1 Linear Response Theory

We now focus on formulating the screening problem in terms of the dielectric-response function. To faciliate this derivation, we first introduce the general formalism of treating slowly varying time-dependent perturbations,namely, linear-response theory. Ultimately, we will apply this approach to calculate the density response of a homogeneous system perturbed by the electric field of an external charge.
Consider a Hamiltonian of the form $H = H_0 + W(t)$. In the presence of the perturbation, W(t), the average value of any observable, Y, will accquire a nontrivial time-dependence through the time evolution of the density matrix. The average value of any dynamical observable, Y, at any time t is determined by

$$\langle Y(t)\rangle = Tr\Big[\rho(t)Y\Big], \tag{1}$$

where $\rho(t)$ is the density matrix appropriately normalized, so that $Tr\rho = 1$. The time evolution of the density matrix

$$\begin{aligned}\dot{\rho} &= -\frac{i}{\hbar}\Big[H,\rho\Big]\\ &= -\frac{i}{\hbar}\Big[H_0,\rho\Big] + \Big[W(t),\rho\Big]\end{aligned} \tag{2}$$

is governed by the Liouville equation of motion. To solve this equation, it is easier to work in the interaction representation. For any operator O, we define $\widehat{O}$ to be the interaction representation,

$$\widehat{O}(t) = S^{-1}OS \tag{3}$$

of O, where $S = e^{-\frac{iH_0t}{\hbar}}$. To simplify notation, we have departed from the convention of using $\widehat{O}$ to denote an operator,because $\widehat{O}$ now indicates an operator in the interaction representation. Rewriting the original average of Y and the Liouville equation in the interaction representation, we obtain,

$$\langle\widehat{Y}(t)\rangle = Tr\Big[\widehat{\rho}(t)\widehat{Y}(t)\Big] \tag{4}$$

and

$$\begin{aligned}i\hbar\dot{\widehat{\rho}} &= -H_0\widehat{\rho} + S^{-1}i\hbar\frac{\partial\rho}{\partial t}S + S^{-1}\rho H_0 S\\ &= -\Big[H_0\widehat{\rho}\Big] + S^{-1}\Big[H_0 + W(t),\rho\Big]S\\ &= \Big[\widehat{W}(t),\widehat{\rho}(t)\Big].\end{aligned} \tag{5}$$

Let ρ_0 be the density matrix before the perturbation is turned on. For a perturbation turned on at $t = -\infty$,the solution to the Liouville equation is the time-ordered product

$$\widehat{\rho}(t) = Texp\Big(\frac{1}{i\hbar}\int_{-\infty}^{t}\Big[\widehat{W}(t'),\widehat{\rho}\Big]dt'\Big)$$
$$= \rho_0 - \frac{i}{\hbar}\int_{-\infty}^{t}\Big[\widehat{W}(t_1),\rho_0\Big]dt_1 - \frac{1}{\hbar^2}\int_{-\infty}^{t}dt_1\int_{-\infty}^{t_1}dt_2\Big[\widehat{W}(t_1),\Big[\widehat{W}(t_2),\rho_0\Big]\Big] + \cdots \tag{6}$$

Consequently, through first order in the perturbation, we find that

$$\langle\widehat{Y}(t)\rangle = \langle\widehat{Y}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t}Tr(\widehat{Y}(t)\Big[\widehat{Y}(t'),\rho\Big])dt'. \tag{7}$$

Cyclically permuting under the trace leads to

$$\langle\widehat{Y}(t)\rangle = \langle\widehat{Y}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t}\chi YW(t,t')dt', \tag{8}$$

in which

$$\chi YW(t,t') = \langle[\widehat{Y}(t),\widehat{W}(t')]\rangle_0 \tag{9}$$

is the two-time response function, and $\langle\cdots\rangle_0$ signifies a trace with the equilibrium or initial density matrix, $\widehat{\rho}_0$. The quantum susceptibility to linear order is $\chi YW(t,t')$. This quantity governs the relaxation of a quantum system. For example, the crux of quantum linear-response theory is that the fluctuation

$$\langle\delta Y(t)\rangle = \langle\widehat{Y}(t)\rangle - \langle\widehat{Y}(t)_0$$
$$= \frac{-i}{\hbar}\int_{-\infty}^{t}\chi YW(t,t')dt' \tag{10}$$

is determined by the time integral of the average value of the commutator of the observable at time t with the perturbation at time t'.A few useful properties of $\chi YW(t,t')$ are

$$\chi YW(t,t') = -\chi YW(t,t') = -\chi Y^{*}W(t,t'). \tag{11}$$

These relationships follow because χYW is a commutator.

1.1 Fluctuation-Dissipation Theorem

Consider the general fluctuation

$$S_{YW}(t,t') = \langle\delta\widehat{Y}(t)\delta\widehat{W}(t')\rangle_0$$
$$= \langle\widehat{Y}(t)\widehat{W}(t')\rangle_0 - \langle\widehat{Y}(t)_0\langle\widehat{W}(t')\rangle_0. \tag{12}$$

The fluctuation-dissipation theorem equates fundamentally the spontaneous fluctuations that occur in an equilibrium system with the relaxation of a non-equilibrium system displaced from equilibrium. The equilibrium density matrix is

$$\rho_0 = e^{-\beta H_0} \tag{13}$$

The correlation function $S_{YW}(t,t')$ is a function of the time difference $t-t'$ rather than of t and t' separately. We want to show that $S_{YW}(t,t')$ is related to χYW. To do this, we first compute

$$\begin{aligned}\langle\widehat{Y}(t)\widehat{W}(t')\rangle_0 &= Tr\Big[e^{-\beta H_0}\widehat{Y}(t)\widehat{W}(t')\Big]\\ &= Tr\Big[e^{-\beta H_0}\widehat{W}(t')e^{-\beta H_0}\widehat{Y}(t)e^{\beta H_0}\Big]\\ &= \langle\widehat{W}(t')\widehat{Y}(t+i\beta\hbar)\rangle_0.\end{aligned} \tag{14}$$

Coupled with the identity

$$\begin{aligned}\langle\widehat{Y}(t)\rangle_0 &= Tr\Big[e^{-\beta H_0}\widehat{Y}(t)\Big] = Tr\Big[e^{-\beta H_0}e^{-\beta H_0}\widehat{Y}(t)e^{\beta H_0}\Big]\\ &= \langle\widehat{Y}(t+i\beta\hbar)\rangle_0,\end{aligned} \tag{15}$$

we arrive at the equality $S_{YW}(t,t') = S_{YW}(t', t+i\beta\hbar)$. In Fourier space, we have

$$\begin{aligned}S_{YW}(\omega) &= \int_{-\infty}^{\infty} d(t-t')S_{YW}(t,t')e^{i\omega(t-t')}\\ &= \int_{-\infty}^{\infty} d(t-t')S_{WY}(t', t+i\beta\hbar)e^{i\omega(t-t')}.\end{aligned} \tag{16}$$

Let $x = t'-t-i\beta\hbar; dx = d(t'-t)$. The Fourier transform of S_{YW} becomes

$$\begin{aligned}S_{YW}(\omega) &= e^{\beta\hbar\omega}\int_{-\infty}^{\infty} dx S_{WY}(x)e^{-i\omega x}\\ &= e^{\beta\hbar\omega}S_{WY}(-\omega).\end{aligned} \tag{17}$$

Combining these results to calculate $\chi YW(\omega)$,

$$\begin{aligned}\chi YW(\omega) &= \int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}\Big\langle\Big[\widehat{Y}(t),\widehat{W}(t')\Big]\Big\rangle_0\\ &= \int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}\Big[S_{YW}(t,t') - S_{WY}(t',t)\Big]\\ &= (1-e^{-\beta\hbar\omega})S_{YW}(\omega).\end{aligned} \tag{18}$$

Consequently, spontaneous fluctuations in equilibrium are related to the linear-response function $\chi YW(\omega)$. This means that relaxation oF fluctuations in a non-equilibrium system is determined by the same laws that govern the relaxation of spontaneous fluctuations in an equilibrium system. This is the fluctuation-dissipation theorem.

1.2 Density Response

Let us apply linear-response theory to density fluctuations. Consider a perturbation of the form

$$H'(t) = \int d\mathbf{r} n(\mathbf{r}, t) W(\mathbf{r}, t), \tag{19}$$

in which the electron density $n(\mathbf{r}, t)$ is changed by the application of an external field, $W(\mathbf{r}, t)$, which commutates with $n(\mathbf{r}, t)$ and H_0. According to linear-response theory,

$$\langle \delta n(\mathbf{r}, t) \rangle = \int_{-\infty}^{t} dt' d\mathbf{r}' \chi_{nn}(\mathbf{r}t, \mathbf{r}'t') W(\mathbf{r}', t'), \tag{20}$$

where

$$\chi_{nn}(\mathbf{r}t, \mathbf{r}'t') = -\frac{i}{\hbar} \langle [n(\mathbf{r}, t), n(\mathbf{r}', t')] \rangle . \tag{21}$$

As several response functions will be introduced, we stress that χ_{nn} represents the response of the system to the external(unscreened) field. We have subsumed the $-\frac{i}{\hbar}$ factor into the definition of the susceptibility. In Eq. (20), the time evolution of the density is determined entirely by H_0.

For free electrons, we define χ°_{nn} to be the response function. We showed previously that

$$n(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{p},\mathbf{p}',\sigma} e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} \, a^{\dagger}_{\mathbf{p}'\sigma} a_{\mathbf{p}\sigma} \tag{22}$$

is the time-independent operator for the electron density at $\mathbf{r}$. We remind the reader that we have dropped the 'hat' on an operator because this symbol is now reserved for the interaction representation. To define $n(\mathbf{r}, t)$, we need the time dependence of $a_{\mathbf{p}\sigma}$. We obtain this through the Heisenberg equations of motion

$$i\hbar \frac{\partial a_{\mathbf{p}\sigma}}{\partial t} = \left[a_{\mathbf{p}\sigma}, H_0 \right] = \sum_{\mathbf{p}',\sigma'} \epsilon_{\mathbf{p}'\sigma'} \left[a_{\mathbf{p}\sigma}, a^{\dagger}_{\mathbf{p}'\sigma'} a_{\mathbf{p}'\sigma'} \right] = \epsilon_{\mathbf{p}} a_{\mathbf{p}\sigma}, \tag{23}$$

where H_0 is the Hamiltanian for free electrons. Integrating the above, we obtain that

$$a_{\mathbf{p}\sigma}(t) = e^{-i\epsilon_p/\hbar} a_{\mathbf{p}\sigma}(t = 0). \tag{24}$$

Let us now evaluate χ_{nn} for a collection of free electrons. To simplify the notation, we define

$$q_{\mathbf{p}_{12}}(\mathbf{r}, t) = e^{i(\mathbf{p}_2-\mathbf{p}_1)\cdot\mathbf{r}/\hbar} \;\; e^{i(\epsilon_{p_1}-\epsilon_{p_2})t/\hbar}, \tag{25}$$

$\delta_{\mathbf{p}_{ij}} = \delta_{\mathbf{p}_i\mathbf{p}_j}$, and $f_{\mathbf{p}_1\mathbf{p}_2} = f_{\mathbf{p}1}(1 - f_{\mathbf{p}2})$. Combining our expression for $a_{\mathbf{p}\sigma}(t)$ together with Eq.(22), it follows that

$$\begin{aligned}\langle n(\mathbf{r},t)n(\mathbf{r}',t')\rangle &= \frac{1}{V^2}\sum_{\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4\sigma_1,\sigma_2}\langle a^\dagger_{\mathbf{p}_1\sigma_1}a_{\mathbf{p}_2\sigma_1}a^\dagger_{\mathbf{p}_3\sigma_2}a_{\mathbf{p}_4\sigma_2}\rangle q_{\mathbf{p}_{12}}(\mathbf{r},t)q_{\mathbf{p}_{34}}(\mathbf{r}',t') \\ &= \langle n(\mathbf{r},t)\rangle\langle n(\mathbf{r}',t')\rangle + \frac{1}{V^2}\sum_{\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4,\sigma_1,\sigma_2}\delta_{\sigma_1\sigma_2}\delta_{\mathbf{p}_{14}}\delta_{\mathbf{p}_{23}}f_{\mathbf{p}_1\mathbf{p}_2}q_{\mathbf{p}_{12}}(\mathbf{r},t)q_{\mathbf{p}_{34}}(\mathbf{r}',t') \\ &= \langle n(\mathbf{r},t)\rangle\langle n(\mathbf{r}',t')\rangle + \frac{1}{V^2}\sum_{\mathbf{p}_1,\mathbf{p}_2,\sigma}f_{\mathbf{p}_1\mathbf{p}_2}q_{\mathbf{p}_{12}}(\mathbf{r}-\mathbf{r}',t-t')\end{aligned} \tag{26}$$

Substitution of Eq. (15) into Eq. (21) illustrates immediately that the response function,

$$\chi^\circ_{nn}(\mathbf{r},t,\mathbf{r}',t') = \frac{1}{i\hbar V^2}\sum_{\mathbf{p}_1,\mathbf{p}_2,\sigma}(f_{\mathbf{p}_1\sigma}-f_{\mathbf{p}_2\sigma})\ q_{\mathbf{p}_{12}}(\mathbf{r}\text{-}\mathbf{r'},t-t') \tag{27}$$

and the density response function depend on the differences **r-r'** and $t-t'$. Hence, this response function is independent of the particular choice of origin in space as well as in time. We will find it most useful to work with the Fourier transform of $\chi^\circ_{nn}(\mathbf{r}t,\mathbf{r}'t')$:

$$\begin{aligned}\chi^\circ_{nn}(\mathbf{k},\omega) &= \int d\mathbf{x}\,dt\,e^{i\mathbf{k}.\mathbf{x}}\,e^{-i\omega t}\,\chi^\circ_{nn}(x,t) \\ &= \frac{2}{i\hbar V}\sum_{\mathbf{p}_1,\mathbf{p}_2}\delta_{\hbar k,\mathbf{p}_2-\mathbf{p}_1}(f_{\mathbf{p}_1}-f_{\mathbf{p}_2})\int_{-\infty}^{0}e^{-i(\hbar\omega+\epsilon_{\mathbf{p}_1}-\epsilon_{\mathbf{p}_2})t/\hbar}dt \\ &= \frac{2}{V}\sum_{\mathbf{p}_1}\frac{f_{\mathbf{p}_1}-f_{\mathbf{p}_1+\hbar\mathbf{k}}}{\hbar\omega+\epsilon_{\mathbf{p}_1}-\epsilon_{\mathbf{p}_1+\hbar\mathbf{k}}}.\end{aligned} \tag{28}$$

In Eq. (28), the factor of 2 comes from the spin summation, and the perturbation coupling to the density was assumed to be turned on at $t=-\infty$ and turned off at $t=0$. It is this expression that will be used to formulate the Lindhard screening function.

Consider the zero-frequency limit of $\chi^\circ_{nn}(\mathbf{k},\omega)$,

$$\chi^\circ_{nn}(\mathbf{k},\omega=0) = 2\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{\partial f_{\mathbf{p}}}{\partial\epsilon_p} = -2\int\frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{\partial f_{\mathbf{p}}}{\partial\mu} = -\frac{\partial n_e}{\partial\mu}, \tag{29}$$

which is precisely the Thomas-Fermi approximation to the screening function. This suggests that there is a fundamental connection between the density response function and screening. To establish the connection formally, we turn to the dielectric-response function.

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