TD n°8 : Out of equilibrium statistical physics (quantum) linear response theory

1 Quantum harmonic oscillator

We study the dynamics of a quantum harmonic oscillator described by the Hamiltonian $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2$, submitted to the time dependent perturbation $H_{\text{pert}}(t) = -x\, f(t)$.

1/ Determine the time dependence of the annihilation operator in the interaction representation $a(t) \stackrel{\text{def}}{=} \mathrm{e}^{\mathrm{i}H_0 t/\hbar} a \mathrm{e}^{-\mathrm{i}H_0 t/\hbar}$.

2/ Deduce the correlation function $C(t) \equiv C_{xx}(t) = \langle x(t)x\rangle$, where $\langle\cdots\rangle$ denotes the canonical averaging. Analyze the classical ($\hbar \to 0$) and zero temperature limits.

3/ Check that the detailed balance relation $\widetilde{C}(-\omega) = \widetilde{C}(\omega)\mathrm{e}^{-\beta\hbar\omega}$ holds. Deduce the symmetrized correlation function $S(t) \stackrel{\text{def}}{=} \frac{1}{2}\langle\{x(t), x\}\rangle$.

4/ Compute the spectral function $\xi(t) \stackrel{\text{def}}{=} \frac{1}{2\hbar}\langle[x(t), x]\rangle$ and the response function $\chi(t) \equiv \chi_{xx}(t)$. Are these results dependent on the nature of the average $\langle\cdots\rangle$? Compute $\widetilde{\chi}(\omega)$ and $\widetilde{\xi}(\omega)$.

5/ Compute the Kubo correlation function $K(t) \equiv K_{xx}(t) = \frac{1}{\beta}\int_0^\beta \mathrm{d}\lambda\, \langle x(-\mathrm{i}\hbar\lambda)x(t)\rangle$. Check the relation with the response function.

6/ Verify that the response function coincides with the classical result. Give the origin of this observation.
Hint : Write the equation of motion in *Heisenberg* representation for $x_H(t)$ and $p_H(t)$. Justify that the response of the quantum harmonic oscillator is purely *linear*.

7/ Check that the correlation functions satisfy the Fluctuation-Dissipation theorem.

2 Conductivity of the electron gas

We consider a gas of (non interacting) free electrons and study its response to an electric field. Perturbation takes the form $H_{\text{pert}}(t) = -e\,\vec{\mathcal{E}}(t)\cdot\vec{r}$ (where $\vec{r}$ is the position operator for *one* electron). The spatially averaged current density is $\vec{j} = \frac{e}{V}\vec{v}$ where $\vec{v}$ is the speed operator for the electron. Conductivity (for $\vec{q} = 0$) is defined by $\langle j_i(t)\rangle_{\mathcal{E}} = \int \mathrm{d}t'\, \sigma_{ij}(t-t')\mathcal{E}_j(t')$ (with implicit summation over repeated index).

1/ Compute the conductivity $\sigma_{ij}^{(1\,e^-)}(t)$ for a single electron.

2/ Deduce the conductivity for the Fermi gas of N electrons at temperature T.

3/ Compute the Fourier tansform $\widetilde{\sigma}_{ij}(\omega)$. Interpret physically the $\omega \to 0$ behaviour.

4/ Sum rule.– Give $\sigma_{ij}(t=0)$ and then $\int \mathrm{d}\omega\, \tilde{\sigma}_{ij}(\omega)$.

3 Response function for identical particles

We introduce the basis of one particle stationary states $\{|\,\varphi_\alpha\,\rangle\}$. We denote h the one body Hamiltonian and $H = \sum_{i=1}^N h^{(i)}$ the many body Hamiltonian, acting in the N particle Hilbert space $\mathscr{H}_N = \mathscr{H}_1^{\otimes N}$. We denote by a_α and $a_\alpha^\dagger$ the annihilation/creation operators acting in the Fock space $\mathscr{F} = \bigoplus_{N=0}^\infty \mathscr{H}_N$. They obey $\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha,\beta}$ for fermions and $[a_\alpha, a_\beta^\dagger] = \delta_{\alpha,\beta}$ for bosons. We consider two observables Q and P, sum of one body operators, $Q = \sum_i q^{(i)}$ and $P = \sum_i p^{(i)}$. We recall that, in the Fock space, these operators can be represented as

$$Q = \sum_{\alpha,\beta} q_{\alpha\beta}\, a^\dagger_\alpha\, a_\beta \tag{1}$$

where $q_{\alpha\beta} \stackrel{\text{def}}{=} \langle\, \varphi_\alpha\, |q|\, \varphi_\beta\, \rangle$ is the matrix element of the one body operator.

We introduce the grand canonical averaging

$$\langle \cdots \rangle \stackrel{\text{def}}{=} \mathrm{Tr}\,\{\rho \cdots\} \qquad \text{with } \rho = \frac{1}{\mathcal{Z}} \mathrm{e}^{-\beta(H-\mu N)} \tag{2}$$

where $\mathrm{Tr}\,\{\cdots\}$ is a trace in $\mathscr{F}$ and N the particle number operator.

1/ Compute $\langle a^\dagger_\alpha\, a_\beta \rangle$. We introduce the notation $f_\alpha \equiv f(\varepsilon_\alpha) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_\alpha-\mu)}\pm 1}$ where $h|\, \varphi_\alpha\, \rangle = \varepsilon_\alpha |\, \varphi_\alpha\, \rangle$.

2/ Verify

$$[AB, CD] = A[B,C]D + [A,C]BD + CA[B,D] + C[A,D]B \tag{3}$$

$$[AB, CD] = A\{B,C\}D - \{A,C\}BD + CA\{B,D\} - C\{A,D\}B \tag{4}$$

and deduce $[a^\dagger_\alpha\, a_\beta, a^\dagger_\mu\, a_\nu]$.

3/ Show that the following relation

$$\boxed{\langle [P,Q] \rangle = \mathrm{Tr}\,\{\rho\,[P,Q]\} = \mathrm{tr}\,\{f(h)[p,q]\}} \tag{5}$$

holds both for bosons *and* fermions, where $\mathrm{tr}\{\cdots\}$ is a trace in the one body Hilbert space $\mathscr{H}_1$.

4/ Note that $\langle PQ \rangle \neq \mathrm{tr}\{f(h)pq\}$.

5/ **IMPORTANT :** Deduce the spectral representation for the response function $\widetilde{\chi}_{PQ}(\omega)$ in terms of one-body matrix elements $q_{\alpha\beta}$ and $p_{\alpha\beta}$. Conclusion ?

4 Compressibility of the free fermionic gas

The operator "density of particle"' is denoted $\hat{n}(r)$ and its Fourier component $\hat{n}_q$ (I drop the arrows on vectors). We consider that the system is in a box of finite size V and study its response to an external scalar potential $V^{\text{ext}}(r,t)$.

1/ Density-density response function $\chi(r,t;r',0)$ is defined by

$$\langle \hat{n}(r,t) \rangle_{V^{\text{ext}}} = \overbrace{n}^{\text{mean density}} + \int \mathrm{d}r'\mathrm{d}t'\, \chi(r,t;r',t')\, V^{\text{ext}}(r',t') + \cdots \tag{6}$$

Express $\hat{H}_{\text{pert}}(t)$ in terms of $\hat{n}_q$. Deduce $\int \mathrm{d}(r-r')\, \mathrm{e}^{-\mathrm{i}q(r-r')}\, \chi(r,t;r',0)$ as a correlator of the density operator $\hat{n}_q$.

2/ We now consider the free fermion gas. One particle eigenstates are the plane waves $\varphi_k(r) = \frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}kr}$ with energy ε_k. For one fermion, the density operator is $\hat{n}(r) = \delta(r - \hat{r})$. Compute the matrix element $\langle\, \varphi_k\, |\hat{n}_q|\, \varphi_{k'}\, \rangle$.

3/ Show that $\widetilde{\chi}(q,\omega) = \int \mathrm{d}(r-r')\, \mathrm{e}^{-\mathrm{i}q(r-r')} \int \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, \chi(r,t;r',0)$ can be represented as a sum over one-particle eigenstates

$$\widetilde{\chi}(q,\omega) = \frac{1}{V} \sum_k \frac{f_k - f_{k+q}}{\hbar\omega + \varepsilon_k - \varepsilon_{k+q} + \mathrm{i}0^+} \tag{7}$$

where $f_k \equiv f(\varepsilon_k)$ is the Fermi-Dirac distribution.

4/ *Static case* $\omega = 0$.– Compute $\widetilde{\chi}(q \ll k_F, 0)$. Interpret the result physically.