PH325: Advanced Statistical Mechanics

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Semester I, 2014–2015

PROBLEM SET 3, DUE: OCT. 30, 2014

3/1. **(C/T) Tight binding:** Consider fermions hopping on a 1D chain given by the hamiltonian

$$\mathcal{H} = -t \sum_i \left(c^\dagger_{i+1} c_i + \text{h. c.} \right).$$

The density of fermions is x per site.

(a) "Diagonalize" the hamiltonian.

(b) Assuming that the system is in contact with a particle reservoir which sets the chemical potential to be μ, find the partition function of the system. You MUST use methods and techniques of occupation number formalism to solve this part of the problem.

(c) Obtain an equation of the chemical potential μ as a function of temperature. Solve this equation and make a plot of it.

(d) Find the specific heat of the system as a function of temperature and make a plot of the same. Specifically focus on $T \ll t$ and $T \gg t$. Are you surprised?

3/2. **(C/T) XXZ model:** The XXZ model defined on a 1D-chain consists of spin-1/2s at each site interacting with its neighbours via

$$\mathcal{H} = -J \sum_i \left(\sigma^+_{i+1} \sigma^-_i + \sigma^+_i \sigma^-_{i+1} \right) - J_z \sum_i \sigma^z_{i+1} \sigma^z_i$$

where σs are the usual Pauli matrices.

(a) What are the symmetries of this Hamiltonian? Focus on the internal symmetries.

(b) Use the Jordan-Wigner transformation find an equivalent fermionic model.

(c) Comment on the manifestation of the symmetries that you found in the spin-problem in the fermionic context.

(d) Is it possible to solve this problem exactly?

3/3. **(C/T) Bosons:** In the discussion in class, we had seen how the operators $c^\dagger_i$ describe states of fermions. Bosons on a 1D lattice are created by the operators $a^\dagger_i$.

(a) Find an occupation number basis for the state of bosons on a lattice (use "real-space" representation like we did for fermions in class).

(b) Use the definition of $a^\dagger_i$ and write a state in the occupation number basis using the vacuum state and the operators $a^\dagger_i$.

(c) What should be the algebra of the a-operators for us to correctly obtain the bosonic statistics.

(d) Repeat problem 3/1 with bosons. Are you surprised?

3/4. **(C/T) Bose-Hubbard model and hardcore bosons:** Consider bosons hopping on a 1-d lattice with amplitude t. There is strong repulsion between bosons if they are on the same site, this is described by a scale U. The Hamiltonian is

$$\mathcal{H} = -t \sum_i \left(a^\dagger_{i+1} a_i + \text{h. c.} \right) + U \sum_i a^\dagger_i a^\dagger_i a_i a_i$$

(a) Write out the meaning of the second term in the hamiltonian.

(b) Suppose U were zero, and the filling is one boson per site, then what is the ground state $(t \neq 0)$?

(c) When the filling is one boson per site, what is the ground state when $t = 0$, $U > 0$?

(d) We have seen spins, fermions and (now) bosons in 1D. We have seen that spins are related to fermions. Is there any relationship between the bosons introduced in this problem and spins/fermions? Explore (with care and thought). Hint: it may help you to read the next part of the question.

(e) Now consider the filling of bosons is $x < 1$ per site with $U = \infty$, and $t \neq 0$ – these are called hardcore bosons (why?). What is the ground state of the system? What are the excitations of the system, and what is it specific heat as a function of temperature? (Note that this problem has an exact solution!)

3/5. **(C) Mean field and Feynman:** Show the meanfield theory is a "sub-class" of the Feynman approach. Hint: Consider H_{MFT} as H_0 where $\langle A_\alpha \rangle$ and $\langle B_\alpha \rangle$ are the parameters "λ" of H_0.

3/6. **(C) Feynman and Potts:** Consider the q-state Potts model on a d-cubic lattice with $\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{s_i s_j}$. Use Feynman variational principle to obtain the phase diagram of the system. How well does your results match (with known results, or results that you can infer from intuition) for different ds? Are the results consistent with known results for $J > 0$ and $J < 0$?

3/7. **(C/T) MFT of Ising model:** Construct a mean-field phase diagram of the *anti*-ferro Ising model (with near neighbour interactions) on a d-cubic lattice. Does your answer match the results known prior (see, for example, problem 2/8.)? (Pay careful attention to what "magnetic field" means.)

3/8. **(C/T) MFT of Heisenberg model:** Consider a classical Heisenberg model with 3-component vector spins $\mathbf{S}_i$ at each lattice site of a d-cubic lattice.

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i \mathbf{n} \cdot \mathbf{S}_i$$

where $\langle ij \rangle$ runs over the nearest neighbour bonds, $\mathbf{n}$ is the direction of the magnetic field. Use mean field theory to obtain the phase diagram in the $T - h$ plane. Does your answer depend on the sign of J? Perform a thorough investigation.

3/9. **(C/T) MFT in the quantum setting:** Consider fermions hopping on a 1D lattice with a Hamiltonian

$$H = -t \sum_i \left(c^\dagger_{i+1} c_i + c^\dagger_i c_{i+1} \right) + V \sum_i c^\dagger_{i+1} c^\dagger_i c_i c_{i+1}$$

We are given a filling (average number of fermions per site) $x \ll 1$ of fermions (take $x = 1/10$ to be definite), and our goal is to find out the zero temperature phase diagram as a function of V/t (going from negative to positive).

(a) Treating $c^\dagger_{i+1} c^\dagger_i c_i c_{i+1}$ by mean field ansatz with $\langle c^\dagger_{i+1} c_i \rangle = \Gamma$, obtain a mean field Hamiltonian (watch out for $-$ signs carefully, you are handling fermions!). Find the "best" value of Γ and obtain the ground state energy as a function of V/t. Comment on what symmetry is broken by choosing this type of mean-field.

(b) Now, take $\langle c^\dagger_{i+1} c^\dagger_i \rangle = \Delta$ and find the ground state energy etc. Again, comment on what symmetry is broken in this case?

(c) Construct a zero temperature mean field phase diagram as a function of V/t. Is there a quantum phase transition in this system?

This problem illustrates that mean field theory can be done in multiple ways...one get the physics right typically when one's intuition is right! Later in ths course you will find out that the conclusions of this exercise (even if your calculations are "correct") are not quite right!

3/10. **(C/T) Mean field theory of the Bose-Hubbard model:** Consider the Bose-Hubbard model on a d-cubic lattice.

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left(a^\dagger_i a_j + \text{h. c.} \right) + U \sum_i a^\dagger_i a^\dagger_i a_i a_i - \mu \sum_i a^\dagger_i a_i$$

Using the mean field ansatz to decouple the *kinetic energy* operator[1] as $a^\dagger_i a_j = \langle a^\dagger_i \rangle a_j + a^\dagger_i \langle a_j \rangle - \langle a^\dagger_i \rangle \langle a_j \rangle$ to obtain a zero-temperature phase diagram in the $\mu/U, t/U$ plane.

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[1] This idea was pioneered at IISc many years back!