https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_22/TMP-TA3/index.html

Sheet 9:

Hand-out: Friday, June 24, 2022[1]

Problem 1 Quantum-Classical mapping: XY model

In this problem we consider the 1D quantum XY model, which can be described by the Hamiltonian

$$\hat{\mathcal{H}}_{\mathrm{XY}} = U\sum_j (\hat{n}_j - \overline{n})^2 - t\sum_j \cos\left(\hat{\theta}_{j+1} - \hat{\theta}_j\right). \tag{1}$$

Here $\hat{n}_i = -i\partial_{\theta_i}$ can be thought of as the conjugate (angular) momentum to the variable $\theta_i \in [0, 2\pi)$, with $[\hat{\theta}_i, \hat{n}_j] = i\delta_{i,j}$. The corresponding partition function can be defined by taking the trace in the eigen-basis $\{|\theta_j\rangle\}$ of $\hat{\theta}_j$:

$$Z = \mathrm{tr}\left(e^{-\beta\hat{\mathcal{H}}_{\mathrm{XY}}}\right) = \int_0^{2\pi}\prod_j d\theta_j\ \langle\underline{\theta}|e^{-\beta\hat{\mathcal{H}}_{\mathrm{XY}}}|\underline{\theta}\rangle. \tag{2}$$

(1.a) Before turning to the quantum case above, consider the *classical* anisotropic XY model in 2D, with classical angular variables $\theta_{j,s} \in [0, 2\pi)$ (indices j and s label the two spatial directions) and the energy functional

$$\mathscr{H} = -J_x\sum_{j,s}\cos(\theta_{j,s} - \theta_{j+1,s}) - J_y\sum_{j,s}\cos(\theta_{j,s} - \theta_{j,s+1}). \tag{3}$$

Write down the integral expression for the classical partition function Z_C for this model.

(1.b) Now we return to the quantum problem. Perform a Trotterization of Z in Eq. (2) and introduce identities

$$1 = \int_0^{2\pi}\prod_j d\theta_j|\underline{\theta}\rangle\langle\underline{\theta}|, \tag{4}$$

to derive a formal path-integral expression for Z, without evaluating any matrix-elements at this point. Use imaginary time steps $\delta\tau = \beta/N$ (later $N \to \infty$) and discrete imaginary times $\tau_s = s\delta\tau$.

(1.c) In (1.b) you encounter matrix elements of the form

$$\langle\underline{\theta}(\tau_{s+1})|e^{-\delta\tau\hat{\mathcal{H}}_{\mathrm{XY}}}|\underline{\theta}(\tau_s)\rangle. \tag{5}$$

Simplify these matrix elements by using $\langle\theta|n\rangle = e^{in\theta}$ and introducing another identity,

$$1 = \prod_j\sum_{n_j}|\underline{n}\rangle\langle\underline{n}|, \tag{6}$$

[1] If you would like to present your solution(s), feel free to send them to Henning Schlömer until Fri, July 01.

and using the Poisson summation formula and Villain approximation:

$$\sum_n e^{-Cn^2+in\theta} = \sqrt{\frac{\pi}{2C}} \sum_p e^{-\frac{1}{4C}(\theta+2\pi p)^2} \approx \text{const} \times \exp\left[\frac{1}{2C}\cos\theta\right]. \tag{7}$$

(1.d) From your results in (1.c) show for $\overline{n} \in \mathbb{Z}$ that

$$Z \propto Z_C. \tag{8}$$

In particular, discuss the Berry-phase contributions to the path integral and why integer $\overline{n} \in \mathbb{Z}$ ensures that Berry phase terms have no effect.

Problem 2 Charge-density wave instability in the 1D Fermi-Hubbard model

In this problem we study charge-density wave instabilities in the 1D spin-$1/2$ weakly attractive ($g > 0$) Fermi gas described by the Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}} = -t\sum_{j,\sigma}\left(\hat{c}^\dagger_{j+1,\sigma}\hat{c}_{j,\sigma} + \text{h.c.}\right) - g\sum_j \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}. \tag{9}$$

(2.a) Describe the ground state of the system at $g = 0$, and calculate $\langle\hat{n}_j\rangle = \sum_\sigma\langle\hat{n}_{j,\sigma}\rangle$. Assume half-filling and periodic boundaries.

(2.b) The effect of a weak staggered potential $V_j = -(-1)^j V_0$ is to induce a staggered charge density $\langle\hat{n}_{j,\sigma}\rangle = \langle\hat{n}_{j,\sigma}\rangle_{V_0=0} + (-1)^j\Delta_j/g$. In the interacting model at low temperatures this charge-density wave order will remain even after the staggered field V_0 is removed. Derive the following mean-field Hamiltonian, by ignoring fluctuations $\delta\hat{n}_j^2$ of the staggered charge density:

$$\hat{\mathcal{H}}_{\text{int}} \to \sum_j\left(-(-1)^j\Delta_j\hat{n}_j + \frac{\Delta_j^2}{g}\right) + \mathcal{O}(\delta\hat{n}_j^2). \tag{10}$$

(2.c) Describe how the transformation in (2.b) can be obtained as an exact result using a path-integral, using the Hubbard-Stratonovich trick. Note that the order parameter is real, not complex.

(2.d) Calculate the excitation spectrum of the mean-field Hamiltonian in the presence of uniform staggered order $\Delta_j \equiv \Delta \neq 0$. Note: You may use analogies with BCS formalism and utilize the spinor field $\hat{\Psi}_{k,\sigma} = (\hat{c}_{k,\sigma}, \hat{c}_{k+\pi,\sigma})^T$.

(2.e) Calculate the free energy $F[\Delta]$ and derive the gap equation for $\Delta(T)$ at finite temperatures T. Discuss how order can develop spontaneously at low T and sketch your result for $F[\Delta]$ for different temperatures.