

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN Fakultät für Physik im WiSe 2023/24 TA1: Condensed matter physics Dozent: Dr. Sebastian Paeckel Exercises: Zhaoxuan Xie



https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_24_25/TA1_theoretical_ condensed_matter/index.html

Problem set 3

Problem 1 Neutron scattering and magnetic moments

In the lecture we ignored the fact that the neutron carries a spin S = 1/2, in this exercise we want to account for that simplification by also incorporating a spin-spin interaction into the interaction Hamiltonian $\hat{H}_{\rm int}$. Assume that the latter is now given by

$$\hat{H}_{\rm int} = \alpha \sum_{j} \delta(\vec{R} - \vec{r}_{j}) \hat{\vec{S}}_{\rm n} \cdot \hat{\vec{S}}_{j} , \qquad (1)$$

where $\hat{\vec{S}}_n$ denotes the spin operator of the neutron and $\hat{\vec{S}}_j$ may describe the spin of the nucleus (but it can be considered to also represent the magnetic moment of an atomic or molecular orbital). Show that the dynamical structure factor of this interaction (using the same notation as in the lecture) is given by

$$S^{-+}(\vec{q},\omega) = \frac{1}{N} \int_{-\infty}^{\infty} dt \, \mathrm{e}^{\mathrm{i}\omega t} \sum_{j,l=1}^{N} \langle\!\langle \hat{S}_{j}^{-}(t) \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{r}_{j}(t)} \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}_{l}} \hat{S}_{l}^{+} \rangle\!\rangle \,. \tag{2}$$

Hint: You may assume, that the spin of the incident neutron is polarized along the z-direction.

Problem 2 Polarization function of the harmonic oscillator

We consider a harmonic oscillator of a particle with mass M and oscillator frequency Ω , which is described by the Hamiltonian

$$H = \frac{P^2}{2M} + \frac{1}{2}M\Omega^2 X^2 ,$$
 (3)

where P denotes the (center of mass) momentum and X the displacement from its equilibrium position.

(2.a) Let us first consider the classical case. Show that the classical polarization function is given by

$$\Pi(q,t) = \langle e^{iqX(t)}e^{-iqX} \rangle = e^{-q^2 \langle X_0^2 \rangle (1 - \cos(\Omega t))} ,$$
(4)

with the initial condition $X_0 = X(t = 0)$.

- (2.b) Compute the dynamical structure factor $S(q, w) = \int_{-\infty}^{\infty} dt e^{i\omega t} \Pi(q, t)$.
- (2.c) Now we consider the quantum mechanical case replacing $X \to \hat{X}$ and $P \to \hat{P}$ which obey the canonical commutation relation for position and momentum operator. In this problem, use the relation $\langle\!\langle e^{\bar{\alpha}\hat{a}^{\dagger}}e^{\alpha\hat{a}}\rangle\!\rangle = e^{-|\alpha|^2 n(\beta)}$ where $\hat{a}^{(\dagger)}$ denotes the usual ladder operators for

the harmonic oscillator, $\alpha \in \mathbb{C}$ and $n(\beta) = \frac{1}{e^{-\beta\Omega}-1}$. Show that quantum mechanically, the polarization function is given by

$$\Pi(q,t) = e^{q^2 g(t)} , \qquad (5)$$

with $g(t) = \langle \hat{X}^2 \rangle (\cos(\Omega t) - 1) - ix_0^2 \sin(\Omega t)$ and the characteristic length scale $x_0 = \sqrt{\frac{\hbar}{2M\Omega}}$ of the harmonic oscillator.