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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

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

Solution

1. Relations between response functions (5 points)

a) For solving this one, we need two basic ingredients:

1. **The convolution theorem**. With a Fourier transform given by

$$f(\omega) = \mathcal{F}(f(t)) = \int dt' f(t') e^{i\omega t'} \tag{1}$$

and a function h defined as

$$h(t) = \int dt' f(t') g(t - t'), \tag{2}$$

we have

$$h(\omega) = f(\omega) g(\omega). \tag{3}$$

2. **Fourier differentiation rules**. As should be known, the Fourier transform of the derivative of a function is

$$\mathcal{F}(df(t)/dt) = -i\omega f(\omega). \tag{4}$$

With these tricks at hand, we find that

$$\boldsymbol{j}(\boldsymbol{q}, \omega) = \sigma(\boldsymbol{q}, \omega) \boldsymbol{E}(\boldsymbol{q}, \omega), \tag{5}$$

$$\delta\rho(\boldsymbol{q}, \omega) = e\chi_{\rho\rho}(\boldsymbol{q}, \omega)\phi(\boldsymbol{q}, \omega). \tag{6}$$

Moreover, one can calculate that

$$\mathcal{F}(\nabla \cdot \boldsymbol{j}) = i\boldsymbol{q} \cdot \boldsymbol{j}(\boldsymbol{q}, \omega), \tag{7}$$

$$\boldsymbol{E}(\boldsymbol{q}, \omega) = -i\phi(\boldsymbol{q}, \omega)\boldsymbol{q}, \tag{8}$$

$$\mathcal{F}(\dot{\rho}) = -i\omega\rho(\boldsymbol{q}, \omega). \tag{9}$$

Plugging all of this in, one obtains finally

$$\chi_{\rho\rho}(\boldsymbol{q}, \omega) = \frac{-i\boldsymbol{q}^2}{e^2\omega} \sigma(\boldsymbol{q}, \omega). \tag{10}$$

b) As can be learned from chapter 6 of [1], there is the relation

$$\sigma(\boldsymbol{q}, \omega) = \frac{ie^2}{\omega} \Pi^R(\boldsymbol{q}, \omega), \tag{11}$$

where

$$\Pi^R(\boldsymbol{r} - \boldsymbol{r'}, t - t') = -i\theta(t - t')\langle \big[\hat{\boldsymbol{J}}(\boldsymbol{r}, t), \hat{\boldsymbol{J}}(\boldsymbol{r'}, t')\big] \rangle, \tag{12}$$

with $\hat{\boldsymbol{J}}$ the current operator. Therefore, we are now able to obtain the density response function of a system by measuring the conductivity, which in turn is related to the current in the system.

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

a) By using space inversion, we find

$$\begin{aligned} -\delta \boldsymbol{P}(t) &= \int dt' dt'' \chi^{(2)}_{PEE}(t;t',t'')(-\boldsymbol{E}(t'))(-\boldsymbol{E}(t'')) \\ &= \int dt' dt'' \chi^{(2)}_{PEE}(t;t',t'')\boldsymbol{E}(t')\boldsymbol{E}(t''), \end{aligned} \tag{13}$$

from which we conclude that $\delta \boldsymbol{P}(t) = -\delta \boldsymbol{P}(t)$, which means $\delta \boldsymbol{P}(t) = 0$, and so $\chi^{(2)}_{PEE}(t;t',t'') = 0$.

b)

$$\begin{aligned} \delta \boldsymbol{P}(2\omega) &= \int dt dt' dt'' e^{2i\omega t} \chi^{(2)}_{PEE}(t;t',t'')\boldsymbol{E}(t')\boldsymbol{E}(t'') \\ &= \int dt dt' dt'' e^{i\omega(2t-t'-t'')} e^{i\omega t'} e^{i\omega t''} \chi^{(2)}_{PEE}(t;t',t'')\boldsymbol{E}(t')\boldsymbol{E}(t'') \\ &= \chi^{(2)}_{PEE}(2\omega;\omega,\omega)\boldsymbol{E}(\omega)\boldsymbol{E}(\omega). \end{aligned} \tag{14}$$

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

a) Here I follow the chapter 1 of [2]. The momentum eigen function is $\phi_{\boldsymbol{k}}(\boldsymbol{x}) = e^{i\boldsymbol{k}\cdot\boldsymbol{x}}/\sqrt{V}$ with sqrt root of the volume $\sqrt{V}$ as normalization factor.

$$\int \phi_{\boldsymbol{k}}(\boldsymbol{x})\phi_{\boldsymbol{k}'}(\boldsymbol{x})d^3x = \delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{15}$$

Generally the one particle potential can be written as,

$$T = \sum_{ij} t_{ij} c_i^\dagger c_j \tag{16}$$

where $t_{ij} = \langle i|t|j\rangle$, $c^\dagger$ and c are creation and annihilation operators. In our case,

$$\begin{aligned} T &= \sum_{\boldsymbol{p}'\boldsymbol{p}} t_{\boldsymbol{p}'\boldsymbol{p}} c^\dagger_{\boldsymbol{p}'} c_{\boldsymbol{p}} \\ &= \sum_{\boldsymbol{p}'\boldsymbol{p}} \int \phi^*_{\boldsymbol{p}'}(\boldsymbol{x})(-\nabla^2/2m)\phi_{\boldsymbol{p}}(\boldsymbol{x})d^3x \\ &= \sum_{\boldsymbol{p}'\boldsymbol{p}} \delta_{\boldsymbol{p}',\boldsymbol{p}} \frac{\boldsymbol{p}^2}{2m} c^\dagger_{\boldsymbol{p}'} c_{\boldsymbol{p}} \\ &= \sum_{\boldsymbol{p}} \frac{\boldsymbol{p}^2}{2m} c^\dagger_{\boldsymbol{p}} c_{\boldsymbol{p}} \end{aligned} \tag{17}$$

b) Here I simply use p for vectors rather than $\boldsymbol{p}$, and px for $\boldsymbol{p}\cdot\boldsymbol{x}$.

$$\begin{aligned}
&\langle i,j|f^{(2)}|k,m\rangle \\
&= \frac{1}{V^2}\int d^3x\, d^3x'\, e^{-ip'x}e^{-ik'x'}V(x-x')e^{ikx'}e^{ipx} \\
&= \frac{1}{V^3}\sum_q V_q \int d^3x\, d^3x' e^{-ip'x-ik'x'+iq(x-x')+ikx'+ipx} \\
&= \frac{1}{V^3}\sum_q V_q V\delta_{-p'+q+p,0}V\delta_{-k'-q+k,0}
\end{aligned} \tag{18}$$

Now use the second quantization form for the two particle potential,

$$\begin{aligned}
&\sum_{i,j,k,m}\langle i,j|f^{(2)}|k,m\rangle c_i^\dagger c_j^\dagger c_m c_k \\
&= \frac{1}{2}\sum_{p,k',p,k}\frac{1}{V}\sum_q V_q\delta_{-p'+q+p,0}\delta_{-k'-q+k,0}c_{p'}^\dagger c_{k'}^\dagger c_k c_p \\
&= \frac{1}{2V}\sum_{q,p,k}V_q c_{p+q}^\dagger c_{k-q}^\dagger c_k c_p
\end{aligned} \tag{19}$$

The momentum conservation is obvious. This process corresponds to two particles exchanged a momentum q after the scattering. In above I used the fact that $\sum_{i>j}V(r_i-r_j) = \frac{1}{2}\sum_{ij}\underbrace{V(x_i-x_j)}_{f^{(2)}}$. And the Fourier transformation,

$$\begin{aligned}
V(x-x') &= \frac{1}{V}\sum_q V_q e^{iq(x-x')} \\
\frac{1}{V}\int e^{iqx}d^3x &= \delta_{q,0}
\end{aligned} \tag{20}$$

References

[1] H. Bruus and K. Flensberg. *Many-body quantum theory in condensed matter physics: an introduction.* Oxford University Press, 2004.

[2] Franz Schwabl. *Advanced quantum mechanics.* Springer Science & Business Media, 2005.