

RG Methods in Statistical Field Theory:

Problem Set 9

due: Friday, December 1, 2006

To get a feel for fermionic systems and Grassmann number methods, let us consider a simple example: the single-site Hubbard model. The lattice version of this model has been one of the most intensely studied physical problems of the last forty years, and has still not been solved exactly in more than one dimension. It describes a system of electrons localized at lattice sites, with two possible interactions: (i) the electrons can tunnel to neighboring lattice sites; (ii) if an up-spin and down-spin electron sit on the same site, they feel a strong Coulomb repulsion. The model was originally developed to describe electrons in narrow bands in solids, but in recent years has achieved prominence as one of the leading candidates to explain high-temperature superconductivity.

In the one-site version of the Hubbard model the electrons have nowhere to tunnel, so the only interaction is Coulomb repulsion. We will first solve the model by operator methods (which is very easy), and then see how we can reformulate the problem in terms of integrals over Grassmann numbers. The two approaches will give the same answer, but in working through the Grassmann method, we will encounter particular problems which will help motivate the idea of path integrals in the next lecture.

Our system consists of a single site with four possible states: the site is empty, singly occupied by an up- or down-spin electron, or doubly occupied by two electrons of opposite spins. We will denote these states by the kets $|\circ\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\uparrow\downarrow\rangle$ respectively. To describe these states we need two different sets of creation/destruction operators: c_{\uparrow}^{\dagger} , c_{\uparrow} for up-spin electrons, and c_{\downarrow}^{\dagger} , c_{\downarrow} for down-spin electrons. These satisfy the anticommutation relations:

$$\{c_{\sigma}, c_{\sigma'}^{\dagger}\} = \delta_{\sigma\sigma'}, \quad \{c_{\sigma}, c_{\sigma'}\} = \{c_{\sigma}^{\dagger}, c_{\sigma'}^{\dagger}\} = 0$$

where $\sigma, \sigma' = \uparrow$ or \downarrow , and $\delta_{\sigma\sigma'}$ is the Kronecker delta. In terms of these operators our four states are:

$$|\circ\rangle, \quad |\uparrow\rangle \equiv c_{\uparrow}^{\dagger}|\circ\rangle, \quad |\downarrow\rangle \equiv c_{\downarrow}^{\dagger}|\circ\rangle, \quad |\uparrow\downarrow\rangle \equiv c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}|\circ\rangle$$

Note that the order of the c_{\downarrow}^{\dagger} and c_{\uparrow}^{\dagger} operators in the definition of $|\uparrow\downarrow\rangle$ is a convention: if we had reversed the order it means multiplying the state by an overall minus sign. However, once we fix the convention, make sure to always write $|\uparrow\downarrow\rangle$ in the same way, so as to avoid mistakes.

Let us define the following number operators: $n_{\uparrow} \equiv c_{\uparrow}^{\dagger}c_{\uparrow}$ and $n_{\downarrow} \equiv c_{\downarrow}^{\dagger}c_{\downarrow}$, which count the number of \uparrow and \downarrow electrons respectively. The total number operator is then $N \equiv n_{\uparrow} + n_{\downarrow}$. The Hamiltonian for our system is:

$$\mathcal{H}_0 = \Omega_0 N + U n_{\uparrow} n_{\downarrow}$$

Thus when the site is singly occupied the energy is Ω_0 , but if it is doubly occupied there is an additional Coulomb repulsion U , making the total energy $2\Omega_0 + U$.

(a) Let us work in the grand canonical ensemble, with a Hamiltonian $\mathcal{H} = \mathcal{H}_0 - \mu N$ and grand partition function $Z = \text{Tr} e^{-\beta \mathcal{H}}$. Using standard quantum mechanics techniques, calculate the trace in the basis of eigenstates and find Z .

(b) Find the free energy $A = -(1/\beta) \ln Z$ and calculate the average particle number $\langle N \rangle = -\partial A / \partial \mu$. Plot $\langle N \rangle$ as a function of μ for $\Omega_0 = U = 1$ and large β . Show that in the limit of $T \rightarrow 0$ ($\beta \rightarrow \infty$) we get the following behavior:

$$\langle N \rangle = \begin{cases} 0 & \mu < \Omega_0 \\ 1 & \Omega_0 < \mu < \Omega_0 + U \\ 2 & \mu > \Omega_0 + U \end{cases}$$

This has a very simple interpretation: for $\mu < \Omega_0$ the state with the lowest free energy has no electrons; for $\Omega_0 < \mu < \Omega_0 + U$ we have enough chemical potential to inject a single electron into the system, but there is still not enough to overcome the Coulomb repulsion U ; finally when $\mu > \Omega_0 + U$ we can add two electrons.

(c) Now let us try to rederive the above results using the Grassmann approach. We first need to define a basis of coherent states. In class, we considered a system with a single fermion state, and thus a single set of creation/destruction operators c^\dagger, c , and we found that a coherent state could be specified by a single Grassmann number ψ : the ket $|\psi\rangle \equiv |0\rangle - \psi|1\rangle = \exp(-\psi c^\dagger)|0\rangle$, where we use the simple Taylor expansion $\exp(-\psi c^\dagger) = 1 - \psi c^\dagger$. Our system here has two different fermion states: the electrons at the lattice site can be either spin-up or spin-down, and there are two sets of creation/destruction operators. It turns out we will need two different Grassmann numbers to specify a coherent state. If we denote these numbers ψ_\uparrow and ψ_\downarrow , then the coherent state is given by:

$$|\psi_\uparrow, \psi_\downarrow\rangle \equiv \exp(-\psi_\uparrow c_\uparrow^\dagger - \psi_\downarrow c_\downarrow^\dagger)|\circ\rangle$$

To prove that this is a coherent state, let us first derive a useful identity. By expanding out both sides, show that:

$$\exp(-\psi_\uparrow c_\uparrow^\dagger - \psi_\downarrow c_\downarrow^\dagger) = \exp(-\psi_\uparrow c_\uparrow^\dagger) \exp(-\psi_\downarrow c_\downarrow^\dagger)$$

This is a consequence of a general theorem that says $e^{A+B} = e^A e^B$ if A and B commute, $AB = BA$. (Note that $\psi_\uparrow c_\uparrow^\dagger$ commutes with $\psi_\downarrow c_\downarrow^\dagger$.) Now prove that:

$$c_\uparrow |\psi_\uparrow, \psi_\downarrow\rangle = \psi_\uparrow |\psi_\uparrow, \psi_\downarrow\rangle = |\psi_\uparrow, \psi_\downarrow\rangle \psi_\uparrow, \quad c_\downarrow |\psi_\uparrow, \psi_\downarrow\rangle = \psi_\downarrow |\psi_\uparrow, \psi_\downarrow\rangle = |\psi_\uparrow, \psi_\downarrow\rangle \psi_\downarrow$$

Thus $|\psi_\uparrow, \psi_\downarrow\rangle$ is a simultaneous eigenstate of c_\uparrow and c_\downarrow , with eigenvalues ψ_\uparrow and ψ_\downarrow respectively.

(d) The completeness identity in the basis $\{|\circ\rangle, |\uparrow\rangle, |\downarrow\rangle, |\updownarrow\rangle\}$ is:

$$\mathbf{1} = |\circ\rangle\langle\circ| + |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\updownarrow\rangle\langle\updownarrow|$$

We would like to write an analogous completeness identity for the basis of coherent states. Using the definitions in part (c) and your knowledge of Grassmann integration from class, prove that:

$$\mathbf{1} = \int |\psi_{\uparrow}, \psi_{\downarrow}\rangle \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| \exp(-\bar{\psi}_{\downarrow}\psi_{\downarrow} - \bar{\psi}_{\uparrow}\psi_{\uparrow}) d\bar{\psi}_{\uparrow} d\psi_{\uparrow} d\bar{\psi}_{\downarrow} d\psi_{\downarrow}$$

Note that the coherent state bra $\langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}|$ is defined as:

$$\langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| \equiv \langle \circ| \exp(-c_{\uparrow}\bar{\psi}_{\uparrow} - c_{\downarrow}\bar{\psi}_{\downarrow})$$

and satisfies:

$$\langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| c_{\uparrow}^{\dagger} = \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| \bar{\psi}_{\uparrow} = \bar{\psi}_{\uparrow} \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}|, \quad \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| c_{\downarrow}^{\dagger} = \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| \bar{\psi}_{\downarrow} = \bar{\psi}_{\downarrow} \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}|$$

(e) Before we can rewrite the partition function Z in terms of Grassmann integrals, we need one more result. Prove the following:

$$\langle n|\psi_{\uparrow}, \psi_{\downarrow}\rangle \langle \bar{\psi}_{\uparrow}, \bar{\psi}_{\downarrow}| e^{-\beta\mathcal{H}}|n\rangle = \langle -\bar{\psi}_{\uparrow}, -\bar{\psi}_{\downarrow}| e^{-\beta\mathcal{H}}|n\rangle \langle n|\psi_{\uparrow}, \psi_{\downarrow}\rangle$$

where $|n\rangle$ is any one of the basis states $\{|\circ\rangle, |\uparrow\rangle, |\downarrow\rangle, |\updownarrow\rangle\}$.

(f) Finally we are ready to rewrite Z . Using the results of parts (d) and (e), show that partition function Z can be written as:

$$\begin{aligned} Z &= \sum_{n=0}^3 \langle n| e^{-\beta\mathcal{H}}|n\rangle \\ &= \int \langle -\bar{\psi}_{\uparrow}, -\bar{\psi}_{\downarrow}| e^{-\beta\mathcal{H}}|\psi_{\uparrow}, \psi_{\downarrow}\rangle \exp(-\bar{\psi}_{\downarrow}\psi_{\downarrow} - \bar{\psi}_{\uparrow}\psi_{\uparrow}) d\bar{\psi}_{\uparrow} d\psi_{\uparrow} d\bar{\psi}_{\downarrow} d\psi_{\downarrow} \end{aligned}$$

(g) After great efforts, we have turned our original boring partition function into something that looks much cooler. Let us now see whether we can evaluate the integrals. The key is to calculate $\langle -\bar{\psi}_{\uparrow}, -\bar{\psi}_{\downarrow}| e^{-\beta\mathcal{H}}|\psi_{\uparrow}, \psi_{\downarrow}\rangle$. As a first step, show that \mathcal{H} can be written as:

$$\mathcal{H} = (\Omega_0 - \mu)(c_{\uparrow}^{\dagger}c_{\uparrow} + c_{\downarrow}^{\dagger}c_{\downarrow}) + Uc_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}c_{\downarrow}c_{\uparrow}$$

Note that we have *normal ordered* the operators in the Hamiltonian: they have been rearranged so that in each term all the creation operators are to the left of all the destruction operators. We do this because for normal ordered terms it is easy to calculate matrix elements between coherent states. As an example, show that:

$$\langle -\bar{\psi}_{\uparrow}, -\bar{\psi}_{\downarrow}|\mathcal{H}|\psi_{\uparrow}, \psi_{\downarrow}\rangle = [(\Omega_0 - \mu)(-\bar{\psi}_{\uparrow}\psi_{\uparrow} - \bar{\psi}_{\downarrow}\psi_{\downarrow}) + U\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\psi_{\downarrow}\psi_{\uparrow}] e^{-\bar{\psi}_{\downarrow}\psi_{\downarrow} - \bar{\psi}_{\uparrow}\psi_{\uparrow}}$$

(h) Wouldn't life be nice if $\langle -\bar{\psi}_{\uparrow}, -\bar{\psi}_{\downarrow}| e^{-\beta\mathcal{H}}|\psi_{\uparrow}, \psi_{\downarrow}\rangle$ was just the exponential of the above result? Unfortunately, this is not the case. When you expand out $e^{-\beta\mathcal{H}}$ in a Taylor series, the higher order terms do *not* disappear (feel free to check this for yourself). And even

though \mathcal{H} is normal ordered, higher powers like $\mathcal{H}^2, \mathcal{H}^3, \dots$, are not normal ordered. Thus it seems you have to repeat part (g) for each power of \mathcal{H} , writing it out in terms of operators and rearranging them into normal ordered form, possibly generating additional terms in the process. At this point you should be horrified: calculating $\langle -\bar{\psi}_\uparrow, -\bar{\psi}_\downarrow | e^{-\beta\mathcal{H}} | \psi_\uparrow, \psi_\downarrow \rangle$ appears to be a highly non-trivial task. Here's the good news: the path integral approach which we will learn in the next lecture provides a beautiful way to solve the normal ordering problem. The bad news: you don't know the path integral approach yet. So you will somehow have to figure out how to normal order $e^{-\beta\mathcal{H}}$ the old-fashioned way: brute force. Happily, there are a few tricks:

To begin with, show that the operators n_\uparrow and n_\downarrow commute, and that $n_\uparrow^2 = n_\uparrow, n_\downarrow^2 = n_\downarrow$. Now look at the k th power of \mathcal{H} ,

$$\mathcal{H}^k = [(\Omega_0 - \mu)(n_\uparrow + n_\downarrow) + Un_\uparrow n_\downarrow]^k$$

Clearly when we multiply out the k factors and simplify, there will only be two types of operator terms: terms proportional to $(n_\uparrow + n_\downarrow)$, and terms proportional to $n_\uparrow n_\downarrow$. Since this is true for every power k , we know that the exponential $e^{-\beta\mathcal{H}}$ must equal:

$$e^{-\beta\mathcal{H}} = 1 + A(n_\uparrow + n_\downarrow) + Bn_\uparrow n_\downarrow$$

where A and B are some constants. To find A and B , apply both sides of the above equation to each of the eigenstates of \mathcal{H} . This will give you a set of equations that can be solved for A and B . Thus you have now written $e^{-\beta\mathcal{H}}$ in a way that can be easily normal ordered. Calculate $\langle -\bar{\psi}_\uparrow, -\bar{\psi}_\downarrow | e^{-\beta\mathcal{H}} | \psi_\uparrow, \psi_\downarrow \rangle$.

(i) At long last we are ready to find the answer: evaluate the Grassmann integrals for Z , and show that the result is the same as in part (a). Physics works! (Even if you use bizarre, confusing methods.) While the Grassmann approach may seem like overkill for the single-site Hubbard model, we will see that when combined with the path integral formulation, it will be the most elegant way of studying complicated fermionic systems. To generalize from this problem set to lattice models is easy: instead of just two sets of creation/destruction operators $c_\sigma^\dagger, c_\sigma$ for $\sigma = \uparrow, \downarrow$, we will have a different set of operators for every lattice site i , which we can label as: $c_{i\sigma}^\dagger, c_{i\sigma}$. These satisfy anticommutation relations:

$$\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}, \quad \{c_{i\sigma}, c_{j\sigma'}\} = \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0$$

Amazingly, almost every identity we derived in this problem set naturally generalizes to the lattice case (except the normal ordering results; that would make life too easy). We will explore the consequences of this next lecture.