OPTI 507 - Solid State Optics F2002 -1-
Solutions by TA - Jason Auxier
HW # 4 - Chapter 5 problems

5.1. The Lagrangian of a system is

p.1482 Cohen-Tannoudji QM V. II

$$L(\vec{r}_i, \dot{\vec{r}}_i, t) \equiv KE - PE \quad \left(\dot{\vec{r}} \equiv \frac{d\vec{r}}{dt}\right)$$
$$= \frac{1}{2}\sum_{i=1}^{N} m_i (\dot{\vec{r}}_i)^2 - V(\vec{r}_i)$$
($\vec{r}_i \equiv$ position of ith particle)

Lagrange's equation of motion are

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i},$$

where q_i is the ~~...~~ coordinate. for the ith particle.

Notice that $\frac{d}{dt}$ is a total time-derivative, i.e., $\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \sum_{i=1}^{N} \dot{q}_i \frac{\partial}{\partial q_i} + \sum_{i=1}^{N} \ddot{q}_i \frac{\partial}{\partial \dot{q}_i}$.

This is because q_i and $\dot{q}_i$ are implicit functions of time. Now, care must be taken here. All these partials act only on explicit dependence of the variables (i.e., $\frac{\partial}{\partial t}(m\dot{x}) = 0$, $\frac{\partial}{\partial x}(m\dot{x}) = 0$, $\frac{\partial}{\partial \dot{x}}(m\dot{x}) = m$)

Now, for background, the EM field can be described by potentials:

$$\vec{B} = \nabla \times \vec{A}$$
$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

The Lorentz force is (No external forces/potentials)

$$\vec{F} = q\left(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}\right)$$
$$\Rightarrow m\ddot{\vec{r}} = q\left(\vec{E} + \frac{1}{c}\dot{\vec{r}} \times \vec{B}\right)$$

5.1 (cont.) The x-coord. is

$$m\ddot{x} = q\left[-\frac{\partial\phi}{\partial x} - \frac{1}{c}\frac{\partial A_x}{\partial t} + \frac{\dot{y}}{c}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) - \frac{\dot{z}}{c}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\right]$$

The cooresponding Lagrangian is

$$L(\vec{r}, \dot{\vec{r}}, t) = \frac{1}{2}m\dot{\vec{r}}^2 + \frac{q}{c}\dot{\vec{r}}\cdot\vec{A} - q\phi$$

To see this, let's use Lagrange's eq. (x-coord.):

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x} + \frac{q}{c}A_x$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial \dot{x}}\right) + \sum_{i=1}^{3}\left(\dot{x}_i\frac{\partial}{\partial x_i}\left(\frac{\partial L}{\partial \dot{x}}\right) + \ddot{x}_i\frac{\partial}{\partial \dot{x}_i}\left(\frac{\partial L}{\partial \dot{x}}\right)\right)$$

$$= \frac{q}{c}\frac{\partial A_x}{\partial t} + \left(\frac{q}{c}\dot{x}\frac{\partial A_x}{\partial x} + \frac{q}{c}\dot{y}\frac{\partial A_x}{\partial y} + \frac{q}{c}\dot{z}\frac{\partial A_x}{\partial z}\right) + m\ddot{x}$$

$$\frac{\partial L}{\partial x} = +\frac{q}{c}\dot{x}\frac{\partial A_x}{\partial x} + \frac{q}{c}\dot{y}\frac{\partial A_y}{\partial x} + \frac{q}{c}\dot{z}\frac{\partial A_z}{\partial x} - q\frac{\partial \phi}{\partial x}$$

Now, $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x}$

$$\Rightarrow m\ddot{x} + \frac{q}{c}\left[\frac{\partial A_x}{\partial t} + \dot{\vec{r}}\cdot\nabla A_x\right] = \frac{q}{c}\left[\dot{x}\frac{\partial A_x}{\partial x} + \dot{y}\frac{\partial A_y}{\partial x} + \dot{z}\frac{\partial A_z}{\partial x} - \frac{\partial \phi}{\partial x}\right]$$

$$\Rightarrow m\ddot{x} = q\left[-\frac{\partial\phi}{\partial x} - \frac{1}{c}\frac{\partial A_x}{\partial t} + \frac{\dot{y}}{c}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) + \frac{\dot{z}}{c}\left(\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right)\right]$$

This is the same eq. of motion we derived from the Lorentz force. You would find similar agreement for the y- & z-components. Thus, L is the correct Lagrangian.

Now, we can calculate the momentum:

$$\vec{p} = \frac{\partial L}{\partial \vec{v}} = \frac{\partial L}{\partial \dot{\vec{r}}}$$

$$\vec{p} = m\dot{\vec{r}} + \frac{q}{c}\vec{A}$$

$$\Rightarrow \dot{\vec{r}} = \frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)$$

5.1 (cont.) The Hamiltonian is defined as

$$H = KE + PE \quad \text{(Now, I will add the Lattice potential } W(\vec{r})\text{)}$$

$$\equiv \vec{p}\cdot\dot{\vec{r}} - L \equiv 2KE - L$$

Using $\dot{\vec{r}} = \frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)$, we obtain

$$H = \vec{p}\cdot\frac{1}{m}\left(\vec{p} - \frac{q}{c}\vec{A}\right) - \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 - \frac{q}{cm}\left(\vec{p} - \frac{q}{c}\vec{A}\right)\cdot\vec{A} + q\phi + W(\vec{r})$$

$$= \frac{1}{m}\left(p^2 - \frac{q}{c}\vec{p}\cdot\vec{A} - \frac{q}{c}\vec{p}\cdot\vec{A} + \frac{q^2}{c^2}A^2\right) - \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi + W(\vec{r})$$

$$\boxed{H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + W(\vec{r}) + q\phi}$$

This is the eq. we want with $m \to m_e$, $q \to e$.

5.2 Show $[f(\vec{r}), \vec{P}] = i\hbar \nabla f(\vec{r})$

We know $[x, p_x] = i\hbar$, $\vec{P} = -i\hbar\nabla$.

Now, $[f, -i\hbar\nabla]g = -i\hbar f\nabla g + i\hbar\nabla(fg)$

$$= -i\hbar f\nabla g + i\hbar(f\nabla g + g\nabla f)$$

$$= i\hbar\, g\nabla f$$

$$= (i\hbar\nabla f)g$$

$\therefore$ $\underline{[f, \vec{P}] = i\hbar\nabla f}$

5.3. Show $[H_0, \vec{r}] = \frac{\hbar\vec{P}}{i m_0}$ with $H \equiv -\frac{\hbar^2}{2m_0}\nabla^2 + W(\vec{r})$

Notice: $[A+B, C] = (A+B)C - C(A+B)$

$$= AC + BC - CA - CB$$

$$= (AC - CA) + (BC - CB)$$

$$= [A, C] + [B, C]$$

$\Rightarrow [A+B, C] \equiv [A, C] + [B, C]$

Also, $[W(\vec{r}), \vec{r}] = 0$ since $W(\vec{r})$ can be written as a Taylor expansion about $\vec{r}=0$.

so, $[H_0, \vec{r}] = [-\frac{\hbar^2}{2m_0}\nabla^2, \vec{r}] = -\frac{\hbar^2}{2m_0}[\nabla^2, \vec{r}]$

Now, $[\frac{\partial^2}{\partial x^2}, x]g = \frac{\partial^2(xg)}{\partial x^2} - x\frac{\partial^2 g}{\partial x^2} \equiv [\nabla^2, \vec{r}]_x g$

$$= \left(g\frac{\partial^2}{\partial x^2}(x) + 2\frac{\partial}{\partial x}(x)\frac{\partial g}{\partial x} + \cancel{x}\frac{\partial^2 g}{\partial x^2}\right) - x\frac{\partial^2 g}{\partial x^2}$$

$$= 2\frac{\partial g}{\partial x} = 2\nabla_x g$$

Extrapolating for other two components,

$$[\nabla^2, \vec{r}] = 2\nabla$$

$\therefore [H_0, \vec{r}] = -\frac{\hbar^2}{m_0}\nabla = -\frac{\hbar^2}{m_0}\frac{1}{-i\hbar}(-i\hbar\nabla) = \frac{\hbar\vec{P}}{i m_0}$

$\Rightarrow [H_0, \vec{r}] = \frac{\hbar\vec{P}}{i m_0}$

See Appendix I for a clever way to prove this.

5.4. Eq. (5.22) says

$$H = \frac{p^2}{2m_0} + W(\vec{r}) - \frac{e}{m_0 c}\vec{A}\cdot\vec{p} + \frac{e^2}{2m_0c^2}A^2$$

Show $(\vec{A}\cdot\vec{p}$ term$) \gg (A^2$ term$)$. $\frac{p}{\hbar} = 10^5 \frac{1}{cm}$ & $I_0 = 10^6 \frac{W}{cm^2}$

Now, $\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$ $\quad \boxed{E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}}$

$\vec{E} = \vec{E_0}e^{-i\omega t} \Rightarrow \vec{E_0} = i\frac{\omega}{c}\vec{A_0}$ $\quad \nabla\cdot\vec{A} = 0$

$\Rightarrow A_0 \sim \frac{c}{\omega}E_0 = 30\frac{c}{\omega}\sqrt{I_0}$

Look at the largest intensity in the range with an optical freq. in the visible ($\lambda = 500nm$).

$\omega = \frac{2\pi c}{\lambda} \Rightarrow A_0 = 30\frac{(0.5\times10^{-4}cm)}{2\pi}10^3\, V/cm$

$A_0 \approx 0.2V$

Now, $\hbar = 6.59\times10^{-16}\,eV\cdot s$

$\Rightarrow p = (10^5\frac{1}{cm})(6.6\times10^{-16}\,e\cancel{V}\cdot s) = 6.6\times10^{-11}\frac{eV\cdot s}{cm}$

1st term: $\frac{e}{m_0 c}\vec{A}\cdot\vec{p} \approx \frac{e^2}{m_0}\frac{(0.2V)(6.6\times10^{-11}V\cdot\frac{1}{cm/s})}{2.9979\times10^{10}\,cm/s}$

$= 4.4\times10^{-22}\frac{V^2}{(cm/s)^2}\frac{e^2}{m_0}$

2nd term: $\frac{e^2}{2m_0c^2}A^2 = \frac{e^2}{m_0}\frac{(0.2V)^2}{2(2.99\times10^{10}\,cm/s)^2}$

$= 2.2\times10^{-23}\frac{V^2}{(cm/s)^2}\frac{e^2}{m_0}$

$\therefore \frac{1st\ term}{2nd\ term} \approx 20$

Thus at $I_0 = 10^6\,W/cm^2$, the 1st term is 20X larger than the second. Since $A \sim \sqrt{I_0}$ as you decrease I_0, the margin between the terms will increase.

Appendix I Prove $[H_0, \vec{r}] = \frac{\hbar \vec{p}}{i m_0}$

This is a very useful commutator:

$$[AB, C] = ABC - CAB$$
$$= ABC - ACB + ACB - CAB$$
$$= A[B, C] + [A, C]B$$

$$\therefore [\vec{p}^2, \vec{r}] = \vec{p}[\vec{p}, \vec{r}] + [\vec{p}, \vec{r}]\vec{p} = -2i\hbar \vec{p}$$

$$\therefore [H_0, \vec{r}] = [\tfrac{1}{2m_0}\vec{p}^2, \vec{r}] = -\frac{i\hbar}{m_0}\vec{p}$$

$$\Rightarrow [H_0, \vec{r}] = \frac{\hbar \vec{p}}{i m_0}$$

Appendix II Delta Function Representations

Properties: (See Gaskill or Barrett or Zemanian)

$$\delta(x - x_0) = 0 \quad x \neq x_0$$
$$\int_{x_1}^{x_2} f(\alpha)\,\delta(\alpha - x_0)\,d\alpha = f(x_0), \quad x_1 < x_0 < x_2$$
$$\delta(ax - x_0) = \frac{1}{|a|}\,\delta\!\left(x - \frac{x_0}{a}\right)$$
$$\delta(-x + x_0) = \delta(x - x_0)$$
$$\delta(-x) = \delta(x)$$
$$f(x)\,\delta(x - x_0) = f(x_0)\,\delta(x - x_0)$$
$$\delta(x)\,\delta(x - x_0) = 0, \quad x_0 \neq 0$$
$$\int_{-\infty}^{+\infty} \delta(\alpha - x_0)\,\delta(x - \alpha)\,d\alpha = \delta(x - x_0)$$

Limiting Representations:

$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\epsilon}\,\mathrm{rect}\!\left(\frac{x}{\epsilon}\right)$$
$$\delta(x) = \lim_{\epsilon \to 0} \frac{\epsilon/\pi}{x^2 + \epsilon^2}$$
$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{2\epsilon}\, e^{-\frac{|x|}{\epsilon}}$$
$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{2\epsilon}\,\mathrm{sech}^2\!\left(\frac{|x|}{\epsilon}\right)$$
$$\delta(x) = \lim_{n \to \infty} \frac{n}{\sqrt{\pi}}\, e^{-n^2 x^2}$$
$$\delta(x) = \lim_{k \to \infty} k\,\mathrm{sinc}(kx) = \lim_{k \to \infty} \frac{\sin(\pi k x)}{\pi x}$$

Closure: $\delta(x) = \int_{-\infty}^{+\infty} d\nu\, e^{2\pi i \nu x}$