# Lecture note Magnetism (13)

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Last week, we saw that the HF approximation on the Hubbard model leads to the Stoner condition, which brings about an energy difference between the ↑-band and the ↓-band. This modeling and the approximation enable us to explain some experimental facts like Slater-Paulings' curve qualitatively. On the other hand, the approximation still has qualitative and quantitative problems naturally for such a simple approximation. In such situations, self-consistent renormalization (SCR) spin-fluctuation theory gave satisfactory results at least for the ground states. This week we would like to reach the entrance of SCR theory but before that we need a bit heavy preparation, to which most of the lecture time is devoted.

## 6.4 Dynamic susceptibility

So far we have seen responses of materials to static magnetic fields. Here we turn our attention to responses to vibrating external fields. In such a case, we need to use the linear response theory.

### 6.4.1 Linear response

Let $\mathscr{H}_{\rm ext}(t)$ be the Hamiltonian of time-dependent external field. The total Hamiltonian is expressed as $\mathscr{H}_0+\mathscr{H}_{\rm ext}(t)$. From the time dependence of density matrix $\rho$ defined in the previous section in eq. (6.9) is,

$$i\hbar\frac{\partial\rho}{\partial t}=[\mathscr{H}_0+\mathscr{H}_{\rm ext}(t),\rho(t)], \tag{6.54}$$

where only time $t$ is shown explicitly as a variable. The initial state, for time $t=-\infty$, is set to the thermal equilibrium state of $\mathscr{H}_0$, that is

$$\rho(-\infty)=\rho_{\rm eq}=\frac{1}{Z_0}\exp\left(-\frac{\mathscr{H}_0}{k_{\rm B}T}\right), \tag{6.55}$$

where $Z_0={\rm Tr}[\exp(-\mathscr{H}_0/k_{\rm B}T)]$ is the partition function of unperturbed state.

As shown in Appendix 13A, the density matrix satisfies the following integral equation.

$$\rho(t)=\rho_{\rm eq}+\frac{1}{i\hbar}\int_{-\infty}^{t}dt'[U_0(t-t')\mathscr{H}_{\rm ext}(t')U_0^{-1}(t-t'),U_0(t-t')\rho(t')U_0^{-1}(t-t')] \tag{6.56}$$

$$=\rho_{\rm eq}+\frac{1}{i\hbar}\int_{-\infty}^{t}dt'U_0(t-t')[\mathscr{H}_{\rm ext}(t'),\rho(t')]U_0^{-1}(t-t'), \tag{6.57}$$

where also as in (13A.1),

$$U_0(t)\equiv\exp\left(\frac{\mathscr{H}_0}{i\hbar}t\right). \tag{6.58}$$

Since the commutation relation in the right hand side of eq. (6.57) is the response to an external field in addition to $\rho_{\rm eq}$, the lowest order in it is the first order of $t$. In the same way, $\mathscr{H}_{\rm ext}$ is a time-dependent part with no constant. As long as we consider the liner response, $\rho(t')$ in the commutation relation in eq. (6.57) can be replaced with time-independent $\rho_{\rm eq}$. $\rho_{\rm eq}$ commutes with Hamiltonian $\mathscr{H}_0$, being made from the eigenstates of it. Then we can write

$$\rho(t)\simeq\rho_{\rm eq}+\frac{1}{i\hbar}\int_{-\infty}^{t}dt'[U_0(t-t')\mathscr{H}_{\rm ext}(t')U_0^{-1}(t-t'),\rho_{\rm eq}]. \tag{6.59}$$

Now we assume the Hamiltonian of external field can be written in the form of

$$\mathscr{H}_{\rm ext}(t) = -PF(t), \tag{6.60}$$

where $F(t)$ is a quantity to represent the strength of the field and $P$ is the operator corresponding to the field. With this density matrix, an expectation value of a general physical quantity $Q$ can be obtained as $\mathrm{Tr}\{\rho(t)Q\}$[1, 2] in the following.

$$\langle Q(t)\rangle = \mathrm{Tr}\{\rho(t)Q\} = \langle Q_{\rm eq}\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t} dt' \,\langle [P, Q(t-t')]\rangle\, F(t'). \tag{6.61}$$

Here $\langle Q_{\rm eq}\rangle$ and $Q(t)$ are defined as

$$\langle Q_{\rm eq}\rangle = \mathrm{Tr}\{\rho_{\rm eq}Q\}, \quad Q(t) = U_0(t)^{-1}QU_0(t). \tag{6.62}$$

From eq. (6.61), we know that the expectation value $\langle [P, Q(t-t')]\rangle$ is a pure imaginary.

Now we consider the external field of frequency $\omega$ and write

$$F(t) = F_0\cos(\omega t) = \mathrm{Re}[F_0 e^{-i\omega t}]. \tag{6.63}$$

We here define the susceptibility $\chi(\omega)$ as

$$\mathit{\Delta} Q(t) = \langle Q(t)\rangle - \langle Q_{\rm eq}\rangle = \mathrm{Re}[\chi(\omega)F_0 e^{-i\omega t}]. \tag{6.64}$$

On the other hand, from eq. (6.61)

$$\mathit{\Delta} Q(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} dt' \,\langle [P, Q(t-t')]\rangle\, \mathrm{Re}[F_0 e^{-i\omega t'}]. \tag{6.65}$$

Now we know that the right-hand sides of eq. (6.64) equates eq. (6.65). The right hand side of (6.64) can be written as

$$\mathrm{Re}[\chi(\omega)F_0 e^{-i\omega t}] = \frac{F_0}{2}[\chi^*(\omega)e^{i\omega t} + \chi(\omega)e^{-i\omega t}]. \tag{6.66}$$

Similarly (6.65) is developed to

$$\frac{F_0}{2i\hbar}\left\{\left[\int_0^\infty d\tau\,\langle [P, Q(\tau)]\rangle\, e^{-i\omega\tau}\right] e^{i\omega t} + \left[\int_0^\infty d\tau\,\langle [P, Q(\tau)]\rangle\, e^{i\omega\tau}\right] e^{-i\omega t}\right\}, \tag{6.67}$$

where $\tau = t - t'$). By remembering $\langle [P, Q(\tau)]\rangle$ is a pure imaginary, we compare the above two to obtain the following.

Kubo formula

$$\chi_{QP}(\omega) = \frac{i}{\hbar}\int_0^\infty \langle [Q(\tau), P]\rangle\, e^{i\omega\tau} d\tau. \tag{6.68}$$

Here we add a subscript to $\chi$, which shows the relation of response $P \to Q$. Equation (6.68) is one of the formulas called **Kubo formula**, which give linear response functions[3]. This can be viewed as a terminus ad quem of the linear response theory initiated by Nyquist and by others. The Kubo formula has been applied to a vast field of science with fruitful results. It should be used probably forever in science. On the other hand, there are various different formalisms in linear response. We need to select one of them according tot the character of the problem[2].

### 6.4.2 Fluctuation-dissipation theorem

Equation (6.68) is a Fourier transformation from (time) to (frequency). At the same time it is a response of a physical quantity $Q$ to the external field in eq. (6.60). The correlation function $\langle [Q(\tau), P]\rangle$ represents transfer on time ($\tau$) axis to the susceptibility [*1]. Then we define a Green's function for physical quantity $P$, $Q$ as

$$G^{\pm}_{QP}(t) = \mp \frac{i}{\hbar}\theta(\pm t)\left\langle [Q(t), P] \right\rangle, \tag{6.69}$$

in which we restore the symbol for time as $\tau \to t$. Here $\theta(t)$ is the Heaviside function defined as

$$\theta(t) = \begin{cases} 1 & (t \geq 0), \\ 0 & (t < 0). \end{cases} \tag{6.70}$$

We also call $G^{+}_{QP}(t)$ as a retarded Green's function, $G^{-}_{QP}(t)$ an advanced Green's function. Then eq. (6.68) is a Fourier transformation of $G^{+}_{QP}(t)$, and can be written in the form

$$\chi_{QP}(\omega) = -\mathcal{G}^{+}_{QP}(\omega) = -\mathscr{F}_{\omega}\{G^{+}_{QP}(t)\}, \tag{6.71}$$

where $\mathscr{F}_{\omega}\{\cdots\}$ expresses the Fourier transform of $\cdots$ to $\omega$-space.

A Fourier transform of a correlation function of a perturbation and a response:

$$\mathcal{S}_{QP}(\omega) = \int_{-\infty}^{\infty} dt \left\langle Q(t), P \right\rangle e^{i\omega t} \tag{6.72}$$

is called a dynamical form factor. Here we can show the following as in Appendix 13B.

$$\mathcal{S}_{QP}(\omega) = \frac{i}{1 - e^{-\beta\hbar\omega}}[\mathcal{G}^{+}_{QP}(\omega) - \mathcal{G}^{-}_{QP}(\omega)], \tag{6.73}$$

where $\beta \equiv (k_{\mathrm{B}}T)^{-1}$. The left-hand side of eq. (6.73) is a Fourier transform of a correlation function and the right-hand side is a susceptibility of linear response. Such formulas that show linear relations between correlation functions and coefficients of linear responses are called **fluctuation dissipation theorem**. Of course fluctuations and energy-dissipations are different physical quantities. The theorems are not saying that they are the same but that fluctuations can be expressed by coefficients of linear response, which are parameters of energy dissipation.

Let $\{|n\rangle\}$ be a complete set of eigenfunctions of $\mathscr{H}$, then

$$\mathcal{G}^{+}_{QP}(\omega) = \sum_{n,m} \langle n|Q|m\rangle \langle m|P|n\rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_n - E_m + \hbar\omega + i\eta}. \tag{6.74}$$

### 6.4.3 Random Phase Approximation (RPA)

We consider an external magnetic field

$$\boldsymbol{B}(\boldsymbol{r}, t) = \boldsymbol{B}(\boldsymbol{q}, \omega) e^{i(\boldsymbol{q}\cdot\boldsymbol{r} - \omega t)}, \tag{6.75}$$

applied on a Hubbard model

$$\mathscr{H} = \sum_{i,j,s} t_{ij} c^{\dagger}_{is} c_{js} + U \sum_{i}^{N} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{6.25}$$

We write the local magnetization density in unit of $-g\mu_{\mathrm{B}}$ as

$$\boldsymbol{S}(\boldsymbol{r}) = \frac{1}{2}\sum_{i}\sum_{\alpha,\beta} \delta(\boldsymbol{r} - \boldsymbol{r}_i) c^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta}, \tag{6.76}$$

[*1] Green's function was invented by George Green (1973-1841). As you probably used in the electromagnetism, it is frequently used for finding solutions of differential equations. A Green's function generally expresses an effect of some local cause to an away point. It appears in various formalisms and the name "Green's function" is now also applied to general correlation (transfer) functions. I should note that according to ref. [4], the naming "Green's function" is strange and we should call it "Green function."

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector with Pauli matrices as elements. Accordingly, Hamiltonian(6.60) in the present case is

$$\mathscr{H}_{\rm ext}(t) = g\mu_{\rm B}\int \boldsymbol{B}(\boldsymbol{r},t)\cdot\boldsymbol{S}(\boldsymbol{r})d^3\boldsymbol{r} = g\mu_{\rm B}\boldsymbol{S}_{-\boldsymbol{q}}\cdot\boldsymbol{B}(\boldsymbol{q},\omega)e^{-i\omega t}. \tag{6.77}$$

Here Fourier-$\boldsymbol{q}$ components of magnetization $S_{\boldsymbol{q}}$ are defined as follows.

$$\left.\begin{aligned} S_{\boldsymbol{q}+} &= S_{\boldsymbol{q}x} + iS_{\boldsymbol{q}y} = \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \\ S_{\boldsymbol{q}-} &= S_{\boldsymbol{q}x} - iS_{\boldsymbol{q}y} = \sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\uparrow}, \\ S_{\boldsymbol{q}z} &= (1/2)\sum_{\boldsymbol{k}}(a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\uparrow} - a^\dagger_{\boldsymbol{k}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}). \end{aligned}\right\} \tag{6.78}$$

In comparison of eq. (6.77) and eq. (6.60), the quantity which corresponds to $P$ is $g\mu_{\rm B}\boldsymbol{S}_{-\boldsymbol{q}}$. On the other hand, the response is also magnetization and in linear response, that is $g\mu_{\rm B}\boldsymbol{S}_{\boldsymbol{q}}$. Hence the $z$-component of dynamic susceptibility is

$$\chi_{zz}(\boldsymbol{q},\omega) = (g\mu_{\rm B})^2\frac{i}{\hbar}\int_0^\infty dt\,\langle[S_{\boldsymbol{q}z}(t), S_{-\boldsymbol{q}z}]\rangle\, e^{i\omega t}. \tag{6.79}$$

Similarly, considering non-zero part after taking correlation function, the transverse component is written as

$$\chi_{+-}(\boldsymbol{q},\omega) = (g\mu_{\rm B})^2\frac{i}{\hbar}\int_0^\infty dt\,\langle[S_{\boldsymbol{q}+}, S_{-\boldsymbol{q}-}]\rangle\, e^{i\omega t}. \tag{6.80}$$

Let us calculate $\chi_{+-}(\boldsymbol{q},\omega)$ in the following way. We take a $\boldsymbol{k}$ term in the expression of $S_{\boldsymbol{q}+}(t)$ in eq. (6.78). The corresponding Green's function is

$$G^+_{\boldsymbol{k}\boldsymbol{q}}(t) = -i\theta(t)\,\langle[a^\dagger_{\boldsymbol{k}\uparrow}(t)a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}(t), S_{-\boldsymbol{q}-}]\rangle\,. \tag{6.81}$$

Henceforth we omit $+$ to specify "retarded." The time derivative of this Green's function (equation of motion) is

$$i\hbar\frac{\partial G_{\boldsymbol{k}\boldsymbol{q}}}{\partial t} = -i\theta(t)\,\langle[e^{i\mathscr{H}t/\hbar}[a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}]e^{-i\mathscr{H}t/\hbar}, S_{-\boldsymbol{q}-}]\rangle + \delta(t)\hbar\,\langle[a^\dagger_{\boldsymbol{k}\uparrow}(t)a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}(t), S_{-\boldsymbol{q}-}]\rangle\,. \tag{6.82}$$

We divide the Hubbard Hamiltonian into the kinetic energy term $\mathscr{H}_{\rm k}$ and the on-site interaction term $\mathscr{H}_{\rm int}$, and calculate the commutation relation in the right-hand side as follows.

$$\begin{aligned} [a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, S_{-\boldsymbol{q}-}] &= \sum_{\boldsymbol{k}'}[a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, a^\dagger_{\boldsymbol{k}'+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}'\uparrow}] \\ &= a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow} - a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, && (6.83\text{a}) \\ [a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}_{\rm k}] &= (\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}})a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, && (6.83\text{b}) \\ [a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, \mathscr{H}_{\rm int}] &= (U/N)\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{p}}[a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}, a^\dagger_{\boldsymbol{k}_1+\boldsymbol{p}\uparrow}a^\dagger_{\boldsymbol{k}_2-\boldsymbol{p}\downarrow}a_{\boldsymbol{k}_2\downarrow}a_{\boldsymbol{k}_1\uparrow}] \\ &= -(U/N)\left[\sum_{\boldsymbol{k}_1,\boldsymbol{p}}a^\dagger_{\boldsymbol{k}\uparrow}a^\dagger_{\boldsymbol{k}_1+\boldsymbol{p}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow}a_{\boldsymbol{k}_1\uparrow} + \sum_{\boldsymbol{k}_2,\boldsymbol{p}}a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow}a^\dagger_{\boldsymbol{k}_2-\boldsymbol{q}\downarrow}a_{\boldsymbol{k}_2\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\right]. && (6.83\text{c}) \end{aligned}$$

There are terms with four (2+2) operators products term of annihilation-creation operators in eq. (6.83c) representing the interaction, to which we apply mean field approximation. That is, we replace two of the four operators with the average of them in $[\cdots]$ as

$$\begin{aligned} -\sum_{\boldsymbol{p}}a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow}\,\langle a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow}\rangle + \sum_{\boldsymbol{k}_1}a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\,\langle a^\dagger_{\boldsymbol{k}_1\uparrow}a_{\boldsymbol{k}_1\uparrow}\rangle& \\ -\sum_{\boldsymbol{k}_2}a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\,\langle a^\dagger_{\boldsymbol{k}_2\downarrow}a_{\boldsymbol{k}_2\downarrow}\rangle + \sum_{\boldsymbol{p}}a^\dagger_{\boldsymbol{k}+\boldsymbol{p}\uparrow}a_{\boldsymbol{k}+\boldsymbol{q}+\boldsymbol{p}\downarrow}\,\langle a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\rangle\,.& \end{aligned} \tag{6.84}$$

Mean field approximation to such dynamic quantity is generally called **Random Phase Approximation(RPA)**. The naming means a quantity with a phase factor ($\exp(i\theta)$) of randomized phase ($\theta$) should vanish.

In eq. (6.84), a difference between an average on $\uparrow$ and that on $\downarrow$ is taken in the second and the thrid terms. In the paramagnetic states, they cancel each other, and the time derivative of Green's function in RPA (6.81)is

$$i\hbar\frac{\partial G_{\boldsymbol{kq}}}{\partial t} = (\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}})G_{\boldsymbol{kq}}(t) - (U/N)(\langle a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow}\rangle - \langle a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\rangle)\sum_{\boldsymbol{p}} G_{(\boldsymbol{k}+\boldsymbol{p})\boldsymbol{q}}(t) + (\langle a^\dagger_{\boldsymbol{k}\uparrow}a_{\boldsymbol{k}\uparrow}\rangle - \langle a^\dagger_{\boldsymbol{k}+\boldsymbol{q}\downarrow}a_{\boldsymbol{k}+\boldsymbol{q}\downarrow}\rangle)\delta(t). \quad (6.85)$$

Taking Fourier transformation of both side we get

$$\mathcal{G}_{\boldsymbol{kq}}(\omega) = \frac{f_{\boldsymbol{k}\uparrow} - f_{\boldsymbol{k}+\boldsymbol{q}\downarrow}}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}}\left[1 - \frac{U}{N}\sum_{\boldsymbol{p}}\mathcal{G}_{\boldsymbol{pq}}(\omega)\right], \quad (6.86)$$

where $f_{\boldsymbol{k}s} = \langle a^\dagger_{\boldsymbol{k}s}a_{\boldsymbol{k}s}\rangle$ is the Fermi distribution function. Summation over $\boldsymbol{k}$ gives

$$\chi_{+-}(\boldsymbol{q},\omega) = N(g\mu_{\rm B})^2\frac{2\chi^{(0)}(\boldsymbol{q},\omega)}{1 - 2U\chi^{(0)}(\boldsymbol{q},\omega)}, \quad (6.87)$$

where

$$\chi^{(0)}(\boldsymbol{q},\omega) = \frac{1}{2N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}+\boldsymbol{q}\downarrow} - f_{\boldsymbol{k}\uparrow}}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}}} \quad (6.88)$$

is the susceptibility of non-interacting system per site normalized by $(g\mu_{\rm B})^2$.

For the calculation of above $\chi^{(0)}(\boldsymbol{q},\omega)$ we calculate the following. Here for clearness of expression, we adopt $\hbar \to 1$, the unit of wavenumber is taken to $k_{\rm F}$, the unit of energy is taken to $\epsilon_{\rm F}$. With 3D Jacobian, the integral is written as

$$\frac{1}{2N}\sum_{\boldsymbol{k}}\frac{f_{\boldsymbol{k}}}{\omega + \epsilon_{\boldsymbol{k}-\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}} = \frac{1}{2}\rho(\epsilon_{\rm F})\int_0^1 k^2dk\int_{-1}^1\frac{d(\cos\theta)}{\omega + q^2 - 2kq\cos\theta} = \frac{1}{2}\rho(\epsilon_{\rm F})\int_0^1 k^2dk\frac{1}{2kq}\log\frac{\omega + q^2 + 2kq}{\omega + q^2 - 2kq}. \quad (6.89)$$

From a mathematical identity

$$\int x\log(ax+b)dx = \frac{1}{2}\left[x^2 - \left(\frac{b}{a}\right)^2\right]\log(ax+b) - \frac{x^2}{4} + \frac{b}{2a}x,$$

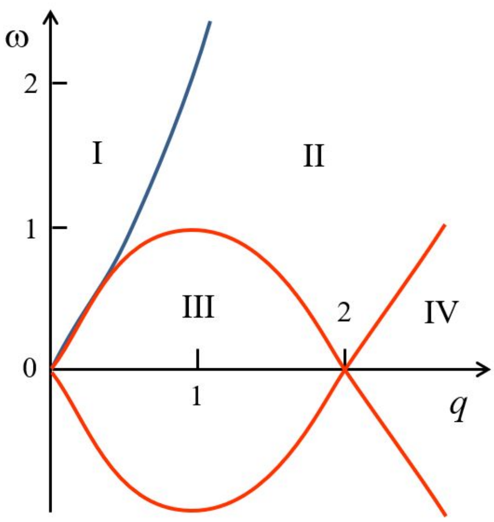


**Fig.** 6.4 Boundary lines of Kohn anomaly expressed in eq. (6.91), and four regions separated by them in the upper half of $q$-$\omega$ plane.

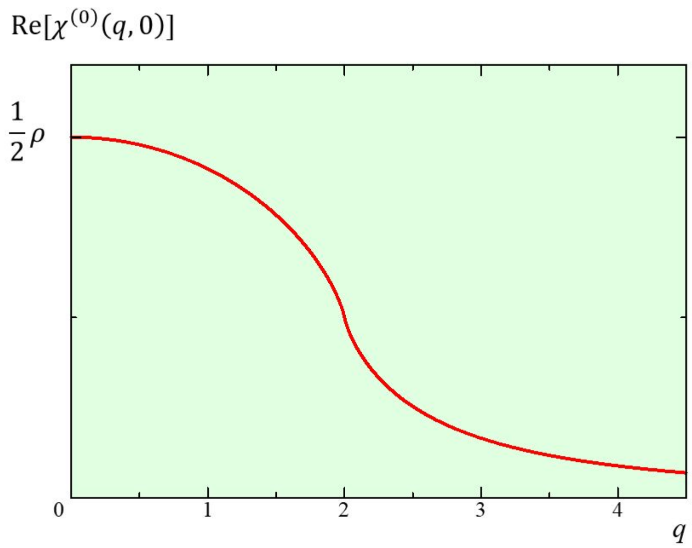


**Fig.** 6.5  Plot of the real part of $\chi^{(0)}(q,0)$ in eq. (6.93). The derivative diverges at $q=2$.

the integration can be performed as

$$\chi^{(0)}(q,\omega)=\frac{\rho(\epsilon_F)}{2}\frac{1}{2q}\left\{\frac{1}{2}\left[1-\left(\frac{\omega+q^2}{2q}\right)^2\right]\log\frac{\omega+q^2+2q}{\omega+q^2-2q}+\frac{\omega+q^2}{2q}\right.$$
$$\left.-\frac{1}{2}\left[1-\left(\frac{-\omega+q^2}{2q}\right)^2\right]\log\frac{-\omega+q^2-2q}{\omega+q^2+2q}+\frac{-\omega+q^2}{2q}\right\}. \tag{6.90}$$

In (6.90), when the arguments of log is negative, the susceptibility has a finite imaginary part that leads to damping. The boundary (Kohn anomaly boundary) is given by

$$\omega=\pm(q^2\pm 2q). \tag{6.91}$$

Figure 6.4 shows these boundaries on $q-\omega$ plane. They divide the upper half plane to four regions I∼IV. In regions I and IV, the imaginary part is zero. In region III, the imaginary part is

$$\mathrm{Im}[\chi^{(0)}(q,\omega)]=\frac{\rho(\epsilon_F)}{2}\frac{\pi}{4}\frac{\omega}{q}. \tag{6.92}$$

The real part is for $\omega=0$

$$\mathrm{Re}[\chi^{(0)}(q,0)]=\frac{\rho(\epsilon_F)}{2}\frac{1}{2q}\left\{\left(1-\frac{q^2}{4}\right)\log\left|\frac{2+q}{2-q}\right|+q\right\}. \tag{6.93}$$

This is plotted as a function of $q$ in Fig. 6.5. At the Kohn anomaly boundary $q=2(k_F)$, the curve shows a divergence of derivative by $q$.

From eq. (6.87) the RPA on dynamical susceptibility of Hubbard model predicts appearance of magnetic order for

$$U\chi^{(0)}(\boldsymbol{q}_{\max},0)\geq\frac{1}{2}. \tag{6.94}$$

Here $\boldsymbol{q}_{\max}$ is the wavenumber that gives the maximum value of $\chi^{(0)}$. In the case of $\boldsymbol{q}_{\max}=0$, as can be seen in Fig. 6.5, $chi^{(0)}(\boldsymbol{q}_{\max})\to\rho(\epsilon_F)/2$, then naturally this agrees with the Stoner condition. On the other hand, when $\boldsymbol{q}_{\max}\neq 0$, a magnetic order with finite wavenumber exists. This corresponds to **spin density wave (SDW)**.

## 6.5 Self-consistent renormalization spin fluctuation theory

As we have seen above, the mean field (HF approximation) theory based on the Hubbard model has various problems both in principle and in comparison with experiments. On the other hand, although parameter tuning may be included, it explains some aspects of experiments such as the Slater-Pauling's curve. It is impossible to discuss trends of researches from a single point of view. However a way to view the flows of research on magnetism is that there were two ways to go after the HF approximation. One is to look for different ways from HFA by simplifying models, by considering extreme cases and the strong correlation is taken into account more seriously. The other is improvement of HFA to solve the difficulties. The former has produced many interesting results on mathematical physics and conversely experiments appeared aiming at realizing such mathematical models. A big success of the latter is **self-consistent renormalization (SCR) spin fluctuation** theory[5].

Since it is difficult to see the mathematical scientific direction in the remaining one lecture, I would like to briefly explain the SCR theory and finish it. Many textbooks on mathematical science directions and strongly correlated systems have been published during the last quarter century[6, 7, 8, 9]. If you are interested, please refer to them.

(To be continued)

## Appendix 13A: Derivation of integral equation

We define the interaction representation of $\rho$ ($\rho^{(\mathrm{I})}$) as

$$\rho(t)=e^{\mathscr{H}_0 t/(i\hbar)}\rho_{\mathrm{I}}(t)e^{-\mathscr{H}_0 t/(i\hbar)}=U_0(t)\rho_{\mathrm{I}}(t)U_0^{-1}(t),\quad U_0(t)\equiv\exp\left(\frac{\mathscr{H}_0}{i\hbar}t\right). \tag{13A.1}$$

Here, $\rho_{\mathrm{I}}=U_0^{-1}\rho U_0$, $[\mathscr{H}_0,U_0]=0$. Also

$$\frac{\partial U_0}{\partial t}=\frac{\mathscr{H}_0}{i\hbar}U_0=\frac{1}{i\hbar}U_0\mathscr{H}_0,\quad \frac{\partial U_0^{-1}}{\partial t}=-\frac{\mathscr{H}_0}{i\hbar}U_0^{-1}=-\frac{1}{i\hbar}U_0^{-1}\mathscr{H}_0,\quad U_0^{-1}(t)=U_0(-t).$$

Then from eq. (6.55), the equation of motion for $\rho_{\mathrm{I}}(t)$ is

$$\begin{aligned}
i\hbar\frac{\partial\rho_{\mathrm{I}}}{\partial t}&=i\hbar\left(\frac{\partial U_0^{-1}}{\partial t}\rho U_0+U_0^{-1}\frac{\partial\rho}{\partial t}U_0+U_0^{-1}\rho\frac{\partial U_0}{\partial t}\right)\\
&=i\hbar\left(-\frac{\mathscr{H}_0}{i\hbar}U_0^{-1}\rho U_0+\frac{1}{i\hbar}U_0^{-1}[\mathscr{H}_0+\mathscr{H}_{\mathrm{ext}},\rho]U_0+U_0^{-1}\rho\frac{\mathscr{H}_0}{i\hbar}U_0\right)\\
&=U_0^{-1}(\mathscr{H}_{\mathrm{ext}}\rho-\rho\mathscr{H}_{\mathrm{ext}})U_0\\
&=[U_0^{-1}\mathscr{H}_{\mathrm{ext}}U_0,\rho_{\mathrm{I}}].
\end{aligned} \tag{13A.2}$$

From the condition $\rho=\rho_{\mathrm{eq}}$ and $\mathscr{H}_{\mathrm{ext}}=0$ for $t=-\infty$, by integrating both sides of eq. (13A.2) with $(-\infty,t]$,

$$\rho_{\mathrm{I}}(t)-\rho_{\mathrm{I}}(-\infty)=-\frac{1}{i\hbar}\int_{-\infty}^{t}dt'[U_0^{-1}(t')\mathscr{H}_{\mathrm{ext}}U_0(t'),\rho_{\mathrm{I}}(t')]. \tag{13A.3}$$

The we obtain

$$\begin{aligned}
\rho(t)&=\rho(-\infty)+\frac{1}{i\hbar}U_0(t)\left\{\int_{-\infty}^{t}dt'[U_0^{-1}(t')\mathscr{H}_{\mathrm{ext}}U_0(t'),U_0^{-1}(t')\rho(t')U_0(t')]\right\}U_0^{-1}(t)\\
&=\rho_{\mathrm{eq}}+\frac{1}{i\hbar}\int_{-\infty}^{t}dt'U_0(t-t')[\mathscr{H}_{\mathrm{ext}}(t'),\rho(t')]U_0^{-1}(t-t'),
\end{aligned} \tag{13A.4}$$

which is eq. (6.57).

## Appendix 13B: Fluctuation-dissipation theorem

We change the order of $Q$ and $P$ in

$$\mathcal{S}_{QP}(\omega) = \int_{-\infty}^{\infty} dt \, \langle Q(t), P \rangle \, e^{i\omega t},$$

to write

$$\int_{-\infty}^{\infty} dt \, \langle PQ(t) \rangle \, e^{i\omega t} = \int_{-\infty}^{\infty} dt \frac{1}{Z} \mathrm{Tr}\{e^{-\beta\mathscr{H}} P e^{i\mathscr{H}t/\hbar} Q e^{-i\mathscr{H}t/\hbar}\} e^{i\omega t}. \tag{13B.1}$$

Now we use mathematical identity that for operators $A$, $B$, $C$, $\mathrm{Tr}\{ABC\}$ satisfies

$$\mathrm{Tr}\{ABC\} = \mathrm{Tr}\{CAB\} = \mathrm{Tr}\{BCA\}. \tag{13B.2}$$

Then

$$\begin{aligned}
\int_{-\infty}^{\infty} dt \, \langle PQ(t) \rangle \, e^{i\omega t} &= \int_{-\infty}^{\infty} dt \frac{1}{Z} \mathrm{Tr}\{e^{i\mathscr{H}t/\hbar} Q e^{-i\mathscr{H}t/\hbar} e^{-\beta\mathscr{H}} P\} e^{i\omega t} \\
&= \int_{-\infty}^{\infty} dt \frac{1}{Z} \mathrm{Tr}\{e^{-\beta\mathscr{H}} e^{(i/\hbar)\mathscr{H}(t-i\beta\hbar)} Q e^{-(i/\hbar)\mathscr{H}(t-i\beta\hbar)} P\} e^{i\omega(t-i\beta\hbar)} e^{-\beta\hbar\omega} \\
&= e^{-\beta\hbar\omega} \mathcal{S}_{QP}(\omega).
\end{aligned} \tag{13B.3}$$

Namely we reach

$$\mathcal{S}_{QP}(\omega) = \frac{1}{1 - e^{-\beta\hbar\omega}} \int_{-\infty}^{\infty} dt \, \langle [Q(t), P] \rangle \, e^{i\omega t} = \frac{i}{1 - e^{-\beta\hbar\omega}} [G^{+}_{QP}(\omega) - G^{-}_{QP}(\omega)]. \tag{13B.4}$$

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