Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 12:30, Room D201) **Sheet 11**

Hand in: Mon 14.01.2019 *(questions marked as $*$ are optional)*
Discussion date: Fri 18.01.2019

17. Mean-field theory from the variational principle

In this problem we will rederive the mean-field approximation from the variational principle introduced in our lectures on the Hartree-Fock approximation. Consider the Heisenberg model on the cubic lattice,

$$H = -J \sum_{(i,j)} \vec{\sigma}_i \cdot \vec{\sigma}_j - h \sum_i \sigma_i^z. \tag{1}$$

The system is in the canonical state at temperature T; we denote $\beta = 1/T$. For avoid complication with units, we set $\hbar = 1$, $\mu_B = 1$ and $k_B = 1$ throughout. Recall from the lectures on the Hartree-Fock approximation that the idea is to approximate the canonical state $\rho = e^{-\beta H}/Z$ by a non-interacting one, $\rho_{\text{eff}}(t) = e^{-\beta H_{\text{eff}}}/Z_{\text{eff}}$, with

$$H_{\text{eff}} = -t \sum_i \sigma_i^z. \tag{2}$$

As in the lectures, the effective field t is obtained by minimising the canonical potential (free energy),

$$F[\rho_{\text{eff}}(m)] = \langle H - H_{\text{eff}} \rangle_{\text{eff}} + F_{\text{eff}} \geq F, \tag{3}$$

with $F = -T \ln Z$, $F_{\text{eff}} = -T \ln Z_{\text{eff}}$ and we use the magnetisation $m = \tanh(\beta t)$ to reparametrize H_{eff} for convenience. Note that $\langle \cdot \rangle_{\text{eff}}$ denotes the mean value with respect to the effective non-interacting density operator ρ_{eff}.

(a) (10pts) Derive the explicit expression for $F[\rho_{\text{eff}}(m)]$. You should find, $F[\rho_{\text{eff}}(m)] = -N(zJm + h)m + NT[\frac{1-m}{2} \ln \frac{1-m}{2} + \frac{1+m}{2} \ln \frac{1+m}{2}]$ with $z = 6$ for the cubic lattice.

Hint: You can use $F_{\text{eff}} = \langle H_{\text{eff}} \rangle_{\text{eff}} - TS_{\text{eff}}$, where S_{eff} is the entropy of the effective system (see Problem 0f). Then use the Shannon formula $S = -\sum_i p_i \ln p_i$ to evaluate the entropy S_{eff} (see Problem 0f).

(b) (5pts) Derive the mean-field self-consistent equation for m by minimising $F[\rho_{\text{eff}}(m)]$ with respect to m. Derive the critical temperature T_c where the system develops a spontaneous magnetisation.

(c) (5pts) Sketch $F[\rho_{\text{eff}}(m)]$ as a function of m for $T > T_c$ and $T < T_c$.

18. Critical exponents of the transverse Ising chain

Consider the transverse Ising chain with rescaled parameter $\lambda > 0$,

$$H = -\sum_i [\sigma_i^x + \lambda \sigma_i^z \sigma_{i+1}^z]. \tag{4}$$

Recall how this is solved: one performs the Jordan–Wigner transformation (ignoring the boundary terms), Fourier transformation, and then diagonalises the obtained Hamiltonian (the last step is generically known as Bogolyubov transformation). Eventually one obtains a new diagonal Hamiltonian,

$$H = 2\sum_q \omega_q \eta_q^\dagger \eta_q + \text{const}, \tag{5}$$

where $(\eta_q^\dagger, \eta_q)$ are fermionic operators, $\omega_q = (1 + 2\lambda\cos q + \lambda^2)^{1/2}$ and $\text{const} = -\sum_q \omega_q$.

(a) (10pts) What is the ground state energy E_0 of the system? Remember to transform any sums over momenta to integrals. You are of course not required to perform the elliptic integral explicitly. Show that $\partial E_0/\partial\lambda$ diverges at $\lambda_c = 1$.

(b) (10pts) What is the first excited state E_1 in the system? Show that the gap $\Delta = E_1 - E_0$ vanishes at some $\lambda_c = 1$, signalling a long range correlation in the system (the correlation length is $\xi \sim \Delta^{-1}$). Compute the critical exponent ν, defined by the divergence of the correlation length near the critical point $\xi \sim |\lambda - \lambda_c|^{-\nu}$.