Advanced Quantum Theory

Problem sheet 6
Fermions, Path integral in second quantisation

Set: 2, 5

Due: Monday 13 March 4pm (Solutions can be handed in during the lecture, or in the box in the Maths building, or by email to sebastian.muller@bristol.ac.uk)

1. *Hubbard model without spin*

   We consider a system allowing for indistinguishable *fermionic* particles. The system has three sites, and the operators $a_i^\dagger$ and a_i ($i = 1, 2, 3$) are the creation and annihilation operators for particles on these sites. The Hamiltonian of the system is

   $$\hat{H} = -a_1^\dagger a_2 - a_2^\dagger a_3 - a_2^\dagger a_1 - a_3^\dagger a_2 + \frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$$

   where $\hat{n}_i = a_i^\dagger a_i$. This is the fermionic counterpart of the Bose-Hubbard model studied in question 1 but we are interested in the case of three sites.

   (a) Explain why in the present case the interaction term $\frac{1}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$ does not matter.

   (b) We are interested specifically in the case that our system contains two particles. Write down the basis states of the system with two particles.

   (c) Investigate how the Hamiltonian acts on the basis states determined in (a). Use your result to represent the Hamiltonian (now restricted to the case of two particles) in matrix form and determine its eigenvalues.

2. *Hubbard model with spin*

   Consider the fermionic system with the Hamiltonian

   $$\hat{H} = -a_1^\dagger a_2 - a_2^\dagger a_1 - a_3^\dagger a_4 - a_4^\dagger a_3 + U(\hat{n}_1\hat{n}_3 + \hat{n}_2\hat{n}_4)$$

   where $\hat{n}_i = a_i^\dagger a_i$. Here the states 1 and 2 are spin-up states at the first and the second site, and the states 3 and 4 are spin-down states at the first and the second site. The Hamiltonian contains terms related to jumps between the two sites, and interaction terms that contribute if both the spin-up state and the spin-down state at the same site are occupied.

   Determine the energy levels of the system for the case that three particles are present.

3. *Arbitrarily many sites*

   (From the 2015/16 exam. This was following a question dealing with the special case $K = 3$ so you may want to consider $K = 3$ to get an idea for a solution.) Consider a fermionic (and spinless) quantum system with K single-particle states and the Hamiltonian

   $$\hat{H} = -\sum_{i=1}^{K-1}(a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1}) - \frac{U}{2}\hat{N}(\hat{N} - 1)$$

   where $\hat{N} = \sum_{i=1}^{K} a_i^\dagger a_i$ and U is a real number. We are interested in the energy levels for the case that $K - 1$ particles are present in the system. Determine a matrix H such that all these energy levels are eigenvalues of H. You are not asked to evaluate the energy levels explicitly.

4. *a_i and $a_i^\dagger$ for fermions*

   (a) Show that the creation and annihilation operators for fermions a_i, $a_i^\dagger$ satisfy the anti-commutation relations as given in the lecture.

   (b) Show that if $|\Psi\rangle$ and $|\Phi\rangle$ are two states with arbitrarily many indistinguishable *fermionic* particles and a_i, $a_i^\dagger$ are creation and annihilation operators, we have

$$\langle\Phi|a_i|\Psi\rangle = \langle\Psi|a_i^\dagger|\Phi\rangle^*$$

   i.e. a_i and $a_i^\dagger$ are adjoint operators. In your proof you can use that the scalar product of states with different particle numbers vanishes by definition.

5. *Path integral for systems in second quantisation*

   In the lecture we considered the following path integral for a system with discrete sites in second quantisation

$$\begin{aligned}\text{tr } e^{-\frac{i}{\hbar}\hat{H}t} &= \int D[a_1, a_2, \ldots] \exp\Big[\int_0^t dt'\Big(-\sum_j a_j^*(t')\dot{a}_j(t') \\ &\quad -\frac{i}{\hbar}H(a_1(t'), a_2(t'), \ldots, a_1^*(t'), a_2^*(t'), \ldots)\Big)\Big].\end{aligned}$$

   Here the integral is taken over functions $a_j(t')$ that satisfy the condition $a_j(0) = a_j(t)$.

   (a) Specify the integration measure $\int D[a_1, a_2, \ldots]\ldots$ based on the analogy to the harmonic oscillator discussed in the lecture.

   (b) Write down the path integral for tr $e^{-\frac{i}{\hbar}\hat{H}t}$ for the many-particle Hamiltonian $\hat{H} = \sum_{i,j} h(i,j)a_i^\dagger a_j + \frac{1}{2}\sum_{i,j} U_{\text{int}}(i,j)a_i^\dagger a_j^\dagger a_j a_i$.

   (c) Assume that the creation and annihilation operators are for states fixed at discrete sites with positions $x_j = \frac{j}{K}$. Here the index j runs from 0 to $K-1$ and we have periodic boundary conditions meaning that the K-th site at $x_K = 1$ is identified with the 0-th site at $x_0 = 0$. Also assume that the matrix with the elements $h(i,j)$ has the form

$$h = -\frac{\hbar^2}{2m}K^2 \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ 1 & & & 1 & -2 \end{pmatrix}$$

   where all elements apart from those on the diagonal, next to the diagonal, and in the upper right and lower left corners are zero. This form arises from discretising the kinetic energy in the case of sites with distances $\frac{1}{K}$. Moreover we take $U_{\text{int}}(i,j) = 0$ i.e. there is no interaction. For this setting determine the path integral in (b) in the continuum limit $K \to \infty$. You should obtain an integral involving $a(x,t')$ and $a^*(x,t')$ that still has a factor K in the exponent.

6. *Perturbation theory for the Bose-Hubbard model*

Consider the Bose-Hubbard model

$$\hat{H} = -a_1^\dagger a_2 - a_2^\dagger a_1 + \frac{\epsilon}{2}\sum_i \hat{a}_i^{\dagger 2} a_i^2$$

where the interaction term is taken as proportional to a constant $\epsilon \ll 1$. We want to use perturbation theory to determine $\operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t}$ neglecting terms of order ϵ^4 and higher. Define the analogue of the operator A for this case. You can take as given that it has an integral kernel $G_{jk}(t', t'')$ where the subscripts refer to the two sites and the continuous arguments to time. Write your result in terms of the corresponding trace for $\epsilon = 0$ and the integral kernel. You do not have to determine an explicit formula for either of these two ingredients, and you can assume a natural generalisation of Wick's theorem. (See PS 3, Q 1 for a variant of Wick's theorem with complex variables.)

Drop in sessions: Thu 10:30-11:30, Fri 10:30-11:30 (Howard House 4.08)