Professor Alexander L. Fetter's Lectures at Tsinghua University

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I. SCATTERING AND DENSITY CORRELATION

A. Introduction

In order to get familiar with the important mathematics frequently used in later discussions, the Fourier transform, let's warm up with a simple, yet, nontrivial example, the diffraction gratings. First let me write down the transmittance function for a one dimensional diffraction gratings with period d,

$$U(x) = \sum_n f(x - nd) \tag{1}$$

Now employing an important identity,

$$\Phi(x_0) = \Phi(x) * \delta(x_0) \tag{2}$$

Eqn (1) can be rewritten as

$$U(x) = f(x) * \sum_n \delta(x - nd) \tag{3}$$

Due to the famous convolution theorem,

$$\mathcal{F}[f * g] = \mathcal{F}[f]\mathcal{F}[g] \tag{4}$$

the Fourier transform of the transmittance function is simply

$$U(k) = f(k) \sum_{n=-N/2}^{N/2} \mathrm{e}^{-\mathrm{i}nkd} \tag{5}$$

$$= f(k) \frac{\sin(Nkd)}{\sin(kd)} \times (\text{const phase}) \tag{6}$$

where the constant phase is unimportant since what we are concerned is the intensity which is $I(k) = U(k)U(k)^*$. As N, the number of grooves, gets larger, the peaks get sharper and finally as $N \to \infty$, the peaks are genuine delta functions.

One step is missing in the above derivations, that is, why it is valid to codify the physics of diffraction in terms of Fourier transform. The explanation is as follows. The amplitude at position $\boldsymbol{r}$, is proportional to the sum of all the contributions of the secondary sources populated on the aperture which is modulated by a transmittance function[1],

$$\psi(\boldsymbol{r}) \propto \int d^2x'\, U(\boldsymbol{r}')\, \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{R}\cdot\boldsymbol{k}}}{R} \tag{7}$$

where $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$. And in the far field approximation, namely $r = |\boldsymbol{r}| \gg |\boldsymbol{r}'|$,

$$R = r - \hat{r}' \cdot \boldsymbol{r}' + \dots \tag{8}$$

Eqn (7) becomes

$$\psi(\boldsymbol{r}) \propto \frac{\mathrm{e}^{\mathrm{i}rk}}{r} \int d^2x'\, U(\boldsymbol{r}')\, \mathrm{e}^{-\mathrm{i}\boldsymbol{r}'\cdot\boldsymbol{k}'} \tag{9}$$

and notice the expression is simply a spherical wave times the Fourier transform of the transmittance function and $\boldsymbol{k}' = k\hat{r}'$. To display the patterns on a screen, a lens is utilized to map directions into positions on the screen, which completes the story for diffraction gratings.

B. X-Ray Scattering and Static Structure Factor

The wave length of x-ray is of order 1 Å, while the Compton wavelength of electron is about a hundred times smaller, therefore, the interaction can be treated classically. In natural units, the Compton wavelength is simply $1/m$ which is independent of interaction[2]; if we multiply it by the dimensionless fine structure constant, the electron-photon coupling constant, it becomes the classical electron radius $r_c = \alpha/m$. The cross section is proportional to r_c^2 since stronger the coupling, more evident the scattering phenomenon.

Energy of x-ray is of order 1 keV while usual energy scale of electrons in metal and outer shell of atoms is of order 1 eV, therefore, the electrons can be treated as free electrons. In classical picture, the free electrons are driven by external electric field and in turn, give off dipole radiation. The photon field is given by the formula,

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{\mu_0}{4\pi} \int d^3x'\, \boldsymbol{J}(\boldsymbol{r}') \frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{10}$$

$$\approx \frac{\mu_0}{4\pi} \frac{\mathrm{e}^{\mathrm{i}kr}}{r} \int d^3x'\, \boldsymbol{J}(\boldsymbol{r}') \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'} \tag{11}$$

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[*]The following content is not an exact copy of the board, but an edited version, since I am trying to make it more comprehensive and self-contained.

where we played the same trick again in the second line. The current density is proportional to the electron density, namely,

$$\boldsymbol{J}(\boldsymbol{r}') = -e\boldsymbol{v}(\boldsymbol{r}')n_e(\boldsymbol{r}') \tag{12}$$

where the electron velocity is related to incident plane wave by $\boldsymbol{v}(\boldsymbol{r}') \propto \exp(\mathrm{i}\boldsymbol{k}_i \cdot \boldsymbol{r}')$. Now the vector potential is truly proportional to the Fourier transform of electron density,

$$\boldsymbol{A}(\boldsymbol{r};\boldsymbol{q}) \propto \int d^3x'\, n_e(\boldsymbol{r}')\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k}_i)\cdot\boldsymbol{r}'} = n(\boldsymbol{q}) \tag{13}$$

where $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}_i$ and assume that the scattering is elastic, $k_i = k'$, then $q \leq 2k_i$. If we write the electron density in a form similar to Eqn (3), that is the convolution of atomic distribution of charges[3] $f(\boldsymbol{r})$ and atomic position distribution formulated by a sum of deltas,

$$n_e(\boldsymbol{r}) = f(\boldsymbol{r}) * \sum_j^{\text{atoms}} \delta(\boldsymbol{r} - \boldsymbol{R}_j) \tag{14}$$

then we have the Fourier transform thereof as

$$n_e(\boldsymbol{q}) = f(\boldsymbol{q}) \times \sum_j^{\text{atoms}} \mathrm{e}^{-\mathrm{i}\boldsymbol{R}_j\cdot\boldsymbol{q}} \tag{15}$$

The intensity obtained from detectors situated at different angular directions far from the target is proportional to $|n(q)|^2$,

$$I(\boldsymbol{q}) \propto \langle n(\boldsymbol{q})n(-\boldsymbol{q})\rangle = N|f(\boldsymbol{q})|^2 S(\boldsymbol{q}) \tag{16}$$

where the average can be both ensemble average or ground state expectation value. The static structure factor by definition is simply

$$S(\boldsymbol{q}) = \frac{1}{N}\left\langle \left(\sum_j^{\text{atoms}} \mathrm{e}^{-\mathrm{i}\boldsymbol{R}_j\cdot\boldsymbol{q}}\right)\left(\sum_{j'}^{\text{atoms}} \mathrm{e}^{-\mathrm{i}\boldsymbol{R}_{j'}\cdot\boldsymbol{q}}\right)^* \right\rangle \tag{17}$$

$$= \frac{1}{N}\left\langle \sum_{j,j'}^{\text{atoms}} \mathrm{e}^{-\mathrm{i}(\boldsymbol{R}_j-\boldsymbol{R}_{j'})\cdot\boldsymbol{q}} \right\rangle \tag{18}$$

Information of the many-body density distribution is all contained in the structure factor.

In sum, electrons of atoms respond to external x-ray while we collect the response signals and extract the atomic distribution information, which is what we really want to know.

C. Neutron Scattering and Dynamic Structure Factor

In x-ray scattering, the change in energy of a photon is merely of negligible fraction of the total energy, so only the momentum transfer to target $\hbar\boldsymbol{q}$ was taken into account. In the case of slow neutron scattering (10 meV, 1 Å), we can measure the final speeds of the scattered neutrons and hence, obtain the changes in energy. Apparently, we can learn even more about the many-particle system by carrying out neutron scattering experiments.

In the case of x-ray scattering, the interaction is electron-photon interaction whereas in the neutron scattering, the effective interaction is point-to-point collision between a neutron and a nucleus which was formulated by Fermi in 1930s as

$$V(\boldsymbol{r},\boldsymbol{R}) \approx \frac{4\pi a_s\hbar^2}{2m_r}\delta^3(\boldsymbol{r}-\boldsymbol{R}) \tag{19}$$

where a_s is the s-wave scattering length[4], $\boldsymbol{R}$ is the nucleus location and $m_r = mM/(M+m)$ the reduced mass which approximately the mass of neutron m.

The external potential is the total contribution from all the atoms

$$V^{\text{ex}}(\boldsymbol{r}) = \sum_{l=1}^{N} V(\boldsymbol{r}-\boldsymbol{R}_l) = \frac{4\pi a_s\hbar^2}{2m} n(\boldsymbol{r}) \tag{20}$$

In order to spell out the transition matrix element, we need to first write down the initial state and final state. Neutron is spin-1/2, therefore, the incident wave takes the form $\frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\eta_\lambda$ where η is a Dirac spinor. The outgoing wave is also a plane wave, $\frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}}\eta_{\lambda'}$ where the far field approximation was made implicitly. The initial and final states of the many-body system are $|i\rangle$ and $|f\rangle$. The overall states and direct products of the neutron and many-body system.

Now we are able to assemble the transition matrix element,

$$H_{fi} = \frac{1}{V}\int d^3x\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}}\eta^\dagger_{\lambda'}\langle f|\, V^{\text{ex}}(\boldsymbol{r})\,|i\rangle\,\eta_\lambda \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{21}$$

$$= \frac{4\pi a_s\hbar^2}{2m}\frac{\delta_{\lambda\lambda'}}{V}\int d^3x\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\langle f|\, n(\boldsymbol{r})\,|i\rangle \tag{22}$$

$$= \frac{4\pi a_s\hbar^2}{2m}\frac{\delta_{\lambda\lambda'}}{V}\langle f|\, n(\boldsymbol{q})\,|i\rangle \tag{23}$$

where spin interaction is neglected hence it is conserved and where $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ is the good old momentum transfer.

The transition rate, according to Fermi's golden rule, is

$$R_{i\to f} = \frac{2\pi}{\hbar}|H_{fi}|^2\delta(\hbar\omega - E_f + E_i) \tag{24}$$

and note that the matrix element has dimension of energy and the argument in the delta is also energy, so the dimesion of the transition rate is $[T]^{-1}$. In order to obtain the cross section which is $[L]^2$ from the transition rate R, we have to divide it by a quantity of dimension $[L]^{-2}[T]^{-1}$ which is the flux, particle number per area per time. It can also be expressed as neutron velocity per unit volumn V[5]

$$\text{(incident flux)} = \frac{v_n}{V} = \frac{\hbar k}{mV} \tag{25}$$

The measurable cross section is simply $R_{i\to f}/(\text{flux})$ but since the sample is initially coupled to a heat bath and we have not specify the final state, we should take thermal average of the initial states $|i\rangle$ and sum over all possible final states $|f\rangle$, which gives

$$d^2\sigma = \left\{ \frac{2\pi}{\hbar} \left(\frac{4\pi a_s \hbar^2}{2mV} \right)^2 \sum_{fi} \frac{1}{Z} \mathrm{e}^{-\beta E_i} |\langle f|\, n(\boldsymbol{q})\, |i\rangle|^2 \delta(\hbar\omega - E_f + E_i) \left(\frac{mV}{\hbar k} \right) \right\} \frac{V}{(2\pi)^2} d^3k' \tag{26}$$

where $d^3k' = k'^2 dk' d\Omega' = \frac{m}{\hbar} k' d\frac{\hbar k'^2}{2m} d\Omega' = \frac{m}{\hbar} k' d\omega d\Omega'$ and notice all the V cancels as expected.

Differentiate the cross section with respect to the solid angle Ω' and frequency ω, we have

$$\frac{d^2\sigma}{d\Omega' d\omega} = N a_s^2 \frac{k'}{k} S(\boldsymbol{q}, \omega) \tag{27}$$

where $S(\boldsymbol{q}, \omega)$ is the *dynamic structure factor* which, canceling out all the $\pi, \hbar, m, V$ exactly, is

$$S(\boldsymbol{q}, \omega) = \sum_{fi} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f|\, n(\boldsymbol{q})\, |i\rangle|^2 \delta(\omega - \omega_f + \omega_i) \tag{28}$$

What follows are a few facts about dynamic structure factor.

Static structure factor Simply perform an integral over ω, the frequency dependency automatically vanishes[6] leaving the sum,

$$S(\boldsymbol{q}) = \sum_{fi} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f|\, n(\boldsymbol{q})\, |i\rangle|^2 \tag{29}$$

$$= \sum_{i} \frac{\mathrm{e}^{-\beta E_i}}{NZ} \langle i|\, n^\dagger(\boldsymbol{q}) \Big\{ \sum_f |f\rangle \langle f| \Big\}_{=1} n(\boldsymbol{q})\, |i\rangle \tag{30}$$

$$= \frac{1}{N} \left\langle n^\dagger(\boldsymbol{q}) n(\boldsymbol{q}) \right\rangle \tag{31}$$

which recovers the static structure factor being proportional to density correlation.

Dynamical correlation Rewrite delta function as

$$\delta(\omega - \omega_f + \omega_i) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}\omega_f t} \mathrm{e}^{\mathrm{i}\omega_i t} \tag{32}$$

and put it into Eqn (28), we have

$$S(\boldsymbol{q}, \omega) = \sum_{fi} \int_{-\infty}^{\infty} \frac{dt}{2\pi} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f|\, n(\boldsymbol{q})\, |i\rangle|^2 \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{-\mathrm{i}\omega_f t} \mathrm{e}^{\mathrm{i}\omega_i t} \tag{33}$$

$$= \sum_{fi} \int_{-\infty}^{\infty} \frac{dt}{2\pi} \frac{\mathrm{e}^{-\beta E_i}}{NZ} \langle i|\, \mathrm{e}^{\mathrm{i}\omega_i t} n^\dagger(\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}\omega_f t}\, |f\rangle\, \mathrm{e}^{\mathrm{i}\omega t} \tag{34}$$

$$\times \langle f|\, n(\boldsymbol{q})\, |i\rangle$$

$$= \frac{1}{N} \int_{-\infty}^{\infty} \frac{dt}{2\pi} \left\langle n^\dagger(\boldsymbol{q}; t) n(\boldsymbol{q}; 0) \right\rangle \mathrm{e}^{\mathrm{i}\omega t} \tag{35}$$

$$= \frac{1}{N} \int \frac{d^4x}{(2\pi)^4} \left\langle n^\dagger(x^\mu) n(0) \right\rangle \mathrm{e}^{\mathrm{i}k^\mu x_\mu} \tag{36}$$

where the correlation is about two points separated in spacetime which can be calucualted in terms of Feynman diagrams.

Detailed balance Now we perform a time reversal, that is

$$S(\boldsymbol{q}, -\omega) = \sum_{fi} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f|\, n(\boldsymbol{q})\, |i\rangle|^2 \delta(\omega - \omega_i + \omega_f) \tag{37}$$

$$= \sum_{if} \frac{\mathrm{e}^{-\beta E_f}}{NZ} |\langle i|\, n(\boldsymbol{q})\, |f\rangle|^2 \delta(\omega - \omega_f + \omega_i) \tag{38}$$

$$= \mathrm{e}^{-\beta\hbar\omega} \sum_{if} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f|\, n^\dagger(\boldsymbol{q})\, |i\rangle|^2 \delta(\omega - \omega_f + \omega_i) \tag{39}$$

where in the second line we exchanged the index i, f to restore the original delta and used the constraint

$E_f = E_i + \hbar\omega$ to eliminate E_f and also the fact that $|z| = |z^*|$ for any complex number z. Next notice $n^\dagger(\boldsymbol{q}) = n(-\boldsymbol{q})$, therefore,

$$S(-\boldsymbol{q}, -\omega) = \mathrm{e}^{-\beta\hbar\omega} S(\boldsymbol{q}, \omega) \tag{40}$$

which is the *detailed balance* condition. Since $\omega = (E_f - E_i)/\hbar$, the left hand side corresponds to the process where the many-body system loses energy for some positive ω. At zero temperature, $\beta \to \infty$, there is zero possibility for a ground state to lose energy while at high temperature, the loss and gain are equally probable.

The f-sum rule We evaluate the first moment in ω,

$$\begin{aligned} I(\boldsymbol{q}) &:= \int \omega S(\boldsymbol{q}, \omega) d\omega \quad &(41)\\ &= \sum_{fi} \frac{E_f - E_i}{\hbar} \frac{\mathrm{e}^{-\beta E_i}}{NZ} |\langle f| n(\boldsymbol{q}) |i\rangle|^2 \quad &(42)\\ &= \sum_{fi} \frac{1}{\hbar N} \frac{\mathrm{e}^{-\beta E_i}}{Z} \\ &\times \{ \langle i| n^\dagger(\boldsymbol{q}) |f\rangle \langle f| \mathcal{H}^\dagger n(\boldsymbol{q}) |i\rangle \quad &(43)\\ &\quad - \langle i| n^\dagger(\boldsymbol{q}) |f\rangle \langle f| n(\boldsymbol{q})\mathcal{H} |i\rangle \} \\ &= \frac{1}{\hbar N} \left\langle n^\dagger(\boldsymbol{q})[\mathcal{H}, n(\boldsymbol{q})] \right\rangle \quad &(44)\\ &= \frac{1}{2\hbar N} \left\langle [n^\dagger(\boldsymbol{q}), [\mathcal{H}, n(\boldsymbol{q})]] \right\rangle \quad &(45)\\ &= \frac{\hbar q^2}{2m} \quad &(46) \end{aligned}$$

where the $\mathcal{H}$ is the many-body Hamiltonian. From line (44) to line (45), what is going on is as follows. First, notice that the value of the integral is real, therefore, it equals its complex conjugate

$$\left\langle n^\dagger(\boldsymbol{q})[\mathcal{H}, n(\boldsymbol{q})] \right\rangle = \left\langle [n^\dagger(\boldsymbol{q}), \mathcal{H}] n(\boldsymbol{q}) \right\rangle$$

Second, assume that the specimen is of inversion symmetry, then the substitution $-\boldsymbol{q} \to \boldsymbol{q}$ will leave the integral invariant, namely $I(-\boldsymbol{q}) = I(\boldsymbol{q})$, then

$$I(\boldsymbol{q}) = \frac{1}{2}[I(\boldsymbol{q}) + I(-\boldsymbol{q})]$$

Last, identify the following

$$I(\boldsymbol{q}) \propto \left\langle n^\dagger(\boldsymbol{q})[\mathcal{H}, n(\boldsymbol{q})] \right\rangle$$

$$I(-\boldsymbol{q}) \propto \left\langle [n(\boldsymbol{q}), \mathcal{H}] n^\dagger(\boldsymbol{q}) \right\rangle$$

and add them up which, in turn, gives the outer commutator in line (45).

From line (45) to (46), it is convenient to invoke the explicit expression of $n(\boldsymbol{q})$, a sum of deltas, which is in agreement with the assumption of delta-interaction. From here, I will change the notation of particle density to $\rho(\boldsymbol{r})$ and its Fourier transform $\rho_{\boldsymbol{q}}$. The f-sum rule is a direct consequence of particle conservation[7], where the conservation is expressed as the continuity equation

$$\partial_t \rho + \nabla \cdot \boldsymbol{J} = 0 \tag{47}$$

Take the spatial Fourier transform, it becomes

$$\partial_t \rho_{\boldsymbol{q}} + i\boldsymbol{q} \cdot \boldsymbol{J}_{\boldsymbol{q}} = 0 \tag{48}$$

where the particle density

$$\rho(\boldsymbol{r}) = \sum_j \delta(\boldsymbol{r} - \boldsymbol{r}_j) \tag{49}$$

$$\rho_{\boldsymbol{q}} = \sum_j \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j} \tag{50}$$

and the current density

$$\boldsymbol{J}(\boldsymbol{r}) = \frac{1}{2} \sum_i \left[\frac{\boldsymbol{p}_i}{m} \delta(\boldsymbol{r} - \boldsymbol{r}_i) + \delta(\boldsymbol{r} - \boldsymbol{r}_i) \frac{\boldsymbol{p}_i}{m} \right] \tag{51}$$

$$\boldsymbol{J}_{\boldsymbol{q}} = \frac{1}{2} \sum_i \left[\frac{\boldsymbol{p}_i}{m} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i} + \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i} \frac{\boldsymbol{p}_i}{m} \right] \tag{52}$$

where $\boldsymbol{p}$ and $\boldsymbol{r}$ are both operators and they do not commute. Now it is ready to show that

$$[\rho_{\boldsymbol{q}}, \mathcal{H}] = \left[\rho_{\boldsymbol{q}}, \sum_i \frac{\boldsymbol{p}_i^2}{2m} \right] = \hbar \boldsymbol{q} \cdot \boldsymbol{J}_{\boldsymbol{q}} \tag{53}$$

where $\rho_{\boldsymbol{q}}$ is a function of positions and where the interaction parts of $\mathcal{H}$ is assumed to be velocity-independent and depend solely on positions $\{\boldsymbol{r}_i\}_{i=1}^N$. Therefore, only the kinetic part survives the commutation. However, without invoking the exact expression of the density and current, we can still get this result if you concede the conservation of particle number, that is Eqn (47). The argument is simple: first in Heisenberg picture, the time derivative of $\rho_{\boldsymbol{q}}$ reads

$$\partial_t \rho_{\boldsymbol{q}} = -\frac{\mathrm{i}}{\hbar} [\rho_{\boldsymbol{q}}, \mathcal{H}] \tag{54}$$

and next identify it with Eqn (48), we have the desired Eqn (53) without writing down explicitly the density and many-body Hamiltonian.

Now let's calculate the outer commutator which is

$$[\rho_{\boldsymbol{q}}^\dagger, [\mathcal{H}, \rho_{\boldsymbol{q}}]] = -\hbar \boldsymbol{q} \cdot [\rho_{\boldsymbol{q}}^\dagger, \boldsymbol{J}_{\boldsymbol{q}}] \tag{55}$$

With the explicit expressions of density and current, we have

$$[\rho_{\boldsymbol{q}}^\dagger, \boldsymbol{J}_{\boldsymbol{q}}] = \sum_i^N \mathrm{i}\hbar \times \frac{\mathrm{i}\boldsymbol{q}}{m} = -N\hbar\boldsymbol{q}/m \tag{56}$$

Hence

$$[\rho_{\boldsymbol{q}}^{\dagger},[\mathcal{H},\rho_{\boldsymbol{q}}]] = N\hbar^2\boldsymbol{q}^2/m \tag{57}$$

which gives the final result (46).

The power of f-sum rule lies in the fact that no matter what form the structure factor takes, the integral always comes out simply and it serves as a quick check for however complicated theories.

II. LINEAR RESPONSE AND CAUSAL COMMUTATOR

A. Response to a weak perturbation

Properties of a given many-body system can be inferred from the resulting effects due to a weak perturbation. Namely, the total Hamiltonian reads,

$$\mathcal{H}^{\mathrm{tot}}(t) = \mathcal{H} + \mathcal{H}^{\mathrm{ex}}(t) \tag{58}$$

where the external perturbation $\mathcal{H}^{\mathrm{ex}}(t) = 0$ for $t < 0$ and $\mathcal{H}^{\mathrm{ex}}(t) \ll \mathcal{H}$ for $t > 0$. In previous examples of X-ray and neutron scattering, the perturbation due to the scatterers are both weak. For X-ray scattering, the dimensionless coupling constant is simply the fine-structure constant $\alpha = 1/137 \ll 1$ since the scattering is due to photon-electron interaction. For the neutron case, we can concoct a dimensionless coupling constant from $a_s \sim 10^{-15}$m and thermal wavelength $\lambda_{\mathrm{th}} \sim 10^{-10}$m, and therefore $a_s/\lambda_{\mathrm{th}} \sim 10^{-5} \ll 1$. You may check that longer the wavelength or smaller the effective scattering length, the more probable the neutrons miss the target nucleus, and hence, weaker the coupling.

For $t < 0$, the system evolves according to the unperturbed $\mathcal{H}$, and in Schrödinger picture, the state takes the form

$$\left|\Psi_S^0(t)\right\rangle = \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\left|\Psi_S^0(0)\right\rangle \tag{59}$$

When the perturbation is turned on, we assume, the state takes the following form,

$$\left|\Psi_S(t)\right\rangle = \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}A(t)\left|\Psi_S^0(0)\right\rangle \tag{60}$$

with $A(t)$ to be determined with the boundary condition $A(t < 0) = 1$. And the state satisfies the Schrödinger equation,

$$\mathrm{i}\hbar\left|\dot{\Psi}_S(t)\right\rangle = (\mathcal{H} + \mathcal{H}^{\mathrm{ex}})\left|\Psi_S(t)\right\rangle \tag{61}$$

Now there are two ways of writing the time derivative of the state and from the two results with different forms, we can deduce the equation of motion of $A(t)$.

Firstly, we substitute the state for the ansatz (Eqn (60)) in Eqn (61),

$$\mathrm{i}\hbar\left|\dot{\Psi}_S(t)\right\rangle = (\mathcal{H} + \mathcal{H}^{\mathrm{ex}})\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}A(t)\left|\Psi_S^0(0)\right\rangle \tag{62}$$

$$= \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}(\mathcal{H} + \mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar}\mathcal{H}^{\mathrm{ex}}\mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}) \times A(t)\left|\Psi_S^0(0)\right\rangle \tag{63}$$

$$= \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}(\mathcal{H} + \mathcal{H}_H^{\mathrm{ex}}(t))A(t)\left|\Psi_S^0(0)\right\rangle \tag{64}$$

where $\mathcal{H}_H^{\mathrm{ex}}(t)$ is the Heisenberg operator. Secondly, take time derivative of Eqn (60),

$$\mathrm{i}\hbar\left|\dot{\Psi}_S(t)\right\rangle = \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}(\mathcal{H}A(t) + \mathrm{i}\hbar\dot{A}(t))\left|\Psi_S^0(0)\right\rangle \tag{65}$$

Therefore, we conclude the equation for $A(t)$ is

$$\mathrm{i}\hbar\dot{A}(t) = \mathcal{H}_H^{\mathrm{ex}}(t)A(t) \tag{66}$$

and you may check that the solution satisfies the condition $A(t < 0) = 1$

$$A(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t dt'\mathcal{H}_H^{\mathrm{ex}}(t')\right) \tag{67}$$

Since the perturbation is small, we can keep up to the linear term[8] in $\mathcal{H}_H^{\mathrm{ex}}$, and Eqn (60) becomes

$$\left|\Psi_S(t)\right\rangle = \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\left[1 - \frac{\mathrm{i}}{\hbar}\int_0^t dt'\mathcal{H}_H^{\mathrm{ex}}(t')\right]\left|\Psi_S(0)\right\rangle \tag{68}$$

Now we consider the expectation of an arbitrary observable $\hat{O}(t)$,

$$\left\langle\hat{O}(t)\right\rangle = \left\langle\Psi_S(t)\right|\hat{O}_S(t)\left|\Psi_S(t)\right\rangle \tag{69}$$

$$= \left\langle\Psi_S(0)\right|\left[1 + \frac{\mathrm{i}}{\hbar}\int_0^t dt'\mathcal{H}_H^{\mathrm{ex}}(t')\right]\mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar}\hat{O}_S(t) \times \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar}\left[1 - \frac{\mathrm{i}}{\hbar}\int_0^t dt'\mathcal{H}_H^{\mathrm{ex}}(t')\right]\left|\Psi_S(0)\right\rangle \tag{70}$$

$$= \left\langle\hat{O}_H(t)\right\rangle + \delta\left\langle\hat{O}_H(t)\right\rangle \tag{71}$$

where $\left|\Psi_H\right\rangle = \left|\Psi_S(0)\right\rangle$ and dropping quadratic terms

$$\delta\left\langle\hat{O}_H(t)\right\rangle = -\frac{\mathrm{i}}{\hbar}\int_0^t dt\,\left\langle[\hat{O}_H(t),\mathcal{H}^{\mathrm{ex}}(t')]\right\rangle \tag{72}$$

The average, in this case, is the ground state average but can be extended to ensemble average at finite temperature.

B. Causality and frequency half plane

The t' in Eqn (72) varies in the range $0 < t' < t$. Automatically, $t > t'$ or t is later than t, that is, the external perturbation causes the deviation in the observable and the expression on the RHS is called the causal commutator.

For a generic, square-integrable causal function $f(t)$ which is 0 for $t < 0$ and finite at $t = 0$, the Fourier transform $f(\omega)$ reads

$$f(\omega) = \int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t} f(t) = \int_{0}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t} f(t) \qquad (73)$$

Take $\omega = \omega_1 + \mathrm{i}\omega_2$ with both ω_1 and ω_2 real-valued, then

$$f(\omega) = \int_{0}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega_1 t} \mathrm{e}^{-\omega_2 t} f(t) < \infty \quad \text{for } \omega_2 > 0 \qquad (74)$$

and also the n-th derivatives

$$f^{(n)}(\omega) = \int_{0}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega_1 t} (\mathrm{i}t)^n \mathrm{e}^{-\omega_2 t} f(t) < \infty \qquad (75)$$

for positive imaginary part ω_2. Hence, a causal function is analytic in upper half ω-plane.

The following integral

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t} f(\omega) \qquad (76)$$

is performed in lower half plane ($\mathrm{Im}(\omega) < 0$) when $t > 0$ and in upper half plane ($\mathrm{Im}(\omega) > 0$) when $t < 0$.

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[1] The origin is placed in the plane of the aperture, then $\boldsymbol{r}'$ is simply two-dimensional.

[2] The celebrated Compton effect is merely a result of 4-momentum conservation.

[3] Assume that the atoms are all identical.

[4] a_S can be negative.

[5] One particle in a volumn V, the particle density is $1/V$.

[6] A trivial integral of delta function.

[7] cf. David Pines and Philippe Nozières

[8] This why it is called “linear” response.