One-Particle Excitation
of the Two-Dimensional Hubbard Model

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The real part of the self-energy of interacting two-dimensional electrons has been calculated in the $t$-matrix approximation. It is shown that the forward scattering results in an anomalous term leading to the vanishing renormalization factor of the one-particle Green function, which is a non-perturbative effect of the interaction $U$. The present result is a microscopic demonstration of the claim by Anderson based on the conventional many-body theory. The effect of the damping of the interacting electrons, which has been ignored in reaching above conclusion, has been briefly discussed.

KEYWORDS: Hubbard model, two dimensions, $t$-matrix approximation, forward scattering

The nature of the low-energy excitation of the two-dimensional system is of great interest recently. The Fermi-liquid picture was considered to be valid from diagramatic studies, while it was suggested by Anderson that the anomalous behavior of the forward scattering phase shift leads to the renormalization factor $Z = 0$, i.e., the breakdown of the Fermi-liquid. This remarkable suggestion has attracted much interest and several calculations of the self-energy of the two-dimensional Hubbard model have been carried out based on the $t$-matrix approximation, in which the self-energy is approximated by the summation of ladder diagrams of the particle-particle process. In these calculations, however, only the imaginary part of the self-energy has been considered, and the real part has not been studied in detail.

In this paper, we will calculate explicitly the real part of the self-energy of the two-dimensional Hubbard model by the $t$-matrix approximation, and show that the singularity of the $t$-matrix in the forward scattering region gives rise to an anomalous term to the real part of the self-energy, which leads to the renormalization factor $Z = 0$. This result is in accordance with the claim by Anderson.

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We consider the asymptotic behavior of the self-energy $\Sigma(k, \epsilon + i\delta)$ in the limit of $|k - k_F| \ll k_F, |\epsilon| \ll \epsilon_F$, $k_F$ and $\epsilon_F$ being the Fermi momentum and the Fermi energy. In general, the shape of the Fermi surface near the point $k$ in the momentum space can be approximated as a parabolic curve, as is schematically shown in Fig. 1(a) and 1(b). Linearizing the energy dispersion in the normal direction of the Fermi surface, we assume the following energy dispersion

$$\xi_k \equiv \epsilon_k - \mu \equiv v_0 k_x + \frac{A_0}{2} k_y^2, \quad (1)$$

where we take the origin of momentum at the point nearest to $k$ on the Fermi surface, as is shown in Fig. 1(b), $\mu$, $v_0$ and $A_0$ are the chemical potential, the Fermi-velocity and a constant, respectively. Here, the momentum dependence of the velocity is neglected. We calculate the self-energy $\Sigma(k, \epsilon + i\delta)$ at the point $k = (k, 0)$. In the Hubbard model, the $t$-matrix is given by

$$T(q, x + i\delta) = \frac{-U}{1 + U K(q, x + i\delta)} \quad (2)$$

$$K(q, x + i\delta) = \sum_k \frac{\text{sgn}\xi_{k+q/2} + \xi_{-k+q/2} - x - i\delta}{\xi_{k+q/2} - k_y^2} \quad (3)$$

where $K(q, x + i\delta)$ is the particle-particle correlation function. Noting that $K(q, 0)$ as a function of $q$ is regular in the forward scattering region, $q \approx 2k_F$, we introduce $K_0 \equiv \lim_{q \to 2k_F} \lim_{x \to 0} K(q, x + i\delta)$, which has a contribution from the high-energy region, and reflects the whole band structure. In contrast to this, $q$- and $x$-dependences of $K(q, x + i\delta) - K_0$ in the region of $|q - 2k_F| \ll k_F, |x| \ll \epsilon_F$ reflect details of a scattering process near the Fermi-energy. Hence, we write the $t$-matrix as,

$$T(q, x + i\delta) = \frac{-U_{\text{eff}}}{1 + U_{\text{eff}} [K(q, x + i\delta) - K_0]} \quad (4)$$

$$U_{\text{eff}} \equiv \frac{U}{1 + U K_0}. \quad (5)$$
We will focus only on the contribution of the $t$-matrix to $\Sigma(k, \epsilon + i\delta)$ from the forward scattering region, i.e., the total momentum of the particle-particle ladder is nearly $2k$. In the following calculations, we introduce momentum cut-offs $k_c$ and $k'_c$ for $x$ and $y$ components of the momentum in the energy dispersion, and momentum integrations for intermediate states of a scattering process are carried out within these cut-offs.

In the $t$-matrix approximation, the expressions for the real and imaginary parts of the self-energy are given by

$$
\text{Re}\Sigma(k, \epsilon + i\delta) = \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \text{Re} T(q, x + i\delta) \text{Im} G_0(q - k, x - \epsilon - i\delta)
$$

$$
- \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \text{Im} T(q, x + i\delta) \text{Re} G_0(q - k, x - \epsilon - i\delta)
$$

$$
\text{Im}\Sigma(k, \epsilon + i\delta) = - \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \text{Im} T(q, x + i\delta) \text{Im} G_0(q - k, x - \epsilon - i\delta).
$$

We will evaluate the asymptotic forms of $\text{Re}\Sigma(k, \epsilon + i\delta)$ and $\text{Im}\Sigma(k, \epsilon + i\delta)$ under the condition of $|\epsilon|, |vk| < \epsilon_c$, where $\epsilon_c$ is defined as $\text{Min}(\nu_0 k_c, A_0 k'^2_c)$. Dividing $x$ integration in $[\epsilon, \infty]$ in the first term of eq. (6) into $[0, \epsilon]$ and $[0, \infty]$, we introduce $\text{Re}\Sigma_1(k, \epsilon + i\delta)$, $\text{Re}\Sigma_2(k, \epsilon + i\delta)$ and $\text{Re}\Sigma_3(k, \epsilon + i\delta)$ as

$$
\text{Re}\Sigma_1(k, \epsilon + i\delta) \equiv \text{Re}\Sigma_1(k, \epsilon + i\delta) + \text{Re}\Sigma_2(k, \epsilon + i\delta) + \text{Re}\Sigma_3(k, \epsilon + i\delta)
$$

$$
\text{Re}\Sigma_1(k, \epsilon + i\delta) \equiv \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \left[ \text{Re} T(q, x + i\delta) \text{Im} G_0(q - k, x - \epsilon - i\delta) - \text{Im} T(q, x + i\delta) \text{Re} G_0(q - k, x - \epsilon - i\delta) \right]
$$

$$
\text{Re}\Sigma_2(k, \epsilon + i\delta) \equiv - \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \text{Re} G_0(q - k, x - \epsilon - i\delta) \text{Im} G_0(q - k, x - \epsilon - i\delta)
$$

$$
\text{Re}\Sigma_3(k, \epsilon + i\delta) \equiv - \int \frac{d^2q}{(2\pi)^2} \int_0^{\infty} \frac{dx}{\pi} \left[ \text{Re} T(q, x + i\delta) - \text{Re} T(q, 0) \right] \text{Im} G_0(q - k, x - \epsilon - i\delta).
$$

It is seen that $\text{Re}\Sigma_1(k, \epsilon + i\delta)$ is a function of only $\epsilon - vk$ and $\text{Re}\Sigma_2(k, \epsilon + i\delta)$ a function of only $\epsilon$ for the dispersion given by eq. (13). Reflecting the regular behavior of $\text{Re} T(q, 0)$, $\text{Re}\Sigma_2(k, \epsilon + i\delta)$ is a regular function of $\epsilon$. Actually for $|\epsilon|, |vk| < \epsilon_c$, we obtain

$$
\text{Re}\Sigma_1(k, \epsilon + i\delta) \simeq \text{Re}\Sigma(0, 0) + c_1(\epsilon - vk)
$$

$$
\text{Re}\Sigma_2(k, \epsilon + i\delta) \simeq c_2\epsilon,
$$

where $c_1$ and $c_2$ are constants. On the other hand, we note that $\text{Re}\Sigma_3(k, \epsilon + i\delta)$ and $\text{Im}\Sigma(k, \epsilon + i\delta)$ are real and imaginary parts of a function which has a contribution from only the low-energy region, i.e., $|q_x| < k_c, |q_y| < k'_c, |x| < \epsilon_c$.

$$
\text{Re}\Sigma_3(k, \epsilon + i\delta) + i\text{Im}\Sigma(k, \epsilon + i\delta)
$$

$$
\simeq - \int_{-\lambda}^{\lambda} \frac{d\lambda_x}{2\pi} \int_{-\lambda'}^{\lambda'} \frac{d\lambda_y}{2\pi} \int_0^{\pi} \frac{dx}{\pi} \left[ T(q, x + i\delta) + U_{\text{eff}} \right] \text{Im} G_0(q - k, x - \epsilon - i\delta),
$$

(14)

(15)
where the cut-offs $\lambda$ and $\lambda'$ are small values compared to $k_c$ and $k_\epsilon'$, respectively, and $U_{\text{eff}} \equiv -\lim_{q\to 0} \lim_{x\to 0} T(q, x + i\delta)$. We introduce $\Sigma_s(k, \epsilon + i\delta)$ by subtracting the on-shell value of $\text{Re} \Sigma_3(k, \epsilon + i\delta)$,

$$\Sigma_s(k, \epsilon + i\delta) \equiv [\text{Re} \Sigma_3(k, \epsilon + i\delta) - \text{Re} \Sigma_3(k, \epsilon + i\delta)] + i\text{Im} \Sigma(k, \epsilon + i\delta). \quad (16)$$

$\text{Re} \Sigma_s(k, \epsilon + i\delta)$ is of interest to us, while $\text{Re} \Sigma(k, \epsilon + i\delta) - \text{Re} \Sigma_s(k, \epsilon + i\delta) = \text{Re} \Sigma_1(k, \epsilon + i\delta) + \text{Re} \Sigma_2(k, \epsilon + i\delta) + \text{Re} \Sigma_3(k, \epsilon + i\delta)$ is related to various renormalizations such as the shift of the chemical potential, the renormalization of the Fermi velocity, the effects of which are taken into account by replacing $v_0$ and $A_0$ in eq. (14) and the renormalization factor $Z_0$ of the Green function $G_0(k, \epsilon + i\delta)$. Then, we obtain the renormalized self-energy $\Sigma^*(k, \epsilon + i\delta)$ and the renormalized Green function $G^*(k, \epsilon + i\delta)$ as

$$\Sigma^*(k, \epsilon + i\delta) \equiv [\Sigma_s(k, \epsilon + i\delta)]_{G_0 \to G_0^*} \quad (17)$$

$$G^*(k, \epsilon + i\delta) \equiv \frac{Z_0}{(\epsilon - vk) - \Sigma^*(k, \epsilon + i\delta)}. \quad (18)$$

where $G_0^*(k, \epsilon + i\delta) \equiv Z_0/(\epsilon - \xi_k^*)$ and $\xi_k^* \equiv vk + A_0^2/2$. The subscript $G_0 \to G_0^*$ on the right hand side (r.h.s.) of eq. (17) indicates that the calculation of $\Sigma_s(k, \epsilon + i\delta)$ should be performed using the renormalized Green function, $G_0^*(k, \epsilon + i\delta)$. We note that the on-shell value of $\text{Re} \Sigma_3(k, \epsilon + i\delta)$, $\text{Re} \Sigma_3(k, \epsilon + i\delta)$, is of the order of $(vk)^2$, and that this term gives the renormalization of a quasiparticle energy only of the order of $k^2$.

Next we need to estimate $\Sigma^*(k, \epsilon + i\delta)$. Under the conditions of $|q_x| \ll k_c, |q_y| \ll k_\epsilon', |x| \ll \epsilon_c$, the asymptotic form of $K^*(q, x + i\delta) - K_0^*$ is given by

$$K^*(q, x + i\delta) - K_0^* \simeq \begin{cases} 
\frac{iZ_0^2 x}{4\pi A^{1/2} v(x - q_x - A q_y^2/4)^{1/2}} & (x > q_x + A q_y^2/4) \\
\frac{4\pi A^{1/2} v(-x + q_x + A q_y^2/4)^{1/2}}{4\pi A^{1/2} v(x - q_x - A q_y^2/4)^{1/2}} & (x < q_x + A q_y^2/4),
\end{cases} \quad (19)$$

where the particle-particle correlation function $K^*(q, x + i\delta)$ is calculated using the renormalized Green function $G_0^*(k, \epsilon + i\delta)$. Using these expressions, we obtain the asymptotic form of $\text{Re} \Sigma^*(k, \epsilon + i\delta)$ in the limit of $|\epsilon - vk| \ll -U_{\text{eff}} Z_0^2 k^2$ for the case of $\epsilon > vk$, for example, as

$$\text{Re} \Sigma^*(k, \epsilon + i\delta) \simeq -\frac{Z_0}{4\pi^2 v} \int -\lambda' \lambda' dq_y \int _0^\infty dx \text{Re} \left[ \frac{U_{\text{eff}}} {1 + \frac{iU_{\text{eff}} Z_0^2 x}{4\pi A^{1/2} v(A q_y^2/4 + \epsilon - vk)^{1/2}}} \right] - \frac{U_{\text{eff}}} {1 + \frac{iU_{\text{eff}} Z_0^2 x}{4\pi A^{1/2} v(A q_y^2/4)^{1/2}}} \right] \right]$$

$$\simeq (\epsilon - vk) \frac{2}{\pi Z_0} \int_0^\infty dq_y \left[ \left( \frac{q_y^2}{4} + 1 \right)^{1/2} \arctan \left( \frac{U_{\text{eff}} Z_0^2 \epsilon}{4\pi A^{1/2} v(\epsilon - vk)^{1/2} (q_y^2/4 + 1)^{1/2}} \right) \right] \left( \frac{q_y^2/4 + 1}{4\pi A^{1/2} v(\epsilon - vk)^{1/2} (q_y^2/4 + 1)^{1/2}} \right) \right].$$
The calculations for the case of $\epsilon < vk$ are similar and we obtain the final result in the limit of $|\epsilon - vk| \ll A^{-1} U_{\text{eff}}^2 Z_0^4 k^2$ as

$$\text{Re} \Sigma^* (k, \epsilon + i\delta) \simeq c \frac{(\epsilon - vk)}{Z_0} \log \frac{A |\epsilon - vk|}{U_{\text{eff}}^2 Z_0^4 k^2},$$

where

$$c = \begin{cases} 
\frac{1}{2}, & (\epsilon > vk, k > 0) \\
0, & (\epsilon < vk, k > 0) \\
\frac{1}{2}, & (\epsilon > vk, k < 0) \\
1, & (\epsilon < vk, k < 0) 
\end{cases}$$

Reflecting the existence of a logarithmic singularity, the renormalization factor $Z = \lim_{\epsilon \to vk} (1 - \partial \text{Re} \Sigma / \partial \epsilon)^{-1}$ exhibits an anomalous behavior, $Z = 0$, except in the limit of $\epsilon \to vk - 0$ in the case of $vk > 0$.

In addition to this, we have evaluated the asymptotic form of $\text{Im} \Sigma^* (k, \epsilon + i\delta)$ in the same limit of $|\epsilon - vk| \ll A^{-1} U_{\text{eff}}^2 Z_0^4 k^2$, which is given by

$$\text{Im} \Sigma^* (k, \epsilon + i\delta) \simeq \text{Im} \Sigma^* (k, vk + i\delta)$$

$$+ \left( \frac{(\epsilon - vk)}{Z_0} \right) \left[ - \frac{1}{4\pi} \left( \log \frac{A |\epsilon - vk|}{U_{\text{eff}}^2 Z_0^4 k^2} \right)^2 + a \left( \log \frac{A |\epsilon - vk|}{U_{\text{eff}}^2 Z_0^4 k^2} \right) + b \right]$$

(24)

$$\text{Im} \Sigma^* (k, vk + i\delta) \simeq \frac{U_{\text{eff}}^2 Z_0^4 k^2}{A} \log \frac{U_{\text{eff}}^2 Z_0^4 |k|}{A^{1/2} \epsilon_c^{1/2}} \equiv \Gamma_k,$$

(25)

where $a$ and $b$ are constants which are different in each region of $\epsilon > vk$ and $\epsilon < vk$. Especially for $\epsilon \to vk$, only the first term on the r.h.s. of eq. (24) survives. So far, the real and imaginary parts of the self-energy have been examined, but $\Sigma(k, \epsilon + i\delta)$ must be an analytic function of $\epsilon$. Actually, $\Sigma^* (k, z)$ is given as follows for a complex variable $z$ (Im $z > 0$) in the limit of $|z - vk| \ll A^{-1} U_{\text{eff}}^2 Z_0^4 k^2$.

$$\Sigma^* (k, z) \simeq i \text{Im} \Sigma^* (k, vk + i\delta)$$

$$+ \left( \frac{z - vk}{Z_0} \right) \left[ - \frac{i}{4\pi} \left( \log \frac{A (z - vk)}{U_{\text{eff}}^2 Z_0^4 k^2} \right)^2 + a' \left( \log \frac{A (z - vk)}{U_{\text{eff}}^2 Z_0^4 k^2} \right) + b' \right],$$

(26)
where \( a' \) and \( b' \) are complex constants related to \( a \) and \( b \) in eq. (24). From the analyticity condition, \( \Sigma^*(k, \epsilon + i\delta) \) is interrelated from \( \epsilon > v k \) to \( \epsilon < v k \) through the upper-half complex plane of \( \epsilon \) (Fig. 1(c)), and therefore the constants \( a' \) and \( b' \) in each region are mutually related by a simple relation. When we see \( \Sigma^*(k, z) \) as one analytic function of \( z \), the logarithmic term in the real part is related to the second term of the r.h.s. of eq. (24) in the imaginary part. Actually, we obtain \( \text{Re } a' = -1/2 (1/2) \) for \( v k > 0 (v k < 0) \). The leading term of the imaginary part when \( \epsilon \simeq v k \), however, is not the second term in eq. (24) but the first one. On the other hand, in the case of \( k = k_F \), \( \text{Im}\Sigma(k_F, \epsilon + i\delta) \propto \epsilon^2 \log \epsilon \) was obtained \[1\] which corresponds to the first term on the r.h.s. of eq. (24), and was the basis of the claim of the Fermi-liquid state. As has been demonstrated, however, the present logarithmic term of the real part cannot be deduced from this imaginary part using the Kramers-Kronig transformation. This has not been noted in previous studies.

Our new result of a logarithmic singular behavior in the real part of the self-energy implies that the renormalization factor \( Z \) vanishes in the low-energy limit.

In addition, we note the relationship between the results in the \( t \)-matrix approximation and the second-order perturbation theory. When we focus only on the forward scattering process, the self-energy as an analytic function of complex variable \( z \) is obtained by the second-order perturbation theory as \[2\]

\[
\Sigma^*(k, z) \propto iU^2 z^2 \log \frac{z - v k}{\epsilon_c},
\]

and there is no logarithmic term in the real part of the self-energy. In the case of the \( t \)-matrix approximation, we found that the self-energy is a logarithmic function not only of \( \epsilon - v k \) but also of \( U_{\text{eff}} \), as shown in eq. (26). Hence, the logarithmic term in the real part of the self-energy obtained by the \( t \)-matrix approximation is a non-perturbative effect of \( U \), which implies that \( U = 0 \) can be a singular point in two dimensions.

Investigating the derivation in eq. (20) of the logarithmic term in the real part of the self-energy near the on-shell region, we can see that the logarithmic term is related to the property of the \( t \)-matrix in the region of \( |x - v q_x| < A^{-1} U_{\text{eff}}^2 Z_0^4 k^2, A q_y^2 < A^{-1} U_{\text{eff}}^2 Z_0^4 k^2, 0 < |x| < |\epsilon| \). This indicates that the on-shell electrons are responsible to the logarithmic term of the self-energy.

Anderson proposed that the special feature of the forward scattering process leads to the vanishing renormalization factor, \( Z = 0 \), i.e., the breakdown of the Fermi-liquid, and our results have confirmed this based on the conventional many-body perturbation theory using the Feynman diagrams.

So far the calculations of the self-energy have been carried out based on the Green function without damping, \( \Gamma_k \). The resulting logarithmic behavior in the real part of the self-energy, however, has been seen only in the energy region \( |\epsilon - v k| \ll A^{-1} U_{\text{eff}}^2 Z_0^4 k^2 \Gamma_k \), implying the importance of the self-consistent treatment. Actually, \( \Gamma_k \) results in finite \( Z \) even when \( X \to 0 \), i.e., \( G(k, \epsilon + i\delta) \simeq Z_0 /[a(X)X + i\Gamma_k] \) with \( a(0) \neq 0 \). However, \( a(X) \) will have a strong dependence on \( X = \epsilon - v k \) as
\( a(X) = a_0[1 + O(|X|/\Gamma_k)] \), which is different from a conventional Fermi-liquid.

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\[ k_x = (k, 0) \]

\[ v k_x + 2 \epsilon k_y^2 = 0 \]

\[ |\epsilon - v k| \ll |v k| \]