form

$$\vec{A}(x,t) = \vec{A}_0\cos(\vec{k}\cdot\vec{r} - \omega t)$$

(since we are "picking out" the term in the sum with wavenumber k as said in Piazza)

with

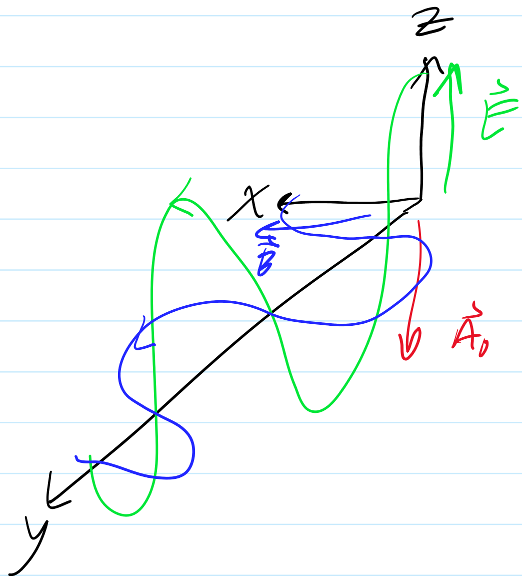
$$\vec{k} = k\hat{y}, \quad \omega = kc.$$

Since $\hat{y}\cdot\vec{r} = y$, we have

$$\vec{A}(x,t) = \vec{A}_0\cos(k(y - ct))$$

$$\vec{A}(x,t) = \vec{A}_0 \cos(k(y-ct))$$

Consider the diagram below:



We know that $\vec{A} = -\hat{z}A_0 \sin(k\overbrace{(y-ct)}^{y'})$ Thus we have

$$H_1 = -\frac{q}{m}\left(-A_0 \cos(ky') \cdot -i\hbar \frac{\partial}{\partial z}\right) + \frac{q^2}{2m} A_0^2 \cos^2(ky')$$
$$-\frac{q}{m} S_x \cdot B_0 \cos(ky')$$

Ignoring the second and third terms in H_1, we find that

$$H_1 = -\frac{q}{m} i\hbar A_0 \cos(ky') \frac{\partial}{\partial z}$$

or, more generally,

$$\boxed{H_1 = -\frac{q}{m} i\hbar \left(A_k e^{iky'} + A_k^* e^{-iky'}\right) \frac{\partial}{\partial z}}$$

with $y' = y - ct = ky - \omega_k t$

and

$$B_0 = kA_0 \qquad \text{(in natural units)}$$

b.) We know that

$$E_0 = k|A_0| = \frac{k}{2}|A_k|$$

Moreover,

$$\vec{A}(x,t) = -\hat{z}\left(A_k e^{iky'} + A_k^* e^{-iky'}\right)$$

Thus,

$$e^{iky} e^{-ikct} \quad e^{-iky} e^{ikct} \quad \omega = kc$$

$$H_p = H_1 \approx -\frac{q}{m} i\hbar \left(A_k \underbrace{e^{ik(y-ct)}} + A_k^* \underbrace{e^{-ik(y-ct)}}\right)\frac{\partial}{\partial z}$$

We now expand this in terms of the tailor series. We choose $A_k = a_k * i$ where i is the imaginary unit (and a_k is real). Therefore, we have

$$H_p = -\frac{q}{m} i\hbar\, a_k\left(i(1 + \cancel{iky}^{\to 0}) e^{-i\omega t} - i(1 - \cancel{iky}^{\to 0}) e^{i\omega t}\right)\partial_z$$

$$= -\frac{q}{m} i\hbar\, a_k\Big(\frac{1}{i}\left(e^{i\omega t} - e^{-i\omega t}\right)$$

$$\cancel{- ky\left(e^{i\omega t} + e^{-i\omega t}\right)}\Big)\partial_z$$

Higher-Order terms.

$$= -\frac{q}{m} i\hbar\, a_k\, 2\sin(\omega t)\,\partial_z$$

We know

We know

$$|\vec{E}| = |\partial_t \vec{A}| = \left| \frac{\partial}{\partial t}\left(a_k \cdot 2\sin(\omega t)\right)\right|$$

$$= 2\omega a_k |\cos\omega t| a_k$$

Thus,

$$\boxed{\begin{aligned} H_p &= -i\hbar \frac{q}{m} \sin(\omega t) \frac{|\vec{E}|}{\omega|\cos\omega t|} \partial_z \\ &\text{or} \\ H_p &= -i\hbar \frac{q}{mk}(\sin\omega t) E_0 \, \partial_z \\ &\text{where} \quad E_0 = \frac{k}{2} a_k \end{aligned}}$$

has time dependence