8.322: Quantum Theory II

Problem Set #8 Solutions
April 23, 2007

1. **Lagrangian and Hamiltonian Schrödinger field theory**

(a) The Lagrangian is

$$L = \int dx \left(i\hbar \Psi^\dagger \dot{\Psi} - \frac{\hbar^2}{2m} \nabla \Psi^\dagger \cdot \nabla \Psi - \Psi^\dagger V(x) \Psi \right)$$

Using the Euler-Lagrange equations,

$$\frac{d}{dt}\frac{\delta L}{\delta \dot{\Psi}^\dagger} = \frac{\delta L}{\delta \Psi^\dagger} \qquad \text{and} \qquad \frac{d}{dt}\frac{\delta L}{\delta \dot{\Psi}} = \frac{\delta L}{\delta \Psi}$$

and integrating by parts on the spatial derivative term, we obtain the Schrödinger equation

$$i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(x)\Psi \tag{0.1}$$

and its conjugate

$$-i\hbar\dot{\Psi}^\dagger = -\frac{\hbar^2}{2m}\nabla^2\Psi^\dagger + \Psi^\dagger V(x) \tag{0.2}$$

Hence we identify

$$\Psi^\dagger = \Psi^*$$

(b) By definition

$$\Pi^\dagger = \frac{\delta L}{\delta \dot{\Psi}^\dagger}$$

and since the Lagrangian does not depend on $\dot{\Psi}^\dagger$, we obtain

$$\Pi^\dagger = 0.$$

The other momentum is nonzero

$$\Pi = i\hbar\Psi^\dagger$$

The Hamiltonian

$$H = \int dx (i\hbar\Psi^\dagger\dot{\Psi} - L) = \int dx \left(\frac{\hbar}{2mi}\nabla\Pi\cdot\nabla\Psi - \frac{i}{\hbar}\Pi V \Psi \right) = H(\Psi, \Pi)$$

(c)

$$\frac{\delta H}{\delta \Pi} = \frac{i\hbar}{2m}\nabla^2\Psi - \frac{i}{\hbar}V\Psi = \dot{\Psi}$$

Thus we get (0.2). Also,

$$\frac{\delta H}{\delta \Psi} = \frac{i\hbar}{2m}\nabla^2\Psi - \frac{i}{\hbar}\Pi V = -\dot{\Pi}$$

and by substituting $\Pi = i\hbar\Psi^\dagger$, we obtain (0.1).

2. **Aspects of second quantization**

(a)

$$H = \int dx \left(\frac{\hbar^2}{2m}\nabla\Psi^\dagger\nabla\Psi + V\Psi^\dagger\Psi\right) = \int dx \left(-\frac{i\hbar}{2m}\nabla\Pi\cdot\nabla\Psi - \frac{i}{\hbar}V\Pi\Psi\right)$$

$$\begin{aligned} i\hbar\dot{\Psi} = [\Psi, H] &= \left[\Psi(x,t),\ \int dx' \left(-\frac{i\hbar}{2m}\nabla\Pi(x',t)\cdot\nabla\Psi(x',t) - \frac{i}{\hbar}V(x')\Pi(x',t)\Psi(x',t)\right)\right] \\ &= \int dx' \left(\frac{i\hbar}{2m}\left[\Psi(x,t),\Pi(x',t)\right]\nabla^2\Psi(x',t) - \frac{i}{\hbar}V(x')\left[\Psi(x,t),\Pi(x',t)\right]\Psi(x',t)\right) \\ &= \int dx' \left(\frac{i\hbar}{2m}\nabla^2\Psi(x',t) - \frac{i}{\hbar}V(x')\Psi(x',t)\right) i\hbar\delta(x-x') \end{aligned}$$

Hence,

$$i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\nabla^2\Psi(x,t) + V(x)\Psi(x,t)$$

(b)

$$\frac{1}{i\hbar}\left[\Psi(x,t),\Pi(x',t)\right] = \left[\Psi(x,t),\Psi^\dagger(x',t)\right] = \delta^3(x-x')$$

$$\left[\sum_i a_i\psi_i(x)e^{-iE_it/\hbar},\ \sum_m a_m^\dagger\psi_m^*(x')e^{iE_mt/\hbar}\right] = \delta^3(x-x')$$

$$\int dx\ \psi_n^*(x)\left[\sum_i a_i\psi_i(x)e^{-iE_it/\hbar},\ \sum_m a_m^\dagger\psi_m^*(x')e^{iE_mt/\hbar}\right] = \psi_n^*(x')$$

$$\left[a_ne^{-iE_nt/\hbar},\ \sum_m a_m^\dagger\psi_m^*(x')e^{iE_mt/\hbar}\right] = \psi_n^*(x')$$

$$\int dx'\ \psi_l(x')\left[a_ne^{-iE_nt/\hbar},\ \sum_m a_m^\dagger\psi_m^*(x')e^{iE_mt/\hbar}\right] = \delta_{ln}$$

$$\left[a_n,\ a_l^\dagger\right]e^{-i(E_n-E_l)t/\hbar} = \delta_{ln}$$

$$\Rightarrow \quad \left[a_n,\ a_l^\dagger\right] = \delta_{ln}$$

Similarly, $[\Psi(x,t),\Psi(x',t)] = 0$, therefore

$$[a_n,\ a_l] = 0$$

(c) We have

$$\phi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

$$\phi(x,t) = \int K(x,t;x',t') \sum_m c_m \psi_m(x') e^{-iE_m t/\hbar} dx'$$

Hence

$$K(x,t;x',t') = \sum_n \psi_n(x)\psi_n(x') e^{iE_n(t'-t)}\ \theta(t-t')$$

Now,

$$\left[\Psi(x,t), \Psi^\dagger(x',t)\right] = \sum_{n,m} \left[a_n,\ a_m^\dagger\right] \psi_n(x)\psi_m(x') e^{-iE_n t/\hbar} e^{iE_m t/\hbar}$$

$$= \sum_n \psi_n(x)\psi_n(x') e^{iE_n(t-t')}$$

and thus

$$K(x,t;x',t') = \theta(t-t') \left[\Psi(x,t), \Psi^\dagger(x',t)\right]$$

(d)

$$[N,H] = \left[\int dx\ \Psi^\dagger(x,t)\Psi(x,t),\ \int dx' \left(\frac{\hbar^2}{2m}\nabla\Psi^\dagger(x',t)\cdot\nabla\Psi(x',t) + V(x',t)\Psi^\dagger(x',t)\Psi(x',t)\right)\right]$$

The commutator of N with the term in H proportional to the potential vanishes. Thus,

$$[N,H] = \int dx \int dx'\ \frac{\hbar^2}{2m} \big(\nabla \big[\Psi^\dagger(x,t)\Psi(x,t),\ \Psi^\dagger(x',t)\big] \nabla\Psi(x',t) + \nabla\Psi^\dagger(x',t)\nabla \big[\Psi^\dagger(x,t)\Psi(x,t),\ \Psi(x',t$$

$$= \int dx \int dx'\ \frac{\hbar^2}{2m} \left\{\nabla\left(\Psi^\dagger(x,t)\delta^3(x-x')\right)\nabla\Psi(x',t) + \nabla\Psi^\dagger(x',t)\nabla\left(-\delta^3(x-x')\Psi(x,t)\right)\right\}$$

$$= \int dx'\ \frac{\hbar^2}{2m}\left(\nabla\Psi^\dagger\cdot\nabla\Psi - \nabla\Psi^\dagger\cdot\nabla\Psi\right) = 0$$

Physically, the eigenvalue of N gives the number of particles in the system.

(e) Reversing the computation in (b) and replacing [ ] by { } yields

$$\{\Psi(x),\ \Psi^\dagger(x')\} = \delta^3(x-x')$$

$$\{\Psi(x),\ \Psi(x')\} = \{\Psi^\dagger(x),\ \Psi^\dagger(x')\} = 0$$

Note that the transition from commutators to anticommutators is possible because

$$[ab,c] = a\{b,c\} - \{c,a\}b = a[b,c] - [c,a]b$$

Explicitly,

$$i\hbar\dot{\Psi}(x,t) = [\Psi(x,t),\ H] = \left[\Psi(x,t),\ \int dx' \left(\frac{\hbar^2}{2m}\nabla\Psi^\dagger(x',t)\cdot\nabla\Psi(x',t) + V(x')\Psi^\dagger(x',t)\Psi(x',t)\right)\right]$$

$$= \int dx' \left(\frac{\hbar^2}{2m}\left[\Psi(x,t),\ \nabla\Psi^\dagger(x',t)\cdot\nabla\Psi(x',t)\right] + V(x')\left[\Psi(x,t),\ \Psi^\dagger(x',t)\Psi(x',t)\right]\right)$$

$$\left[\Psi(x,t),\ \nabla\Psi^\dagger(x',t)\cdot\nabla\Psi(x',t)\right] =$$

$$\nabla\left(\{\Psi(x,t),\ \Psi^\dagger(x',t)\} - \Psi^\dagger(x',t)\Psi(x,t)\right)\nabla\Psi(x',t) + \nabla\Psi^\dagger(x',t)\Psi(x,t)\nabla\Psi(x',t) = \nabla\delta^3(x-x')\cdot\nabla\Psi(x',t)$$

Similarly,

$$\left[\Psi(x,t),\ \Psi^\dagger(x',t)\Psi(x',t)\right] = \delta^3(x-x')\Psi(x',t)$$

Hence,

$$i\hbar\dot{\Psi}(x,t) = \int dx' \left(-\frac{\hbar^2}{2m}\delta^3(x-x')\nabla^2\Psi(x',t) + V(x')\delta^3(x-x')\Psi(x',t)\right)$$

$$i\hbar\dot{\Psi}(x,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(x,t) + V(x)\Psi(x,t)$$

(f) By the anticommutation relations,

$$\left\{a_k^\dagger, a_{k'}^\dagger\right\} = 0$$

we obtain

$$a_k^\dagger a_k^\dagger = -a_k^\dagger a_k^\dagger = 0$$

If we now consider $|k_1, k_2, \ldots, k_n\rangle$ with $k_i = k_j$, then by means of the anticommutation relations we can move $a_{k_i}^\dagger$ next to $a_{k_j}^\dagger$ and we get

$$|k_1, k_2, \ldots, k_n\rangle = \pm\, a_{k_1}^\dagger a_{k_2}^\dagger \cdots a_{k_{j-1}}^\dagger \left(a_{k_i}^\dagger a_{k_j}^\dagger\right) a_{k_{j+1}}^\dagger \cdots a_{k_n}^\dagger |\Omega\rangle$$

Since

$$\left(a_{k_i}^\dagger a_{k_j=k_i}^\dagger\right) = 0$$

the above state is zero.

If $k_i \neq k_j$ for $i \neq j$, then we can move the creation operators in the same way. We only need to figure out the overall sign. If we want to exchange k_i and k_j, then we need to move $a_{k_i}^\dagger$ step–by–step to the j–th position which gives a factor of $(-1)^\alpha$. We also need to move $a_{k_j}^\dagger$ to the i–th position that gives the same sign $(-1)^\alpha$, due to the symmetry. These factors cancel each other. And finally, there is an extra sign coming from the step when we exchanged $a_{k_i}^\dagger$ and $a_{k_j}^\dagger$. Hence,

$$|k_1, k_2, \ldots, k_i, \ldots, k_j, \ldots k_n\rangle = -|k_1, k_2, \ldots, k_j, \ldots, k_i, \ldots k_n\rangle$$

(g) If $k_i = k_j$ for $i \neq j$, then clearly

$$\langle k_1, k_2, \ldots | k_1, k_2, \ldots \rangle = 0$$

If all k_i's are distinct, then by definition

$$\langle k_1, k_2, \ldots | k_1, k_2, \ldots \rangle = \langle \Omega | a_{k_n} a_{k_{n-1}} \cdots a_{k_1} a^{\dagger}_{k_1} a^{\dagger}_{k_2} \cdots a^{\dagger}_{k_n} | \Omega \rangle$$

As in (f), we can move the operators and thus we obtain

$$\langle k_1, k_2, \ldots | k_1, k_2, \ldots \rangle = \langle \Omega | \left(a_{k_n} a^{\dagger}_{k_n} \right) \cdots \left(a_{k_1} a^{\dagger}_{k_1} \right) | \Omega \rangle$$

Using

$$a_{k_i} a^{\dagger}_{k_i} | \Omega \rangle = (1 - a^{\dagger}_{k_i} a_{k_i}) | \Omega \rangle = | \Omega \rangle$$

gives

$$\langle k_1, k_2, \ldots | k_1, k_2, \ldots \rangle = 1$$

(h) We have the expansion

$$\Psi(x,t) = \sum_j a_j \psi_j(x) e^{-iE_j t/\hbar} = \sum_j a_j \psi_j(x,t)$$

where $\psi_j(x,t)$ satisfies the time–dependent Schroedinger equation. Then,

$$\langle \Omega | \Psi(x_1,t_1) \cdots \Psi(x_m,t_m) | k_1, \ldots k_m \rangle = \sum_{p_1, p_2, \ldots} \psi_{p_1}(x_1,t_1) \cdots \psi_{p_m}(x_m,t_m) \; \langle \Omega | a_{p_1} \cdots a_{p_m} a^{\dagger}_{k_1} \cdots a^{\dagger}_{k_m} | \Omega \rangle$$

If $\{p_i\}_{i=1\ldots m}$ is not a permutation of $\{k_j\}_{j=1\ldots m}$, then the state gives zero, since we can move a_{p_i} to $|\Omega\rangle$ by the anticommutation relations. Hence,

$$\langle \Omega | \Psi(x_1,t_1) \cdots \Psi(x_m,t_m) | k_1, \ldots k_m \rangle = \sum_{\sigma} \psi_{\sigma(k_1)}(x_1,t_1) \cdots \psi_{\sigma(k_m)}(x_m,t_m) \; \langle \Omega | a_{\sigma(k_1)} \cdots a_{\sigma(k_m)} a^{\dagger}_{k_1} \cdots a^{\dagger}_{k_m} | \Omega$$

where σ is a permutation. We can rearrange the $a_{\sigma(k_i)}$ annihilation operators to obtain

$$\langle \Omega | \Psi(x_1,t_1) \cdots \Psi(x_m,t_m) | k_1, \ldots k_m \rangle =$$

$$\sum_{\sigma} (\text{sign } \sigma) \psi_{\sigma(k_1)}(x_1,t_1) \cdots \psi_{\sigma(k_m)}(x_m,t_m) \; \langle \Omega | a_{k_1} \cdots a_{k_m} a^{\dagger}_{k_1} \cdots a^{\dagger}_{k_m} | \Omega \rangle$$

$$= \pm \sum_{\sigma} (\text{sign } \sigma) \psi_{\sigma(k_1)}(x_1,t_1) \cdots \psi_{\sigma(k_m)}(x_m,t_m) \; \langle \Omega | a_{k_m} \cdots a_{k_1} a^{\dagger}_{k_1} \cdots a^{\dagger}_{k_m} | \Omega \rangle$$

The above sign depends only on m. The vev gives 1 (see (g) for example) and thus we get the antisymmetric wavefunction for m particles. Comparing this form to the Slater determinant fixes the constant factor to

$$C_m = \frac{1}{\sqrt{m!}}$$

3. **Coulomb interactions in a box**

Including the spin–part, the operator $\Psi(x)$ takes the following form

$$\Psi(x) = \sum_{k,\sigma} a_{k,\sigma}\phi_k(x)\chi_\sigma$$

$$\Psi^\dagger(x) = \sum_{k,\sigma} a^\dagger_{k,\sigma}\phi^*_k(x)\chi^\dagger_\sigma$$

such that $\int_V dx\ \phi^*_k(x)\phi_{k'}(x) = \delta_{kk'}$ and $\chi^\dagger_\sigma\chi_{\sigma'} = \delta_{\sigma\sigma'}$.

Two parallel spins are given by the state

$$|k,\sigma;k',\sigma\rangle = a^\dagger_{k,\sigma}a^\dagger_{k',\sigma}|\Omega\rangle$$

Two antiparallel spins

$$|k,\sigma;k',-\sigma\rangle = a^\dagger_{k,\sigma}a^\dagger_{k',-\sigma}|\Omega\rangle$$

Now,

$$V_{\text{Coulomb}} = \frac{1}{2}\sum_{k_i,\sigma_j}\int d^3x\ d^3y\ \frac{\phi^*_{k_1}(x)\phi_{k_2}(x)\phi^*_{k_3}(y)\phi_{k_4}(y)}{|x-y|}\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4} : a^\dagger_{k_1,\sigma_1}a_{k_2,\sigma_2}a^\dagger_{k_3,\sigma_3}a_{k_4,\sigma_4} :$$

Normal ordering gives

$$: a^\dagger_{k_1,\sigma_1}a_{k_2,\sigma_2}a^\dagger_{k_3,\sigma_3}a_{k_4,\sigma_4} := -a^\dagger_{k_1,\sigma_1}a^\dagger_{k_3,\sigma_3}a_{k_2,\sigma_2}a_{k_4,\sigma_4}$$

Then for $|k,\sigma;k',\sigma'\rangle$ we have

$$\langle V_{\text{Coulomb}}\rangle = -\frac{1}{2}\sum_{k_i,\sigma_j}\int d^3x\ d^3y\ \frac{\phi^*_{k_1}(x)\phi_{k_2}(x)\phi^*_{k_3}(y)\phi_{k_4}(y)}{|x-y|}\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4}\times$$

$$\times\langle\Omega|a_{k',\sigma'}a_{k,\sigma}a^\dagger_{k_1,\sigma_1}a^\dagger_{k_3,\sigma_3}a_{k_2,\sigma_2}a_{k_4,\sigma_4}a^\dagger_{k,\sigma}a^\dagger_{k',\sigma'}|\Omega\rangle$$

We perform Wick contractions on the vev. Thus,

$$\langle V_{\text{Coulomb}}\rangle = -\frac{1}{2}\int d^3x\ d^3y\ \frac{\phi^*_k(x)\phi_{k'}(x)\phi^*_{k'}(y)\phi_k(y)}{|x-y|}\delta_{\sigma\sigma'} - \frac{1}{2}\int d^3x\ d^3y\ \frac{\phi^*_{k'}(x)\phi_k(x)\phi^*_k(y)\phi_{k'}(y)}{|x-y|}\delta_{\sigma\sigma'} +$$

$$+\frac{1}{2}\int d^3x\ d^3y\ \frac{|\phi_k(x)|^2|\phi_{k'}(y)|^2}{|x-y|} + \frac{1}{2}\int d^3x\ d^3y\ \frac{|\phi_{k'}(x)|^2|\phi_k(y)|^2}{|x-y|}$$

Hence, the energy difference of parallel and antiparallel spin alignments

$$\langle\sigma\sigma|V_{\text{Coulomb}}|\sigma\sigma\rangle - \langle\sigma,-\sigma|V_{\text{Coulomb}}|\sigma,-\sigma\rangle = -\int d^3x\ d^3y\ \frac{\phi^*_k(x)\phi_{k'}(x)\phi^*_{k'}(y)\phi_k(y)}{|x-y|}$$

Let $u = x - y$. Then,

$$\Delta E = -\frac{1}{V^2}\int_V \left(\int \frac{e^{i(k'-k)u}}{|u|} du\right) dy = -\frac{1}{V}\int \frac{e^{i(k'-k)u}}{|u|} du = -\frac{4\pi}{V|k-k'|^2}$$

where the integral has been performed in the approximation that the box is infinitely large. This approximation works if $\frac{1}{|\vec{k}-\vec{k}'|} \ll R$, where R is a typical linear dimension of the box. If, however, the momenta are almost equal, the integral must be done more carefully. Consider, for example, the case $\vec{k} = \vec{k}'$. Then the integral yields $\Delta E = ce^2/V^{1/3}$, where c is a constant that depends on the specific shape of the box. This differs from the large box approximation, which appears to diverge as $\vec{k} \to \vec{k}'$.