Problem Set 6:

Handout: Fri, Jul 03, 2020; Solutions: Fri, Jul 17, 2020

Problem 1 Lee-Low-Pines (LLP) transformation I

Consider the unitary transformation introduced for the Fröhlich model in the lecture:

$$\hat{U}_{\rm LLP} = \exp\left[i\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{P}}_{\rm ph}\right], \qquad \hat{\boldsymbol{P}}_{\rm ph} = \int d^d\boldsymbol{k}\ \boldsymbol{k}\ \hat{a}^\dagger_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}}. \tag{1}$$

(1.a) Derive the following relations,

$$\hat{U}^\dagger_{\rm LLP}\ \hat{a}^\dagger_{\boldsymbol{k}}\ \hat{U}_{\rm LLP} = \hat{a}^\dagger_{\boldsymbol{k}}\ e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{x}}} \tag{2}$$

$$\hat{U}^\dagger_{\rm LLP}\ \hat{\boldsymbol{p}}\ \hat{U}_{\rm LLP} = \hat{\boldsymbol{p}} - \hat{\boldsymbol{P}}_{\rm ph} \tag{3}$$

$$\hat{U}^\dagger_{\rm LLP}\ \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\ \hat{U}_{\rm LLP} = \hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}} \tag{4}$$

$$\hat{U}^\dagger_{\rm LLP}\ \hat{\boldsymbol{x}}\ \hat{U}_{\rm LLP} = \hat{\boldsymbol{x}}. \tag{5}$$

(1.b) Using (1.a), derive the transformed Fröhlich Hamiltonian:

$$\begin{aligned}\tilde{\mathcal{H}}_{\rm F} = \hat{U}^\dagger_{\rm LLP}\Big[\frac{\hat{\boldsymbol{p}}^2}{2M} + \int d^3\boldsymbol{k}\ \omega_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}} + \int d^3\boldsymbol{k}\ V_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{x}}}\left(\hat{a}_{\boldsymbol{k}} + \hat{a}^\dagger_{-\boldsymbol{k}}\right)\Big]\hat{U}_{\rm LLP} = \\ = \frac{1}{2M}\left(\hat{\boldsymbol{p}} - \hat{\boldsymbol{P}}_{\rm ph}\right)^2 + \int d^3\boldsymbol{k}\ \omega_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}} + \int d^3\boldsymbol{k}\ V_{\boldsymbol{k}}\left(\hat{a}_{\boldsymbol{k}} + \hat{a}^\dagger_{-\boldsymbol{k}}\right)\end{aligned} \tag{6}$$

Problem 2 Lee-Low-Pines (LLP) transformation II

Consider two *distinguishable* quantum particles (masses M_1, M_2) described by the following Hamiltonian:

$$\hat{\mathcal{H}}_{12} = \frac{\hat{\boldsymbol{p}}_1^2}{2M_1} + \frac{\hat{\boldsymbol{p}}_2^2}{2M_2} + V(\hat{\boldsymbol{x}}_1 - \hat{\boldsymbol{x}}_2). \tag{7}$$

(2.a) Define a LLP transformation $\hat{U}_{\rm LLP}$ which transforms into the co-moving frame with particle 1. Derive the transformed Hamiltonian!

(2.b) Solve the model in (2.a) for $V(x) = \frac{1}{2}m\omega^2 x^2$.

Problem 3 Lee-Low-Pines (LLP) mean-field theory

Consider the general Fröhlich Hamiltonian, with LLP transform $\tilde{\mathcal{H}}_{\mathrm{F}}$ discussed in Problem (1.b). We will use the variational ansatz of coherent states in the LLP frame, $|\tilde{\psi}_{\mathrm{MF}}\rangle = \prod_{\boldsymbol{k}} |\alpha_{\boldsymbol{k}}\rangle \otimes |\boldsymbol{q}\rangle$, which corresponds to the wavefunction $|\psi_{\mathrm{MF}}(\boldsymbol{q})\rangle = \hat{U}_{\mathrm{LLP}}|\tilde{\psi}_{\mathrm{MF}}\rangle \otimes |\boldsymbol{q}\rangle$ in the lab frame.

(3.a) Derive the expression for the mean-field variational energy functional from the lecture – Eq. (72) on p. III-34 in the lecture notes:

$$\mathscr{H}_{\mathrm{MF}}(\boldsymbol{q}, [\alpha_{\boldsymbol{k}}]) = \langle\tilde{\psi}_{\mathrm{MF}}|\langle\boldsymbol{q}|\tilde{\mathcal{H}}_{\mathrm{LLP}}|\boldsymbol{q}\rangle|\tilde{\psi}_{\mathrm{MF}}\rangle = \langle\Psi_{\mathrm{MF}}(\boldsymbol{q})|\hat{\mathcal{H}}_{\mathrm{F}}|\Psi_{\mathrm{MF}}(\boldsymbol{q})\rangle \tag{8}$$

(3.b) From the expression obtained for the energy functional $\mathscr{H}_{\mathrm{MF}}(\boldsymbol{q}, [\alpha_{\boldsymbol{k}}])$, derive the saddle-point equations which become:

$$\alpha_{\boldsymbol{k}} = -\frac{V_{\boldsymbol{k}}}{\Omega_{\boldsymbol{k}}[\alpha_{\boldsymbol{k}}]}, \tag{9}$$

$$\Omega_{\boldsymbol{k}}[\alpha_{\boldsymbol{k}}] = \omega_{\boldsymbol{k}} + \frac{\boldsymbol{k}^2}{2M} - \frac{1}{M}\boldsymbol{k}\cdot\left(\boldsymbol{q} - \boldsymbol{P}_{\mathrm{ph}}^{\mathrm{MF}}[\alpha_{\boldsymbol{k}}]\right), \tag{10}$$

$$\boldsymbol{P}_{\mathrm{ph}}^{\mathrm{MF}}[\alpha_{\boldsymbol{k}}] = \int d^d\boldsymbol{k}\ \boldsymbol{k}\ |\alpha_{\boldsymbol{k}}|^2. \tag{11}$$

(3.c) Simplify $\mathscr{H}_{\mathrm{MF}}(\boldsymbol{q}, [\alpha_{\boldsymbol{k}}])$ for the mean-field saddle-point solution $\alpha_{\boldsymbol{k}}$ from Eq. (9): show that

$$\mathscr{H}_{\mathrm{MF}}(\boldsymbol{q}) = \frac{1}{2M}\left(\boldsymbol{q}^2 - \left(\boldsymbol{P}_{\mathrm{ph}}^{\mathrm{MF}}\right)^2\right) - \int d^d\boldsymbol{k}\ \frac{V_{\boldsymbol{k}}^2}{\Omega_{\boldsymbol{k}}}. \tag{12}$$

Problem 4 Lang-Firsov transformation

Consider the Fröhlich lattice Hamiltonian

$$\hat{\mathcal{H}}_{\mathrm{FL}} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}\left(\hat{c}_{\boldsymbol{i}}^\dagger\hat{c}_{\boldsymbol{j}} + \text{h.c.}\right) + \int d^d\boldsymbol{k}\ \omega_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}^\dagger\hat{a}_{\boldsymbol{k}} + \int d^d\boldsymbol{k}\sum_{\boldsymbol{j}} V_{\boldsymbol{k}}\hat{c}_{\boldsymbol{j}}^\dagger\hat{c}_{\boldsymbol{j}}e^{i\boldsymbol{k}\cdot\boldsymbol{j}}\left(\hat{a}_{\boldsymbol{k}} + \hat{a}_{-\boldsymbol{k}}^\dagger\right). \tag{13}$$

(4.a) Derive the Lang-Firsov transformed Hamiltonian

$$\tilde{\mathcal{H}}_{\mathrm{FL}} = \hat{U}_{\mathrm{LF}}^\dagger\hat{\mathcal{H}}_{\mathrm{FL}}\hat{U}_{\mathrm{LF}}, \qquad \hat{U}_{\mathrm{LF}} = \exp\left[\int d^d\boldsymbol{k}\sum_{\boldsymbol{j}}\hat{c}_{\boldsymbol{j}}^\dagger\hat{c}_{\boldsymbol{j}}\left(\alpha_{\boldsymbol{k},\boldsymbol{j}}\hat{a}_{\boldsymbol{k}}^\dagger - \text{h.c.}\right)\right] \tag{14}$$

discussed in the lecture, including expressions for the modified hopping amplitude $\hat{t}_{\boldsymbol{i},\boldsymbol{j}} = \hat{X}_{\boldsymbol{i}}\hat{X}_{\boldsymbol{j}}^\dagger$, the induced polaron-polaron interaction $\hat{V}$, the amplitudes $\alpha_{\boldsymbol{k},\boldsymbol{j}}$ and the energy shift ΔE:

$$\tilde{\mathcal{H}}_{\mathrm{FL}} = -t\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle}\left(\hat{c}_{\boldsymbol{i}}^\dagger\hat{X}_{\boldsymbol{i}}\hat{X}_{\boldsymbol{j}}^\dagger\hat{c}_{\boldsymbol{j}} + \text{h.c.}\right) + \sum_{\boldsymbol{i},\boldsymbol{j}} V(\boldsymbol{i}-\boldsymbol{j})\hat{n}_{\boldsymbol{i}}\hat{n}_{\boldsymbol{j}} + \int d^d\boldsymbol{k}\ \omega_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}^\dagger\hat{a}_{\boldsymbol{k}} + \Delta E \tag{15}$$

Problem 5 Imaginary-time Green's function

(5.a) By introducing unity, $\hat{1} = \sum_{\boldsymbol{k}} \sum_n |\boldsymbol{k}, n\rangle\langle\boldsymbol{k}, n|$, where $|\boldsymbol{k}, n\rangle$ label all eigenstates of the Fröhlich Hamiltonian $\hat{\mathcal{H}}_{\rm F}$ with total momentum $\boldsymbol{k}$ and eigenenergies $E_n(\boldsymbol{k})$, show that the imaginary-time Green's function approaches

$$\mathcal{G}(\boldsymbol{q}, \tau) = \langle 0|\hat{\psi}_{\boldsymbol{q}}(\tau)\hat{\psi}^\dagger_{\boldsymbol{q}}(0)|0\rangle \simeq Z_0(\boldsymbol{q}) \exp[-E_0(\boldsymbol{q})\tau] \tag{16}$$

asymptotically when $\tau \to \infty$, with the quasiparticle residue:

$$Z_0(\boldsymbol{q}) = |\langle 0|\hat{\psi}_{\boldsymbol{q}}|\boldsymbol{q}, 0\rangle|^2. \tag{17}$$