Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **April 9, 2007**

Assignment 8

DUE APRIL 20, 2007, AT THE END OF THE DAY

Announcements

- Please keep an eye on the website, http://web.mit.edu/8.322/, for updates on the problem set.

Reading topics for this period

Many particle quantum mechanics.

- Second Quantization

Reading Recommendations 8

- On second quantization: Gottfried and Yan, §11.2. You can find more discussion of second quantization in Baym (§19); Merzbacher (§20); and Schiff (§55). If you read only one of these references, Baym or Schiff would be best.
- Degenerate fermi gas: Notes *Degenerate Fermion Systems* posted on line §1.1 — 1.3.

Problem Set 8

Topics covered in the problems

- Classical Schrödinger field theory
- Second Quantization
- Exchange energy

Problems

For clarity, I've kept $\hbar \neq 1$ in these problems.

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

   The aim of this problem is to work through the foundations of second quantization. In lecture I introduced a second field, Φ, into the classical Lagrangian. This problem takes a slightly different approach: Ψ and $\Psi^\dagger$ are taken as independent canonical variables.

   Consider a system governed by the Lagrangian

   $$\mathbf{L} = \int d\mathbf{x} \left(i\hbar \Psi^\dagger \dot{\Psi} - \frac{\hbar^2}{2m} \nabla \Psi^\dagger \cdot \nabla \Psi - \Psi^\dagger V(\mathbf{x}) \Psi \right) \tag{1}$$

   where Ψ and $\Psi^\dagger$ are regarded as independent variables.

   (a) Use the Euler-Lagrange equations,

   $$\frac{d}{dt} \frac{\delta \mathbf{L}}{\delta \dot{q}(\mathbf{x},t)} = \frac{\delta \mathbf{L}}{\delta q(\mathbf{x},t)}$$

   for the "coordinates", $q = \Psi$ and $\Psi^\dagger$, to show that the classical equation of motion for the fields $\Psi(\mathbf{x},t)$ are the Schrödinger equation and the relation $\Psi^\dagger = \Psi^*$.

   (b) Define the momenta canonically conjugate to Ψ and $\Psi^\dagger$ to be

   $$\Pi \equiv \frac{\delta \mathbf{L}}{\delta \dot{\Psi}} \text{ and } \Pi^\dagger \equiv \frac{\delta \mathbf{L}}{\delta \dot{\Psi}^\dagger}.$$

   Show $\Pi^\dagger$ is zero. Then construct the Hamiltonian,

   $$\mathbf{H}(\Psi, \Pi, \Psi^\dagger, \Pi^\dagger) \equiv \int d\mathbf{x} \left(\Pi \dot{\Psi} + \Pi^\dagger \dot{\Psi}^\dagger - \mathcal{L} \right)$$

   and show that it can be written as a function of only Ψ and Π, $\mathbf{H} = \mathbf{H}(\Psi, \Pi)$.

   (c) Verify Hamilton's equation, $\delta\mathbf{H}/\delta\Pi = \dot{\Phi}$ and $\delta\mathbf{H}/\delta\Psi = -\dot{\Pi}$, reduce to the Schrödinger equation for the field Ψ.

2. **Aspects of second quantization**

   Consider the Schrödinger field operator, $\Psi(\mathbf{x},t)$ and its conjugate momentum,

   $$\Pi \equiv i\hbar \Psi^\dagger,$$

   obeying the canonical quantization relations,

   $$\begin{aligned} \left[\Psi(\mathbf{x},t), \Pi(\mathbf{x}',t)\right] &= i\hbar\delta^3(\mathbf{x}-\mathbf{x}') \\ \left[\Psi(\mathbf{x},t), \Psi(\mathbf{x}',t)\right] &= \left[\Pi(\mathbf{x},t), \Pi(\mathbf{x}',t)\right] = 0. \end{aligned} \tag{2}$$

   Let the second quantized Hamiltonian *operator* be

   $$\mathbf{H} = \int d\mathbf{x} \left(\frac{\hbar^2}{2m} \nabla \Psi^\dagger \cdot \nabla \Psi + V(\mathbf{x}) \Psi^\dagger \Psi \right)$$

(a) Show that the quantum equation of motion for $\Psi(\mathbf{x},t)$,

$$i\hbar\dot{\Psi}(\mathbf{x},t) = [\Psi(\mathbf{x},t), \mathbf{H}] \tag{3}$$

reduces to the Schödinger wave equation,

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

Suppose, for simplicity that the *first quantized* Hamiltonian, $H = -\hbar^2\nabla^2/2m + V(\mathbf{x})$, has a discrete spectrum (eigenstates ψ_n, eigenvalues E_n).

(b) Suppose $\Psi(\mathbf{x},t)$ is expanded in the normalized eigenstates, $\{\psi_n\}$, of H,

$$\Psi(\mathbf{x},t) = \sum_n a_n \psi_n(\mathbf{x}) e^{-iE_n t/\hbar}$$

Show

$$[a_n, a_m^\dagger] = \delta_{nm} \quad \text{and} \quad [a_n, a_m] = 0$$

(c) Show that

$$K(\mathbf{x},t;\mathbf{x}',t') = \theta(t-t')[\Psi(\mathbf{x},t), \Psi(\mathbf{x}',t')]$$

is the propagator that we introduced last term. [Note K is a c-number, not an operator.]

(d) Show that the operator

$$\mathbf{N} = \int d\mathbf{x}\Psi^\dagger(\mathbf{x},t)\Psi(\mathbf{x},t)$$

is conserved by showing that it commutes with $\mathbf{H}$. What is the interpretation of $\mathbf{N}$?

Suppose, instead, that we had quantized this system with anticommutation relations,

$$\{a_n, a_m^\dagger\} = \delta_{nm} \quad \text{and} \quad \{a_n, a_m\} = 0.$$

(e) How are the canonical commutation relations of the fields (eq. (2)) altered? Verify that the quantum equation of motion, eq. (3), still yields the Schrödinger equation even though the fields now obey anticommutation relations.

Consider the state:

$$|k_1 k_2 ... k_m\rangle = a_{k_1}^\dagger a_{k_2}^\dagger ... a_{k_m}^\dagger |\Omega\rangle$$

where $|\Omega\rangle$ is the state annihilated by all the $\{a_m\}$,

$$a_m|\Omega\rangle = 0, \text{ for all } m.$$

$|\Omega\rangle$ is normalized, $\langle\Omega|\Omega\rangle = 1$.

(f) Show that $|k_1 k_2 ... k_m\rangle = 0$ if $k_i = k_j$, and that

$$|k_1 k_2 ... k_i ... k_j ... k_m\rangle = -|k_1 k_2 ... k_j ... k_i ... k_m\rangle.$$

(g) What is

$$\langle k_1 k_2 ... k_m | k_1 k_2 ... k_m \rangle?$$

(h) Show that

$$\phi_{k_1 k_2 \ldots k_m}(\mathbf{x_1}, t_1; \mathbf{x_2}, t_2; \ldots \mathbf{x_m}, t_m) = C_m \langle \Omega | \Psi(\mathbf{x_1}, t_1) \Psi(\mathbf{x_2}, t_2) ... \Psi(\mathbf{x_m}, t_m) | k_1 k_2 ... k_m \rangle$$

is the totally antisymmetric Schrödinger wavefunction for m-particles in the states $k_1, k_2, ..., k_m$. What value of C_m normalizes ϕ to unity?

3. **Coulomb interactions in a box**

Two electrons are in plane wave states in a box. [You can take the coordinate space wave functions to be

$$\phi_{\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}}$$

with $\int_V d\mathbf{x}\, \phi^*_{\mathbf{k}}(\mathbf{x}) \phi_{\mathbf{k}'}(\mathbf{x}) = \delta_{\mathbf{k},\mathbf{k}'}$.] The second quantized form of the coulomb interaction is

$$\mathbf{V}_{\text{coul}} = \frac{1}{2} \; : \int d\mathbf{x} d\mathbf{y} \frac{\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})\Psi^\dagger(\mathbf{y})\Psi(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} :$$

Calculate to first order in the coulomb interaction the energy difference of parallel and antiparrallel spin alignments.