

Sheet 9:

Hand-out: Friday, Jun 23, 2023

Problem 1 Quantum-Classical mapping: XY model

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

$$\hat{\mathcal{H}}_{\text{XY}} = U \sum_j (\hat{n}_j - \bar{n})^2 - t \sum_j \cos(\hat{\theta}_{j+1} - \hat{\theta}_j). \quad (1)$$

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 $\hat{\theta}_j$:

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

(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

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

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

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

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 $N \rightarrow \infty$) and discrete imaginary times $\tau_s = s\delta\tau$.

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

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

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

$$1 = \prod_j \sum_{n_j} |n_j\rangle \langle n_j|, \quad (6)$$

and using the Poisson summation formula and Villain approximation:

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

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

$$Z \propto Z_C. \quad (8)$$

In particular, discuss the Berry-phase contributions to the path integral and why integer $\bar{n} \in \mathbb{Z}$ 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

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

(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:

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

(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.