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Physikalisches Institut
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http://www.kroha.uni-bonn.de/teaching

Special Topics in Condensed Matter Theory
Winter term 2016/17

Exercise 1

(Solutions due on 4 November, 2016)

1. Relations between response functions (5 points)

a) The electrical conductivity, σ, is the linear response function describing the response of the electric current density $\vec{j}(\vec{r},t)$ to an externally applied electric field $\vec{E}(\vec{r}',t')$. The density response function $\chi_{\rho\rho}$ describes the linear response of the particle density $\rho(\vec{r},t)$ to an external electrostatic potential $e\Phi(\vec{r}',t')$. Note that, in general, σ and $\chi_{\rho\rho}$ are non-local in space and temporally retarded. That is, we have,

$$\begin{aligned} \vec{j}(\vec{r},t) &= \int d^3r'\,dt'\,\sigma(\vec{r}-\vec{r}',t-t')\,\vec{E}(\vec{r}',t') \qquad \text{(Ohm's law)} \\ \delta\rho(\vec{r},t) &= e\int d^3r'\,dt'\,\chi_{\rho\rho}(\vec{r}-\vec{r}',t-t')\,\Phi(\vec{r}',t')\ . \end{aligned}$$

Charge and current density are related by the continuity equation, $e\,d/dt\,\rho + \nabla\cdot\vec{j} = 0$ (charge conservation) and the external fields by $\vec{E} = -\nabla\Phi$.

Fourier-transform these relations to the momentum ($\vec{q}$) and frequency (ω) domain. Derive the relation between $\sigma(\vec{q},\omega)$ and $\chi_{\rho\rho}(\vec{q},\omega)$.

b) Now write down the definitions of the electrical conductivity $\sigma(\vec{r},t)$ and of the density response function in terms of expectation values of appropriate quantum mechanical operators.

Discuss that the relation of a) and the definition of $\chi_{\rho\rho}$ imply that the intrinsic electron-electron correlations of the system can be otained by measuring the (dynamical) electrical conductivity.

2. Nonlinear response functions and discrete symmetries (5 points)

We consider the *quadratic*, nonlinear response of a system to an external optical laser pulse. In leading order, the laser field couples to the system via electric dipole coupling, $\delta H = -\vec{P}\cdot\vec{E}$, where $\vec{P}$ is the electric polarization of the system. The system's response is an emitted light pulse, proportional to its induced polarization $\delta\vec{P}$. We can safely assume that all light fields are constant in space; spatial dependence is irrelevant for the following. The quadratic response equation then reads

$$\delta\vec{P}(t) = \int dt'dt''\chi^{(2)}_{PEE}(t;t',t'')\vec{E}(t')\vec{E}(t'')\ .$$

a) $\vec{E}$ and $\vec{P}$ have odd parity under space inversion: $\vec{E} \to -\vec{E}$, $\vec{P} \to -\vec{P}$. $\chi^{(2)}_{PEE}$ depends on the system properties only, as shown in the lecture, and not on the external fields. Using the above response equation, show that $\chi^{(2)}_{PEE}(t;t',t'')$ vanishes identically if the system is space inversion symmetric (like a continuous gas or an inversion symmetric crystal).

b) Express $\chi^{(2)}_{PEE}(t;t',t'')$ as an expectation value of $\vec{P}$ (c.f. lecture). Fourier-transform the response eqn. to the frequency domain and show for a driving field of frequency ω,

$$\delta\vec{P}(2\omega) = \chi^{(2)}_{PEE}(2\omega,\omega,\omega)\vec{E}(\omega)\vec{E}(\omega) \ ,$$

i.e., the quadratic response describes 2nd harmonic generation (SHG).

3. Hamilton operator in occupation number representation (10 points)

We consider a system of N particles (bosons or fermions) described by the Hamiltonian in position representation,

$$\hat{H} = \sum_{i=1}^{N} \frac{-\hbar^2\nabla_i^2}{2m} + \sum_{i,j=1|i>j}^{N} V(\vec{r}_i - \vec{r}_j) =: \hat{H}^{(1)} + \hat{V}^{(2)} \ ,$$

where $i,\ j = 1,\ldots,N$ label the particles, $\hat{H}^{(1)} = \sum_{i=1}^{N} -\hbar^2\nabla_i^2/2m$ is the kinetic energy operator, and $\hat{V}^{(2)} = \sum_{i,j=1|i>J}^{N} V(\vec{r}_i - \vec{r}_j)$ is an interaction potential between two particles. A possible spin of the particles is not considered here. $\hat{H}^{(1)}$ is called a single-particle operator, since each term in the sum acts on the state of one particle. $\hat{V}^{(2)}$ is called a two-particle operator, since each of its terms acts on the states of two particles simultaneously.

Consider now the complete, normalized basis of momentum eigenstates of a single particle, $B^{(1)} = \{|\vec{p}\rangle \,|\, \vec{p} \in R^3\}$, and the corresponding basis of N-particle product states (symmetrized or antisymmetrized).

a) Calculate all matrix elements of $\hat{H}^{(1)}$ in the basis of *occupation number eigenstates* $|n_{\vec{p}_1}, n_{\vec{p}_2}, \ \ldots\rangle$ with occupation numbers $n_{\vec{p}_\alpha}$. Show that in this occupation number representation the single-particle operator is diagonal and takes the form

$$\hat{H}^{(1)} \ = \ \sum_{\vec{p}} \frac{\vec{p}^2}{2m} c^\dagger_{\vec{p}} c_{\vec{p}} \ ,$$

where $c^\dagger_{\vec{p}}$ and $c_{\vec{p}}$ are the bosonic or fermionic creation and annihilation operators, respectively, of a particle in state $|\vec{p}\rangle$. Convince yourself, in particular, that $\hat{H}^{(1)}$ has the same form for bosons and fermions.

b) Calculate all matrix elements of the two-particle operator $\hat{V}^{(2)}$ in the basis of *occupation number eigenstates* and express them in terms of expectation values of the two-particle potential $V(\vec{r}_i - \vec{r}_j)$. Show that these matrix elements conserve the total momentum of the system, i.e., the sum of outgoing momenta is equal to the sum of ingoing momenta. Show that in occupation number representation (2nd quantization) $\hat{V}^{(2)}$ takes the form

$$\hat{V}^{(2)} \ = \ \sum_{\vec{p},\vec{p}',\vec{q}} V^{\vec{q}}_{\vec{p},\vec{p}'} c^\dagger_{\vec{p}+\vec{q}} c^\dagger_{\vec{p}'-\vec{q}} c_{\vec{p}'} c_{\vec{p}} \ .$$