FK110 Diagrammatic methods in modern condensed matter physics

Exam problem 1 – Propagators in classical mechanics

Consider a classical damped harmonic oscillator of frequency ω driven by a general force $F(t)$. Its one-dimensional motion is captured by the differential equation

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + m\gamma\frac{\mathrm{d}x}{\mathrm{d}t} + m\omega_0 x^2 = F(t)\,.$$

(a) Determine the corresponding retarded Green's function $G(t,t')$ by solving the above equation with $F(t)$ being a delta-function $\delta(t-t')$ and by imposing the initial condition $G(t,t')=0$ for $t<t'$.

(b) Perform Fourier transform to convert the Green's function from time domain to frequency domain and show that it takes the form

$$G(\omega) = \frac{1}{2m\tilde{\omega}}\left(\frac{1}{\omega+\tilde{\omega}+i\frac{\gamma}{\omega}} - \frac{1}{\omega-\tilde{\omega}+i\frac{\gamma}{\omega}}\right)\,,$$

where $\tilde{\omega}$ stands for the frequency of free damped oscillations.

(c) When extended into the whole complex ω plane, the retarded Green's function obtained in (b) shows two poles below the real frequency axis. As a consequence, the retarded Green's function obeys the Kramers-Kronig relation of the form

$$\mathrm{Re}\,G(\omega) = \frac{1}{\pi}\,\mathcal{P}\int\limits_{-\infty}^{+\infty}\frac{\mathrm{Im}\,G(\omega')}{\omega'-\omega}\,.$$

Check this feature by an explicit evaluation of the integral.

Exam problem 2 – Fluctuation–dissipation theorem

Considering a general equilibrium many-body system, use the spectral representation based on Hamiltonian eigenstates to show that the dynamical correlation function of quantity A defined as

$$C(E) = \langle \hat{A}\hat{A}^\dagger\rangle_E = \int\limits_{-\infty}^{+\infty}\langle\,\hat{A}(t)\hat{A}^\dagger(0)\,\rangle\,\mathrm{e}^{\frac{i}{\hbar}Et}\,\mathrm{d}t$$

and the imaginary part of the corresponding susceptibility

$$\chi(E) = \chi'(E) + i\chi''(E) = \frac{i}{\hbar}\int\limits_{-\infty}^{+\infty}\langle\,[\,\hat{A}(t),\hat{A}^\dagger(0)\,]\,\rangle\,\vartheta(t)\,\mathrm{e}^{\frac{i}{\hbar}Et}\,\mathrm{d}t$$

are connected by fluctuation–dissipation theorem

$$C(E) = 2\hbar\,[N_B(E)+1]\,\chi''(E)$$

with N_B denoting the Natanson-Bose-Einstein factor. The dynamical correlation function captures the fluctuations of a given physical quantity A while the imaginary part of the susceptibility corresponds to the absorption/dissipation of energy taken from the external driving field coupled via A. This theorem may be used, e.g., to relate the dynamical structure factor $S(\boldsymbol{q},E) = \langle S^\alpha_{\boldsymbol{q}} S^\alpha_{-\boldsymbol{q}}\rangle_E$ accessible by neutron scattering to the corresponding spin susceptibility $\chi''_{\alpha\alpha}(\boldsymbol{q},E)$.

Note: To simplify the notation, assume that the eigenstates form a discrete spectrum.

Exam problem 3 – Lindhard function for a free-electron gas

Calculate the Lindhard function for a gas of non-interacting electrons with the usual free-electron dispersion

$$\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m} - E_F$$

in three dimensions. Express the resulting real and imaginary part of the Lindhard function

$$\Pi(\boldsymbol{q}, E) = \frac{2}{\Omega} \sum_{\boldsymbol{k}} \frac{n_F(\varepsilon_{\boldsymbol{k}}) - n_F(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}})}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} - E - i0^+}$$

using the reduced quantities $Q = q/2k_F$ and $W = E/4E_F$. Show that the lowest term in the expansion of the reduced $\widetilde{\Pi} = (2\pi^2\hbar^2/mk_F)\,\Pi$ above the $W = Q+Q^2$ line reads as $\widetilde{\Pi}(Q, W) \approx -\frac{2}{3}(Q/W)^2$. Within the RPA approximation, this result gives the plasmon energy in the $\boldsymbol{q} \to 0$ limit.

Exam problem 4 – System of coupled harmonic oscillators

Consider a system of a bosonic particle a coupled to a large set of bosonic modes b_n, the coupled system being described by the Hamiltonian

$$\mathcal{H} = \hbar\Omega\, a^\dagger a + \sum_n \hbar\omega_n\, b_n^\dagger b_n + \sum_n g_n (a^\dagger b_n + b_n^\dagger a).$$

(a) Using the equation of motion technique, derive a set of differential equations for the thermal propagators related to the a and b_n particles. Note that the form of the Hamiltonian generates also off-diagonal propagators (i.e. those connecting a and b) that need to be included. Perform Fourier transform to Matsubara representation that converts the differential equations into algebraic form and solve this set for the propagator of the particle a. Analytically continue the result to obtain its retarded form and the corresponding spectral function.

(b) Try to express the propagator of a as a series of Feynman diagrams and deduce the above result based on this series. Hint: Focus on the selfenergy of a arising due to the interaction with b_n modes.

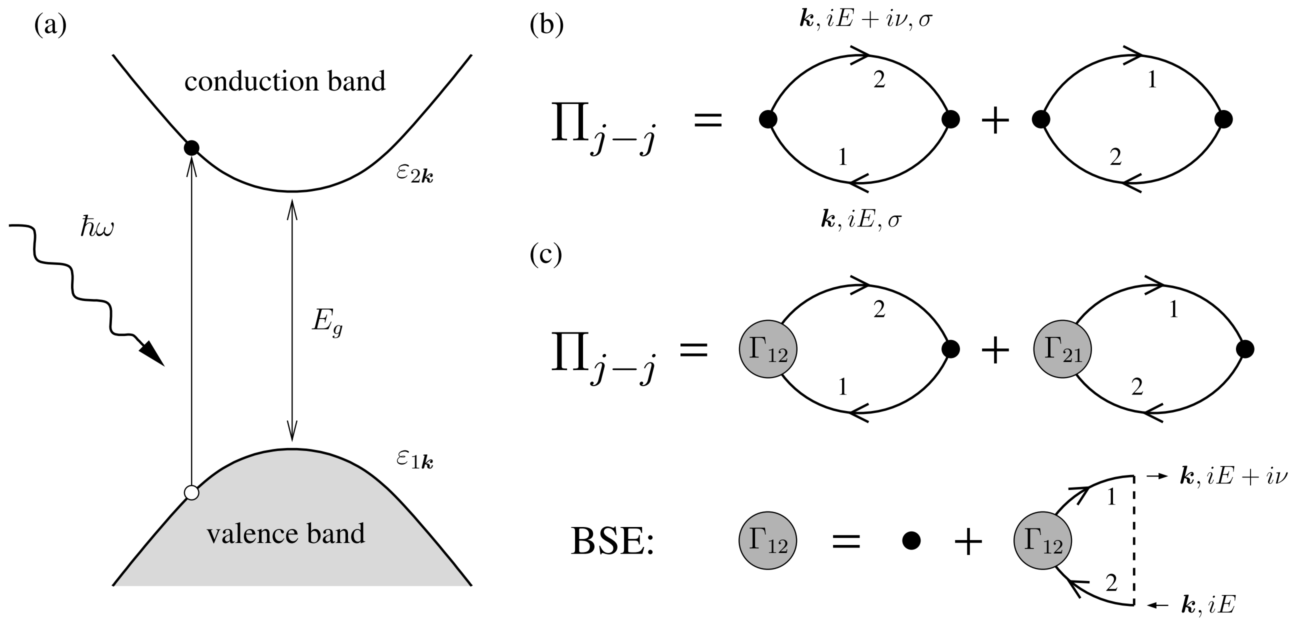
(c) Assuming $N \to \infty$ modes b_n homogeneously covering the interval $\hbar\omega_{\min}$ to $\hbar\omega_{\max}$ and constant $g_n = g/\sqrt{N}$, determine explicitly the selfenergy of the mode a and try to plot a few representative graphs of the selfenergy and the spectral function for varying relative position of Ω with respect to the $[\omega_{\min}, \omega_{\max}]$ interval and varying coupling strength g.

Exam problem 5 – Optical response of a semiconductor and Bethe–Salpeter equation

In this problem you will address the optical response functions via diagrammatic formalism. The key ingredient is the current-density operator $\hat{\mathbf{j}}$ which couples a many-body system to the light field captured by a vector potential $\boldsymbol{A}$. In terms of the Fourier components, the interaction Hamiltonian can be written as $\mathcal{H}_{\text{int}} = -\sum_{\boldsymbol{q}} \hat{\mathbf{j}}_{\boldsymbol{q}} \cdot \boldsymbol{A}_{\boldsymbol{q}}$. To study the optical response, it is sufficient to work with the $\boldsymbol{q} = 0$ components. The imaginary part of the dielectric function, which reflects the optical absorption processes, can be determined via so-called current-current correlation function obtained by including the current-density operator into the general susceptibility definition, namely

$$\operatorname{Im} \epsilon_{\alpha\alpha}(\omega) = \frac{1}{\epsilon_0\, \omega^2} \operatorname{Im} \Pi_{j-j}(\hbar\omega) \qquad \text{with} \qquad \Pi_{j-j}(E) = \frac{i}{\hbar} \int_{-\infty}^{+\infty} \langle [\hat{\jmath}_\alpha(t), \hat{\jmath}_\alpha(0)] \rangle\, \vartheta(t)\, \mathrm{e}^{\frac{i}{\hbar}Et} \mathrm{d}t\,.$$

Consider specifically the case of a semiconductor with the valence band having dispersion ε_{1k} and conduction band having dispersion ε_{2k}, schematically depicted in panel (a). These bands are separated



by the band gap E_g. The current density operator corresponding to interband transitions reads as

$$\hat{\mathrm{j}}_\alpha = \sum_{\boldsymbol{k}\sigma} ie\gamma_{\boldsymbol{k}\alpha}(c^\dagger_{2\boldsymbol{k}\sigma}c_{1\boldsymbol{k}\sigma} - c^\dagger_{1\boldsymbol{k}\sigma}c_{2\boldsymbol{k}\sigma})\,,$$

where $\gamma_{\boldsymbol{k}\alpha}$ is essentially a dipole matrix element for the direction α. We keep it unspecified, note however, that in the above definition, $\gamma_{\boldsymbol{k}\alpha}$ needs to take real values.

(a) In the crudest approximation, the current-current correlator can be evaluated via the diagrams presented in panel (b). These neglect the Coulomb interaction between the electron and hole in the intermediate state. Write down the expressions corresponding to these diagrams, evaluate the doable summations over free variables and obtain $\mathrm{Im}\,\Pi_{j-j}(\hbar\omega)$. The resulting formula has a straightforward interpretation in terms of the interband transitions sketched in the scheme of panel (a).

(b) To account for the Coulomb interaction between the excited electron and hole, the series of ladder diagrams may be considered. These can be compactly expressed by introducing a renormalized current vertex as shown in panel (c). The vertex function $\Gamma_{12}(\boldsymbol{k}, iE, i\nu)$ is the solution of so-called Bethe-Salpeter equation (BSE) also presented in panel (c). Write down the algebraic expressions corresponding to both corrected $\Pi_{j-j}(i\nu)$ and BSE but do not evaluate them. When translating the diagrammatic BSE, denote the Coulomb matrix element (which is in fact reduced by screening) as a general $V_{\boldsymbol{q}}$ with the momentum $\boldsymbol{q}$ specified by the diagram. A deeper look at the BSE shows, that one can actually easily perform the Matsubara summation in the equation. You may optionally include this step. If everything is properly worked out, the corrected Π_{j-j} from panel (c) includes excitonic absorption below the band gap.

Exam problem 6 – Enhancement of AF fluctuations due to Hubbard interaction

Calculate the spin susceptibility of electrons moving in a square lattice renormalized by on-site Hubbard repulsion. The electrons are described by a tight-binding Hamiltonian including nearest-neighbor hopping with an amplitude t and second nearest-neighbor hopping with an amplitude t'

$$\mathcal{H}_{tt'} = -t \sum_{\langle ij\rangle\in\mathrm{NN}} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} - t' \sum_{\langle ij\rangle\in\mathrm{nNN}} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \mathrm{H.c.}$$

(summation over the spin projections is implied) leading to the familiar dispersion

$$\varepsilon_{\boldsymbol{k}} = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a.$$

The total Hamiltonian of the system

$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma} (\varepsilon_{\boldsymbol{k}} - \mu) \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

includes also the Hubbard interaction term that is to be treated within RPA approximation. Using a diagrammatic RPA approach, determine the zz component $\chi_{zz}(\boldsymbol{q}, E)$ of the spin susceptibility and evaluate it numerically. The necessary Brillouin zone (BZ) summations to get the bare susceptibility can be performed by utilizing a regular grid of $\boldsymbol{k}$ points covering the BZ. Use the following values of the parameters: $t = 0.4\,\mathrm{eV}$, $t' = -t/3$, band occupation $n = 0.85$, and plot the results for a few values of U that range from zero to critical U. Your plots should show both real and imaginary parts of $\chi_{zz}(\boldsymbol{q}, E)$ as maps plotted along the conventional path $\Gamma - \mathrm{X} - \mathrm{M} - \Gamma$ in the 2D BZ of the square lattice. Here $\Gamma = (0, 0)$, $\mathrm{X} = (\pi/a, 0)$, and $\mathrm{M} = (\pi/a, \pi/a)$. Additionally, show the BZ maps of static $\chi_{zz}(\boldsymbol{q}, E = 0)$ and the Fermi surface (FS) that will help you to understand the link to FS nesting. Optionally, you can contrast the results for the above nearly half-filled case with those for small ($n \lesssim 0.5$) or large ($n \gtrsim 1.5$) band filling and/or inspect the consequences of varying the t'/t ratio.