Systematic analysis of the magnetic susceptibility in the itinerant electron model

K. Okumura*
Department of Physics, Faculty of Science and Technology, Keio University, Yokohama 223, Japan
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The self-consistent renormalization theory of the itinerant electron model was the first theory to show that the Curie-Weiss behavior of the magnetic susceptibility is not peculiar to the localized model. But the theory was justified on the basis of physical intuition so that the improvement of the approximation is a hard problem. In this paper the susceptibility is studied by the inversion method, in which the way to improve the approximation is always known in principle. The inversion method advances the Stoner theory systematically since the method is a kind of perturbation theory and its first-order calculation reproduces the mean-field theory. The second order of the inversion method is applied for the concrete model, which has been considered to be difficult. It is possible to realize the Curie-Weiss law and the lowering of the critical temperature T_c as a result.

I. INTRODUCTION

Ferromagnetism in the itinerant electron model has been one of the most fundamental issues in solid-state physics and has attracted much attention accordingly. Although the mean-field approach to the problem[1] explained the qualitative features, several serious discrepancies are left unresolved. One of the crucial problems is how one can explain the Curie-Weiss law in the itinerant model, which is a property common to most of the metallic ferromagnetic substances. Another problem is the fact that the Curie temperature T_c calculated from the observed value of the saturation magnetization by the Stoner theory is several times higher than the observed T_c for typical substances.

About 20 years ago the self-consistent renormalization (SCR) theory of the itinerant electron model was proposed by Moriya and Kawabata.[2] This theory reproduces the Curie-Weiss behavior of the susceptibility and the Curie temperature substantially lower than that of the Stoner theory. The SCR theory succeeded in taking into account the effect of the spin fluctuation neglected in the Stoner theory. The approximations used in the SCR theory are considered to be good at least for the weak ferromagnetic substance where the long-wavelength contribution of the spin fluctuation is dominant. This theory shows that the Curie-Weiss law is not unique to the localized electron model although there are many works on Green's function theories of the spin fluctuation or χ,[3–8] which give similar result. Furthermore the SCR theory was developed to see qualitatively excellent agreement with experiment (see, for example, Chap. 4 of Ref. 1 and references therein).

But, as in almost all the theory going beyond the mean-field approach, the SCR theory is based on *the physical approximation*, that is, approximations understandable only when one relies on the physical intuition. One does not know how to improve the theory as a result. To make this point clear the SCR theory is reviewed in Sec. IV.

The viewpoint of this article is that it is worthwhile trying to explain the Curie-Weiss law and lowering of the Curie temperature (compared with the Stoner theory) by resorting only to *mathematically well-defined approximations*—approximations justified without the physical intuition.

As a starting point of this line of approach we apply the inversion method. The approximation can be made better perturbatively up to the desired order in the method. The naive perturbation theory cannot deal with the problem of the symmetry breaking or the critical phenomenon. The inversion method is, however, a technique for making the Legendre transformation perturbatively, and therefore, it is natural that the method be a powerful tool in studying the symmetry-breaking situation.

The inversion method up to its first order is known to correspond to the mean-field result. This fact has been confirmed for the case of the Ising spin systems, the superconductivity of the BCS theory, the theory of the superfluidity of ^{4}He, and the ferromagnetism of the itinerant electrons in addition to several cases in particle physics.[9–13] Many examples have been studied by the inversion method. It is stressed here that the nontrivial result beyond the mean-field approximation is done in this work.

Combined with the on-shell expansion,[14] the inversion method can also be utilized to investigate excitation modes and the scattering among them on the (symmetry-breaking) vacuum. This line of study has already been performed up to the first order of the inversion method for the ferromagnetic phase of the itinerant electron model (the spin-wave theory).[14,15]

The primary purpose of this paper is to *improve the mean-field theory systematically*, for which the inversion method is particularly suited. This method can be summarized in the following four steps.

Step 1: Introduction of the source. Replace the original Hamiltonian $\mathscr{H}$ by

$$\mathscr{H} \rightarrow \mathscr{H} - J\hat{\phi}, \tag{1.1}$$

where the source J is an external c-number field coupled to the operator of the order parameter $\hat{\phi}$ in question. $J\hat{\phi}$ is called the source term. If one deals with the problem of the symmetry breaking, the original Hamiltonian $\mathscr{H}$ keeps the symmetry while the source term $J\hat{\phi}$ breaks it.

Step 2: Calculation of the original series. For the system with the artificial source J, calculate the expectation value ϕ of the operator $\hat{\phi}$ by the conventional perturbation theory to obtain *the original series*

$$\phi=\phi(J)=\phi^{(0)}(J)+\phi^{(1)}(J)+\phi^{(2)}(J)+\cdots. \quad (1.2)$$

Here we have assumed that there exists a small expansion parameter, say U, and $\phi^{(n)}(J)$ is the nth order (in U) contribution to ϕ regarding the source J as order unity.

Step 3: Obtaining the inversion series. Invert (1.2) in favor of J to get *the inversion series*

$$J=J(\phi)=J^{(0)}(\phi)+J^{(1)}(\phi)+J^{(2)}(\phi)+\cdots, \quad (1.3)$$

where $J^{(n)}(\phi)$ is the nth order of J regarding ϕ as order unity. To obtain the explicit form of $J^{(i)}(\phi)$, insert (1.3) into (1.2),

$$\phi=\phi^{(0)}(J^{(0)}+J^{(1)}+J^{(2)}+\cdots)+\phi^{(1)}(J^{(0)}+J^{(1)}+\cdots)+\phi^{(2)}(J^{(0)}+\cdots)+\cdots, \quad (1.4)$$

or

$$\phi=\phi^{(0)}(J^{(0)})+\{\phi^{(0)\prime}(J^{(0)})J^{(1)}+\phi^{(1)}(J^{(0)})\}+\{\phi^{(0)\prime}(J^{(0)})J^{(2)}+\tfrac{1}{2}\phi^{(0)\prime\prime}(J^{(0)})(J^{(1)})^2+\phi^{(1)\prime}(J^{(0)})J^{(1)}+\phi^{(2)}(J^{(0)})\}+\cdots. \quad (1.5)$$

Then we regard ϕ as independent of U or order unity in the last equation to get a set of equations,

$$\phi=\phi^{(0)}(J^{(0)}), \quad (1.6)$$

$$0=\phi^{(0)\prime}(J^{(0)})J^{(1)}+\phi^{(1)}(J^{(0)}), \quad (1.7)$$

$$0=\phi^{(0)\prime}(J^{(0)})J^{(2)}+\tfrac{1}{2}\phi^{(0)\prime\prime}(J^{(0)})(J^{(1)})^2+\phi^{(1)\prime}(J^{(0)})J^{(1)}+\phi^{(2)}(J^{(0)}), \quad (1.8)$$

and so on. In this way we can obtain $J^{(i)}(\phi)$ successively up to the desired order.

Regarding ϕ as independent of U just corresponds to making the Legendre transformation since ϕ and U are dealt with as mutually independent in the Legendre transformation (see Appendix A of Ref. 16 for detail).

Step 4: Turning off the artificial source J. In order to return to the original theory, we require $J=0$, or

$$J^{(0)}(\phi)+J^{(1)}(\phi)+J^{(2)}(\phi)+\cdots=0. \quad (1.9)$$

The key point is that it is possible for this equation of ϕ to have a nonzero (symmetry-breaking) solution.

We have assumed the case in which there is only a single order parameter ϕ. It is straightforward to extend the above steps to the case of many order parameters.

II. APPLYING THE INVERSION METHOD TO THE ITINERANT ELECTRON MODEL

The itinerant electron model is here defined by

$$\mathcal{H}=\sum_{\mathbf{r}\mathbf{r}'}\sum_{\sigma} t_{\mathbf{r}\mathbf{r}'}a^{\dagger}_{\mathbf{r}\sigma}a_{\mathbf{r}'\sigma}+U\sum_{\mathbf{r}} n_{\mathbf{r}\uparrow}n_{\mathbf{r}\downarrow}, \quad (2.1)$$

where the creation and annihilation operators for the electron of spin σ and σ' at the lattice site $\mathbf{r}$ and $\mathbf{r}'$ satisfy anticommutation relations

$$\{a_{\mathbf{r}\sigma},a^{\dagger}_{\mathbf{r}'\sigma'}\}=\delta_{\mathbf{r}\mathbf{r}'}\delta_{\sigma\sigma'}, \quad (2.2)$$

etc. The number operator of the spin σ has been introduced as

$$n_{\mathbf{r}\sigma}=a^{\dagger}_{\mathbf{r}\sigma}a_{\mathbf{r}\sigma}. \quad (2.3)$$

Furthermore $t_{\mathbf{r}\mathbf{r}'}$ represents the hopping term and U the Coulomb interaction. In this paper only the on-site Coulomb interaction will be considered and we assume that $t_{\mathbf{r}\mathbf{r}'}$ is a function of $\mathbf{r}-\mathbf{r}'$.

Step 1: Introduction of the source. Since we have interest in the ferromagnetism at finite temperature, the order parameter is the total spin operator

$$\hat{\mathbf{S}}=\tfrac{1}{2}\sum_{\mathbf{r}}\boldsymbol{\tau}_{\sigma\sigma'}a^{\dagger}_{\mathbf{r}\sigma}a_{\mathbf{r}\sigma'}, \quad (2.4)$$

where $\boldsymbol{\tau}$ is the 2×2 Pauli matrix,

$$\boldsymbol{\tau}=\left[\begin{pmatrix}0&1\\1&0\end{pmatrix},\begin{pmatrix}0&-i\\i&0\end{pmatrix},\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]. \quad (2.5)$$

Although it is natural that one take the source term as $\mathbf{h}\cdot\hat{\mathbf{S}}$, we here introduce the source only for the z component of $\hat{\mathbf{S}}$ for simplicity. Thus the grand canonical Hamiltonian takes the form

$$\mathcal{H}_J=\mathcal{H}-\mu\hat{N}-h\hat{S}_z=\mathcal{H}-J_{\sigma}\hat{N}_{\sigma}, \quad (2.6)$$

where the summation over σ is omitted as we will do unless it is ambiguous. The z component of the spin operator $\hat{S}_z$ and the total number of the electron $\hat{N}$ are given by

$$\hat{S}_z=\tfrac{1}{2}\sum_{\mathbf{r}}(n_{\mathbf{r}\uparrow}-n_{\mathbf{r}\downarrow}), \quad (2.7)$$

$$\hat{N}=\sum_{\sigma}\hat{N}_{\sigma},\quad \hat{N}_{\sigma}=\sum_{\mathbf{r}} n_{\mathbf{r}\sigma}. \quad (2.8)$$

We introduce the total magnetization operator $\hat{M}$ or its density $\hat{m}$ by $\hat{S}_z=-\hat{M}=-V\hat{m}$, where V is the volume of the system. The source J_{σ} and $\hat{N}_{\sigma}$ in (2.6) are given by

$$J_{\sigma}=\frac{\sigma}{2}h+\mu,\quad \hat{N}_{\sigma}=\frac{\hat{N}}{2}+\sigma\hat{S}_z. \quad (2.9)$$

The chemical potential μ has been introduced as usual and is here considered as a part of the source for convenience. The two sources μ and h are combined to the source J_{σ} as in (2.9). The spin index σ is defined to take the value $(+1,-1)$ for $(\uparrow,\downarrow)$. Note that the original Hamiltonian defined in (2.1) has the SU(2) symmetry while the source terms in (2.6) reduce the symmetry down to the Z_2 invariance. The case where a more general source term $\mathbf{h}\cdot\hat{\mathbf{S}}$ is introduced has been also studied up to the first order of the inversion method.[14,15]

Step 2: Conventional perturbative calculation of the order parameter. The thermodynamical potential $\Omega(J_\uparrow,J_\downarrow)/\beta = \bar{\Omega}(h,\mu)/\beta$ is defined here by

$$e^{-\Omega(J_\uparrow,J_\downarrow)} = \mathrm{Tr} e^{-\beta\mathscr{H}_J}, \tag{2.10}$$

where $T=\beta^{-1}$ is the temperature of the system. The expectation values ϕ_σ of the operators $\hat{N}_\sigma/V$ are considered as order parameters for convenience although the original order parameter of the present problem is the expectation value m of the operator $\hat{m}=-\hat{S}_z/V$. The value m is easily given by $m=(\phi_\downarrow-\phi_\uparrow)/2$ once ϕ_σ is known. This is clear from the relation

$$V\phi_\sigma=\langle\hat{N}_\sigma\rangle=\tfrac{1}{2}N+\sigma S_z=\tfrac{1}{2}N-\sigma M, \tag{2.11}$$

where N, S_z, and M are the expectation values of the operators $\hat{N}$, $\hat{S}_z$, and $\hat{M}$, respectively. One can calculate ϕ_σ as a function of J_σ by the conventional perturbation technique since ϕ_σ is given by

$$\beta V\phi_\sigma=-\frac{\partial\Omega}{\partial J_\sigma}. \tag{2.12}$$

The diagrammatic expansion according to the imaginary-time formalism is done as follows. Since the source term $J_\sigma N_\sigma=\Sigma_\sigma J_\sigma\Sigma_{\mathbf{r}}a^\dagger_{\mathbf{r}\sigma}a_{\mathbf{r}\sigma}$ is quadratic, it can be absorbed into the propagator G^J_σ:

$$[G^J_\sigma]^{-1}_{xx'}=G^{-1}_{xx'}-\delta_{\tau\tau'}\delta_{\mathbf{r}\mathbf{r}'}J_\sigma \tag{2.13}$$

with

$$G^{-1}_{xx'}=\delta_{\tau\tau'}\left(\delta_{\mathbf{r}\mathbf{r}'}\frac{\partial}{\partial\tau'}+t_{\mathbf{r}\mathbf{r}'}\right), \tag{2.14}$$

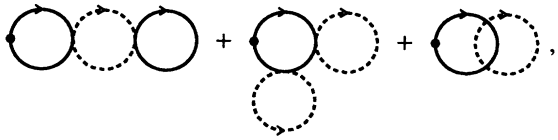
where x and x' denote the sets $(\tau,\mathbf{r})$ and $(\tau',\mathbf{r}')$, respectively. Here τ denotes the imaginary-time variable. Specifically $\phi_\uparrow$ is given by the following graph in which the solid (dashed) line represents the propagator $G^J_\uparrow$ ($G^J_\downarrow$) and the factor U is assigned to the four-point vertex (see the Appendix for the detailed rule including the symmetry factor):

$$\phi_\uparrow=\phi^{(0)}_\uparrow+\phi^{(1)}_\uparrow+\phi^{(2)}_\uparrow+\cdots, \tag{2.15}$$

where

$-\beta V\phi^{(0)}_\uparrow(J_\uparrow,J_\downarrow) =$  , (2.16)

$-\beta V\phi^{(1)}_\uparrow(J_\uparrow,J_\downarrow) =$  , (2.17)

$-\beta V\phi^{(2)}_\uparrow(J_\uparrow,J_\downarrow) =$  , (2.18)

and so on. The solid dot where two propagators meet corresponds to the derivative with respect to $J_\uparrow$ since we have the relation

$$\frac{\partial G^J_\uparrow(y,z)}{\partial J_\uparrow}=\sum_x G^J_\uparrow(y,x)G^J_\uparrow(x,z), \tag{2.19}$$

where $\Sigma_x\equiv\int d\tau\Sigma_{\mathbf{r}}$.

We notice from (2.16) that $\phi^{(0)}_\uparrow(J_\uparrow,J_\downarrow)$ depends only on $J_\uparrow$ so we write it as $\phi^{(0)}_\uparrow(J_\uparrow,J_\downarrow)\equiv\phi_0(J_\uparrow)$:

$$\phi_0(J_\uparrow)=-\frac{1}{\beta V}\sum_x (G^{-1}_{xx}-\delta_{xx}J_\uparrow)^{-1}. \tag{2.20}$$

Then $\phi^{(0)}_\downarrow(J_\uparrow,J_\downarrow)$ can be written by using the same function, that is, $\phi^{(0)}_\downarrow(J_\uparrow,J_\downarrow)=\phi_0(J_\downarrow)$.

By the conventional perturbation approach like above (up to any finite order) the spontaneous magnetization is always zero, that is, one obtains $\phi_\uparrow=\phi_\downarrow$, which means $m=0$, if one sets $h=0$ ($J_\uparrow=J_\downarrow$). This is easily understood if one notices that for the case of $h=0$ the propagators $G^J_\uparrow$ and $G^J_\downarrow$ take the same value to result in $\phi_\uparrow=\phi_\downarrow$.

Step 3: Inversion of $\phi=\phi(J)$ to obtain $J=J(\phi)$. Let us discuss the graphical expressions of the inversion formulas (1.6)–(1.8). From (2.16) the zeroth-order formula (1.6) becomes

$-\beta V\phi_\uparrow =$  , (2.21)

where the line represents not $G^J_\uparrow$ but $G^{(0)}_\uparrow$ defined by

$$[G_\sigma^{(0)}]^{-1}_{xx'} = G^{-1}_{xx'} - \delta_{xx'} J_\sigma^{(0)} . \tag{2.22}$$

Since (2.21) defines $J_\sigma^{(0)}$ implicitly we know that $J_\sigma^{(0)}$ is a function of ϕ_σ which does not depend on $\phi_{-\sigma}$. In other words $J_\sigma^{(0)}$ is given by

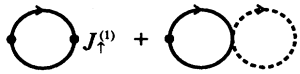
$$\phi_\sigma = \phi_0(J_\sigma^{(0)}) \quad \text{or} \quad J_\sigma^{(0)} = \phi_0^{-1}(\phi_\sigma). \tag{2.23}$$

By noting that

$$-\beta V \left.\frac{\partial \phi_\uparrow^{(0)}(J_\uparrow, J_\downarrow)}{\partial J_\sigma}\right|_{J=J^{(0)}} = -\beta V \frac{\partial \phi_\uparrow}{\partial J_\sigma^{(0)}} = \delta_{\uparrow\sigma}$$

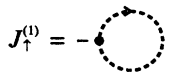
(2.24)

and by using Eq. (2.17), the first-order formula (1.7) becomes



(2.25)

Here and hereafter the line represents not G_σ^J but $G_\sigma^{(0)}$ as in (2.21). Thus we get

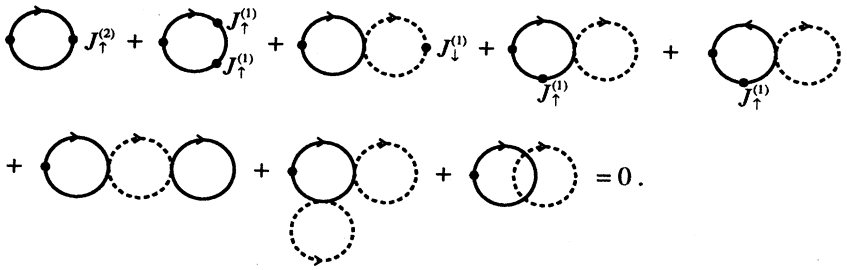


(2.26)

or

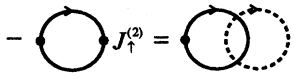
$$J_{-\sigma}^{(1)} = -G^{(0)}_{\sigma\, xx} = \phi_0(J_\sigma^{(0)}) = \phi_\sigma . \tag{2.27}$$

We have used (2.23) and the fact that $G^{(0)}_{\sigma\, xx}$ does not depend on x (assuming the translational invariance). The graphs of the second-order formula (1.8) are obtained by (2.16)–(2.18) through the way similar to the one of getting (2.25):



(2.28)

Inserting the graphic expression of $J_\downarrow^{(1)}$ like (2.26) into this equation, we see that the third and sixth graphs cancel out (taking the symmetry factor into account of course, see the Appendix). The second, fourth, fifth, and the seventh graphs are also summed up to zero. Thus we have the simple result



(2.29)

We can continue this course of study up to the desired order. The result for full order is already known to be given as a simple rule.[16]

We have completed the inversion up to the second order. It is convenient to get the free energy from these results. The Helmholtz free energy $F(M,N)/\beta$ is defined through Legendre transformation:

$$F = \Omega + \beta V \sum_\sigma J_\sigma \phi_\sigma . \tag{2.30}$$

Then F is actually a function of $\phi_\uparrow$ and $\phi_\downarrow$ (or of M and N) with an identity

$$J_\sigma = \frac{1}{\beta V}\frac{\partial F}{\partial \phi_\sigma} . \tag{2.31}$$

We introduce the nth order of F in accordance with (2.31):

$$J_\sigma^{(n)} = \frac{1}{\beta V}\frac{\partial F^{(n)}}{\partial \phi_\sigma} . \tag{2.32}$$

Thus integrating both sides (at $n=0$) we have

$$F^{(0)} = \beta V \sum_\sigma \int J_\sigma^{(0)} \frac{\partial \phi_\sigma}{\partial J_\sigma^{(0)}} dJ_\sigma^{(0)}$$

$$= \beta V \sum_\sigma J_\sigma^{(0)} \phi_\sigma - \sum_{\sigma,x} (\ln[G_\sigma^{(0)}]^{-1})_{xx} . \tag{2.33}$$

We have integrated the second expression by part and have used

$$-\beta V\phi_\sigma=\frac{\partial\Omega^{(0)}[J^{(0)}]}{\partial J_\sigma^{(0)}} \tag{2.34}$$

and

$$\Omega^{(0)}=-\sum_{\sigma,x}(\ln[G_\sigma^{(0)}]^{-1})_{xx} \tag{2.35}$$

to obtain the last expression. The quantity $F^{(1)}$ is readily obtained by integrating (2.27) with respect to $\phi_{\sigma'}$:

$$\frac{1}{\beta V}F^{(1)}=U\phi_\uparrow\phi_\downarrow=U(N^2/4-M^2)/V^2. \tag{2.36}$$

It is easy to see that $F^{(0)}+F^{(1)}$ is the free energy of the Stoner theory. Thus the inversion method up to the first-order coincides with the mean-field result.

Next, $F^{(2)}$ can also be obtained if we notice that

$$J_\uparrow^{(2)}=\frac{1}{\beta V}\frac{\partial F^{(2)}}{\partial\phi_\uparrow}=\frac{1}{\beta V}\frac{\partial J_\uparrow^{(0)}}{\partial\phi_\uparrow}\frac{\partial F^{(2)}}{\partial J_\uparrow^{(0)}}, \tag{2.37}$$

and also that the left-hand side of (2.29) can be written as $\beta V\partial\phi_\uparrow/\partial J_\uparrow^{(0)}\cdot J_\uparrow^{(2)}$. Namely, the right-hand side of (2.29) is just $\partial F^{(2)}/\partial J_\uparrow^{(0)}$. Thereby we get

$F^{(2)}=$  . (2.38)

A more sophisticated way of obtaining $F^{(0)}$, $F^{(1)}$, ... is shown in Ref. 16.

Now we introduce the momentum representation where p or p' represents a set $(n,\mathbf{k})$ or $(n',\mathbf{k}')$, respectively:

$$[G_\sigma^J]^{-1}_{pp'}=\frac{1}{\beta V}\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{\mathbf{r}}\sum_{\mathbf{r}'}\times e^{i\xi_n\tau-i\mathbf{k}\cdot\mathbf{r}}[G_\sigma^J]^{-1}_{xx'}e^{-i\xi_{n'}\tau'+i\mathbf{k}'\cdot\mathbf{r}'} \tag{2.39}$$

$$=(-i\xi_n+t_\mathbf{k}-J_\sigma)\delta_{pp'}\equiv G^J_{\sigma p}\delta_{pp'}, \tag{2.40}$$

where the odd frequency ξ_n and $t_\mathbf{k}$ are given by

$$\xi_n=(2n+1)\pi T, \tag{2.41}$$

$$t_\mathbf{k}\delta_{\mathbf{k}\mathbf{k}'}=\frac{1}{V}\sum_{\mathbf{r}}\sum_{\mathbf{r}'}e^{-i\mathbf{k}\cdot\mathbf{r}}t_{\mathbf{r}\mathbf{r}'}e^{i\mathbf{k}'\cdot\mathbf{r}'}. \tag{2.42}$$

Here we have assumed that $t_{\mathbf{r}\mathbf{r}'}$ is a function of $\mathbf{r}-\mathbf{r}'$. In this way we have from (2.20)

$$\phi_0(a)=-\frac{1}{\beta V}\sum_{n,\mathbf{k}}\frac{1}{-i\xi_n+t_\mathbf{k}-a}=\frac{1}{V}\sum_\mathbf{k}f_\beta(t_\mathbf{k}-a), \tag{2.43}$$

where

$$f_\beta(x)=\frac{1}{e^{\beta x}+1}. \tag{2.44}$$

Thus we have

$$\phi_\sigma=\phi_0(J_\sigma^{(0)})=\frac{1}{V}\sum_\mathbf{k}f_\beta(t_\mathbf{k}-J_\sigma^{(0)}). \tag{2.45}$$

Let us examine the physical meaning of $J_\sigma^{(0)}$. When $T>T_c$ and $h=0$, one gets $\phi_\uparrow=\phi_\downarrow=n/2$ because $m=0$, and thus we have $J_\uparrow^{(0)}=J_\downarrow^{(0)}\equiv\mu_0$. The physical meaning of μ_0 is the chemical potential for the system with $m=0$ ($T>T_c$, $h=0$) and $U=0$ (noninteracting) at finite temperature. This is understood from (2.45) for the case of $\phi_\uparrow=\phi_\downarrow=n/2$ or

$$\frac{N}{2}=\sum_\mathbf{k}f_\beta(t_\mathbf{k}-\mu_0). \tag{2.46}$$

Thus $J_\sigma^{(0)}$ is the usual chemical potential in this case.

The algebraic expression of $F^{(2)}$ is given by

$$F^{(2)}=-\frac{U^2}{2}\sum_{x,y}G^{(0)}_{\uparrow xy}G^{(0)}_{\uparrow yx}G^{(0)}_{\downarrow xy}G^{(0)}_{\downarrow yx}$$

$$=-\frac{U^2}{2}\frac{1}{(\beta V)^2}\sum_k\left(\sum_{p_1}G^0_{\uparrow p_1}G^{(0)}_{\uparrow p_1+k}\right)\times\left(\sum_{p_2}G^{(0)}_{\downarrow p_2}G^{(0)}_{\downarrow p_2+k}\right), \tag{2.47}$$

where $G^{(0)}_{\sigma p}=(-i\xi_n+t_\mathbf{k}-J_\sigma^{(0)})^{-1}$ with $p=(n,\mathbf{k})$. For later convenience we introduce $F^{(2)}(J_1,J_2)$ as follows:

$$F^{(2)}(J_1,J_2)=-\frac{U^2}{2}\sum_k\chi_k^0(J_1)\chi_k^0(J_2), \tag{2.48}$$

where

$$\chi_p^0(J)=-\frac{1}{\beta V}\sum_{p'}G^J_{p'}G^J_{p'+p} \tag{2.49}$$

and $G_p^J=(-i\xi_n+t_\mathbf{k}-J)^{-1}$ with $p=(n,\mathbf{k})$. Then $F^{(2)}$ is given by

$$F^{(2)}=F^{(2)}(J_1,J_2)|_{J_1=J_\uparrow^{(0)},J_2=J_\downarrow^{(0)}}. \tag{2.50}$$

The quantity $\chi_p^0(J)$ reduces to the dynamical susceptibility of the free-electron system ($U=0$) in zero magnetic field if we set $J=\mu_0$ and further reduces to the Pauli (static) susceptibility when $p=(n,\mathbf{k})=0$. This is because $\chi_p^0(J)$ can be rewritten as

$$\chi_p^0(J)=\frac{1}{V}\sum_{\mathbf{k}'}\frac{f_\beta(t_{\mathbf{k}'+\mathbf{k}}-J)-f_\beta(t_{\mathbf{k}'}-J)}{i\omega_n+t_{\mathbf{k}'}-t_{\mathbf{k}'+\mathbf{k}}}, \tag{2.51}$$

where ω_n is the even frequency:

$$\omega_n=2n\pi T. \tag{2.52}$$

Step 4: Turning off the source. In order to go back to the starting theory we set $h=0$ at this stage. This is done by the following replacement,

$$\frac{1}{\beta V}\frac{\partial F}{\partial\phi_\sigma}=J_\sigma=\frac{\sigma}{2}h+\mu\Rightarrow\mu. \tag{2.53}$$

Specifically this equation is written, by using (2.33), (2.36), and (2.48), as

$$\mu=J_\sigma^{(0)}+U\phi_{-\sigma}$$
$$-\frac{U^2}{2}\frac{1}{\beta V}\frac{\partial J_1}{\partial\phi_\sigma}\sum_k\frac{\partial\chi_k^0(J_1)}{\partial J_1}\chi_k^0(J_2)\Big|_{J_1=J_\sigma^{(0)},J_2=J_{-\sigma}^{(0)}}. \tag{2.54}$$

Two equations (2.54) for $\sigma=\uparrow$ and $\downarrow$ can be looked upon as relations determining the magnetization M and the chemical potential μ as functions of the total number of electrons N. If we neglect the last term in (2.54) we have

$$J_\sigma^{(0)}=\mu-U\phi_{-\sigma}. \tag{2.55}$$

By operating ϕ_0 on the above equation we get from (2.23)

$$\phi_\sigma=\phi_0(\mu-U\phi_{-\sigma})=\frac{1}{V}\sum_{\mathbf{k}} f_\beta(t_{\mathbf{k}}+U\phi_{-\sigma}-\mu). \tag{2.56}$$

Hence we arrive at

$$N=\sum_{\mathbf{k}}[f_\beta(t_{\mathbf{k}}-Um-\tilde{\mu})+f_\beta(t_{\mathbf{k}}+Um-\tilde{\mu})], \tag{2.57}$$
$$m=\frac{1}{2V}\sum_{\mathbf{k}}[f_\beta(t_{\mathbf{k}}-Um-\tilde{\mu})-f_\beta(t_{\mathbf{k}}+Um-\tilde{\mu})],$$

where $\tilde{\mu}=\mu-Un/2$. These two equations are the self-consistent equations of m and μ for a given N in the Stoner theory. Thus we see again that the inversion method up to the first order reproduces the mean-field result.

III. STUDY OF THE SUSCEPTIBILITY FOR $T>T_c$

The inverse of the static susceptibility is given by the second derivative of the free energy with respect to M. The susceptibility χ for $T>T_c$ with $h=0$ is given by

$$\chi^{-1}=\frac{1}{\beta V}\frac{\partial^2 F}{\partial m^2}\Big|_{J_\uparrow^{(0)}=J_\downarrow^{(0)}=\mu_0}$$
$$=\frac{1}{\beta V}(F_{\uparrow\uparrow}+F_{\downarrow\downarrow}-2F_{\uparrow\downarrow})_{J_\uparrow^{(0)}=J_\downarrow^{(0)}=\mu_0}, \tag{3.1}$$

where $F_{\sigma\sigma'}=\partial^2F/\partial\phi_\sigma\partial\phi_{\sigma'}$. [Note that in the above equation the subscript $J_\uparrow^{(0)}=J_\downarrow^{(0)}=\mu_0$ does not imply that the derivative with respect to m is taken by fixing $J^{(0)}$ but implies merely that $J^{(0)}$ is set to μ_0 after the derivative, see below (2.45).] Hence the zeroth-order of the inverse of the susceptibility is obtained as

$$[\chi^{-1}]^{(0)}=\sum_\sigma\frac{\partial J_\sigma^{(0)}}{\partial\phi_\sigma}\Big|_{J_\sigma^{(0)}=\mu_0}. \tag{3.2}$$

By noting (2.45) we get

$$[\chi^{-1}]^{(0)}=2[\phi_0'(\mu_0)]^{-1}, \tag{3.3}$$

where $\phi_0'(J)=\partial\phi_0(J)/\partial J$ and $\phi_0(J)=-\Sigma_k G_k^J/\beta V$. The first order is easily given from (2.36):

$$[\chi^{-1}]^{(1)}=-2U. \tag{3.4}$$

Therefore we have

$$\chi_{\mathrm{MF}}^{-1}\equiv[\chi^{-1}]^{(0)}+[\chi^{-1}]^{(1)}=2\{[\phi_0'(\mu_0)]^{-1}-U\}, \tag{3.5}$$

which corresponds to the mean-field result. If we denote $\phi_0'(\mu_0)$ by the graph in (2.24), the graphs of χ_{MF} are represented by so-called ring diagrams. Thus we see that as the result of the inversion an infinite number of graphs has been summed up to reproduce the Stoner theory.

In order to derive the second order of the inverse of the susceptibility we first note

$$F_{\uparrow\downarrow}^{(2)}=\frac{\partial J_1}{\partial\phi_\uparrow}\frac{\partial J_2}{\partial\phi_\downarrow}\frac{\partial}{\partial J_1}\frac{\partial}{\partial J_2}F^{(2)}(J_1,J_2)|_{J_1=J_\uparrow^{(0)},J_2=J_\downarrow^{(0)}}, \tag{3.6}$$

$$F_{\uparrow\uparrow}^{(2)}=\left\{\frac{\partial^2 J_1}{\partial\phi_\uparrow^2}\frac{\partial}{\partial J_1}+\left(\frac{\partial J_1}{\partial\phi_\uparrow}\right)^2\frac{\partial^2}{\partial J_1^2}\right\}F^{(2)}(J_1,J_2)|_{J_1=J_\uparrow^{(0)},J_2=J_\downarrow^{(0)}}. \tag{3.7}$$

Since the susceptibility for $T>T_c$ and $h=0$ is evaluated at $J_\uparrow^{(0)}=J_\downarrow^{(0)}=\mu_0$, in the above equations, $\partial J_i/\partial\phi_\sigma$ reduces to $[\phi_0'(\mu_0)]^{-1}$ as before and the quantity

$$\frac{\partial^2 J_i}{\partial\phi_\sigma^2}=\frac{\partial}{\partial\phi_\sigma}\left(\frac{\partial\phi_\sigma}{\partial J_i}\right)^{-1}=-\left(\frac{\partial\phi_\sigma}{\partial J_i}\right)^{-3}\frac{\partial^2\phi_\sigma}{\partial J_i^2} \tag{3.8}$$

reduces to $-[\phi_0'(\mu_0)]^{-3}\phi_0''(\mu_0)$. Thus from (3.1) and (2.48) the second order of χ^{-1} is given by

$$\Delta\chi^{-1}\equiv[\chi^{-1}]^{(2)}$$
$$=\left(\frac{U}{\phi_0'(\mu_0)}\right)^2\left\{\frac{\phi_0''(\mu_0)}{\phi_0'(\mu_0)}\frac{\partial}{\partial J_1}-\frac{\partial^2}{\partial J_1^2}+\frac{\partial}{\partial J_1}\frac{\partial}{\partial J_2}\right\}$$
$$\times\frac{1}{\beta V}\sum_k\chi_k^0(J_1)\chi_k^0(J_2)\Big|_{J_1=J_2=\mu_0}. \tag{3.9}$$

We now obtain the inverse of the susceptibility for $T>T_c$ and $h=0$ up to the second order of the inversion method, which is given by

$$\chi^{-1}=\chi_{\mathrm{MF}}^{-1}+\Delta\chi^{-1} \tag{3.10}$$

with (3.5) and (3.9). This expression is exact except for the approximation by the inversion method so that we expect that it approaches the correct value if the coupling constant U becomes small. We note here that without further approximation the even-frequency summation in (3.9) [see ω_n appearing in (2.51)] can be performed although the result is not used explicitly in what follows:

$$\frac{1}{\beta V}\sum_k\chi_k^0(J_1)\chi_k^0(J_2)$$
$$=\frac{1}{2V^3}\sum_{\mathbf{k},\mathbf{k}_1,\mathbf{k}_2}\{f_\beta(\tilde{\mu}_1)-f_\beta(\mu_1)\}\{f_\beta(\tilde{\mu}_2)-f_\beta(\mu_2)\}$$
$$\times\frac{\coth(\beta\varepsilon_2/2)-\coth(\beta\varepsilon_1/2)}{\varepsilon_1-\varepsilon_2}, \tag{3.11}$$

where $\tilde{\mu}_i=t_{\mathbf{k}_i+\mathbf{k}}-J_i$, $\mu_i=t_{\mathbf{k}_i}-J_i$, $\varepsilon_i=t_{\mathbf{k}_i+\mathbf{k}}-t_{\mathbf{k}_i}$.

To examine (3.10) numerically we make two approximations.

(1) Use a parabolic band with cutoff momentum. We employ the parabolic band structure $t_{\mathbf{k}}=\mathbf{k}^2/2m$ where the upper boundary of the band is taken into account by cutting off the momentum integration at k_c.

(2) Keep only the zeroth-order of the Sommerfeld expansion. We keep only the first term of the following expansion:

$$\frac{\partial}{\partial\varepsilon}\frac{1}{e^{\beta(\varepsilon-\mu)}+1}=-\delta(\varepsilon-\mu)-\frac{\pi^2}{6\beta^2}\frac{\partial^2}{\partial\varepsilon^2}\delta(\varepsilon-\mu)+O(T^4). \tag{3.12}$$

This amounts to the assumption $1\gg(\pi^2/12)(T/T_F)^2$.

We stress here the fact that T/T_F may be smaller than 0.1 in most of real substances even at the temperature of melting point where T_F is the Fermi temperature. With these approximations the following replacement can be used:

$$\phi_0'(\mu_0)\to D_F, \tag{3.13}$$

$$\frac{\phi_0''(\mu_0)}{\phi_0'(\mu_0)}\to\frac{1}{2\varepsilon_F}, \tag{3.14}$$

$$\mu_0\to\varepsilon_F, \tag{3.15}$$

$$f_\beta(\varepsilon-\mu_0)\to\theta(\varepsilon_F-\varepsilon), \tag{3.16}$$

where ε_F has the following relation with μ_0:

$$\mu_0=\varepsilon_F\left(1-\frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2+\cdots\right),\quad T_F=\varepsilon_F. \tag{3.17}$$

D_F is the density of states at Fermi surface of the free electron:

$$D_F=\frac{3n}{4\varepsilon_F}. \tag{3.18}$$

In addition we have the well-known relations

$$\varepsilon_F=\frac{k_F^2}{2m},\quad k_F^2=3\pi^2n, \tag{3.19}$$

where k_F and n are the Fermi momentum and the number density of the free Fermi gas, respectively.

By the approximation $f_\beta(x)\to\theta(-x)$ one gets from (2.51)

$$\chi_p^0(J)=\frac{1}{V}\sum_{\mathbf{k}'}\frac{\theta(J-t_{\mathbf{k}'+\mathbf{k}})-\theta(J-t_{\mathbf{k}'})}{t_{\mathbf{k}'}-t_{\mathbf{k}'+\mathbf{k}}+i\omega_n} \tag{3.20}$$

with $p=(n,\mathbf{k})$. Now we introduce dimensionless quantities

$$\mathbf{K}=\frac{\mathbf{k}}{k_F},\quad \bar\omega_n=\frac{\omega_n}{\varepsilon_F},\quad \bar J=\frac{J}{\varepsilon_F}. \tag{3.21}$$

Thus in these approximations we have to set $\bar J=1$ in the end. One then obtains, with the approximation $t_{\mathbf{k}}=\mathbf{k}^2/2m$,

$$\chi_p^0(J)=\frac{D_F}{2K}\int_0^{\sqrt{\bar J}}dK'K'\ln\frac{(K'+K/2)^2+(\bar\omega_n/2K)^2}{(K'-K/2)^2+(\bar\omega_n/2K)^2}, \tag{3.22}$$

where the upper limit of the integral of K' is automatically set to $\sqrt{\bar J}$ by the θ function. Here $K\equiv|\mathbf{K}|$.

On the other hand, $\Delta\chi^{-1}$ is given from (3.9) as follows with the above approximations:

$$\Delta\chi^{-1}=\left(\frac{U}{D_F}\right)^2\frac{1}{\beta V}\sum_p\frac{1}{\varepsilon_F^2}\left\{\left(\frac{1}{2}\frac{\partial\chi_p^0(J)}{\partial\bar J}-\frac{\partial^2\chi_p^0(J)}{\partial\bar J^2}\right)\chi_p^0(J)+\left(\frac{\partial\chi_p^0(J)}{\partial\bar J}\right)^2\right\}_{\bar J=1} \tag{3.23}$$

with $p=(n,\mathbf{K})$. By introducing the quantities

$$f_{nK}=\frac{1}{2}\ln\frac{K^2(2+K)^2+\bar\omega_n^2}{K^2(2-K)^2+\bar\omega_n^2}, \tag{3.24}$$

$$g_{nK}=\frac{K^2(4-K^2)+\bar\omega_n^2}{4K^2}, \tag{3.25}$$

$$h_{nK}=4K^3\frac{K^2(4-K^2)-\bar\omega_n^2}{\bar\omega_n^4+2K^2(4+K^2)\bar\omega_n^2+K^4(4-K^2)^2}, \tag{3.26}$$

$$l_{nK}=\frac{\bar\omega_n}{2}\left(\arctan\frac{2K+K^2}{\bar\omega_n}+\arctan\frac{2K-K^2}{\bar\omega_n}\right), \tag{3.27}$$

one gets, after some calculation using the above expression for $\chi_p^0(J)$ in (3.22),

$$\Delta\chi^{-1}=\frac{U^2}{4\beta}\sum_{n=-\infty}^{\infty}\int_0^{K_c}\frac{4\pi K^2}{(2\pi)^3}dK\frac{k_F^3}{\varepsilon_F^2}\left\{\frac{f_{nK}+h_{nK}}{2K}\times\left(1+\frac{f_{nK}g_{nK}-l_{nK}}{K}\right)+\left(\frac{f_{nK}}{K}\right)^2\right\}, \tag{3.28}$$

where we have introduced the cutoff momentum $K_c=k_c/k_F$. We get in this way a formula for the normalized (dimensionless) susceptibility:

$$1/\bar\chi=1-\alpha+\frac{\alpha^2}{2}A(\bar T) \tag{3.29}$$

with

$$A(\bar T)=\frac{1}{2}\bar T\sum_{n=-\infty}^{\infty}\int_0^{K_c}dK\{\tfrac{1}{2}(f_{nK}+h_{nK})(K+f_{nK}g_{nK}-l_{nK})+f_{nK}^2\}, \tag{3.30}$$

where

$$\bar\chi=\frac{\chi}{D_F/2},\quad \alpha=UD_F,\quad \bar T=T/T_F=T/\varepsilon_F. \tag{3.31}$$

Note here that in the Stoner theory $\bar\chi$ is given by $1/\bar\chi=1-\alpha+R\bar T^2$ where R is determined by the derivatives of the density of states at the Fermi level. Equation (3.29) for $\bar\chi$ is estimated numerically. As is clear from the expression, parameters of this theory are K_c and $\alpha=UD_F$. The parameter α is directly related to the Stoner criteria $\alpha>1$, which

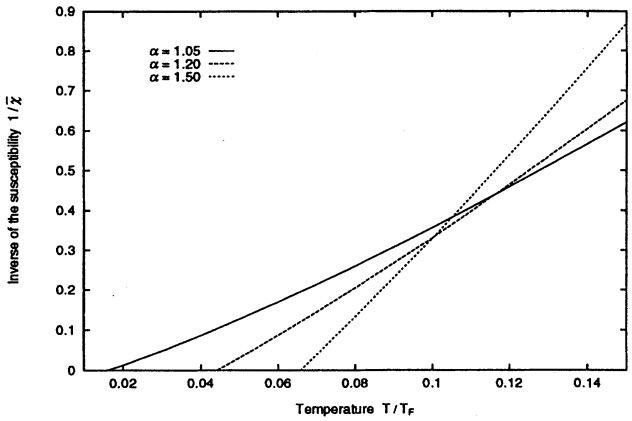


FIG. 1. The relation between $1/\bar{\chi}$ and $\bar{T}$. The values of α indirectly determine the critical temperature T_c. The Curie-Weiss law is well reproduced.

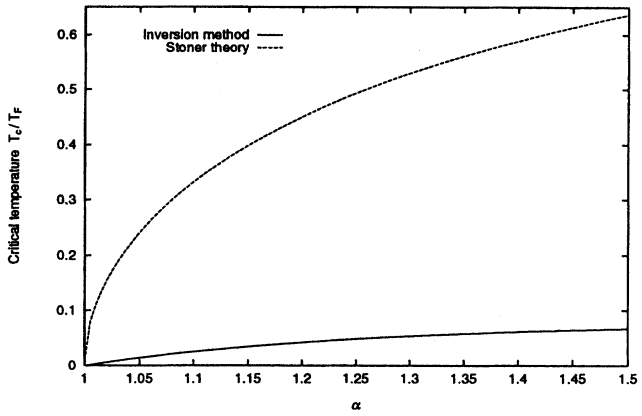


FIG. 2. The relation between α and $\bar{T}_c$. The critical temperature T_c in the present theory is generally lower than that in the Stoner theory.

gives a sufficient condition for realizing the ferromagnetic phase in the mean-field approximation.

Through the numerical calculation we confirm that the $A(\bar{T})$ in (3.29), which is α independent, is almost linearly dependent on $\bar{T}$ if K_c is slightly smaller than 2.0 (see below) and $\bar{T}=0.01$–0.15. Note that since the typical value of T_F for metal may be about 10^5 K, this range of temperature covers that of the normal experiment situation on the susceptibility. Thus for rather special value of K_c we obtain the linear dependence of the inverse susceptibility on temperature—an important property realized in most kind of metals.

The significance of the special value of K_c can be considered as follows. The integrand in (3.30) is singular for $n=0$ at $K=2$. This singularity is originated from the adaptation of the parabolic band which may be unphysical if we do not require cutoff. Thus it is natural that we cut off the momentum integration at smaller value than the singular point that corresponds to twice the Fermi momentum. By letting the K_c close to the singular point from below, the contribution from the $n=0$ term in (3.30) which is independent of the temperature comes to dominate, resulting in the linear behavior of $A(\bar{T})$. The fact that the reproduction of the Curie-Weiss law requires K_c to be slightly smaller than 2 implies that the present theory is sensitive to the behavior of the density of states near the singularity.

Furthermore we interpret the result as follows. The temperature-independent part of the correction term, namely $A(0)$, has the role to renormalize α so that the renormalized α takes its critical value at $\alpha=1$ as in the Stoner theory; $1-\alpha+(\alpha^2/2)A(0)=1-\alpha_r$. Thus we simply keep only the temperature-dependent part of $A(\bar{T})$ in what follows. This interpretation will be reconsidered later. In this way we arrive at Fig. 1 where the Curie-Weiss law is well reproduced. Furthermore as seen from Fig. 2 we see that the Curie temperature T_c is substantially lowered in the present theory compared with that in the Stoner theory, which is more agreeable to the real situation than the Stoner theory. The parameter K_c in these figures is 1.9999. We made sure that the linearity in Fig. 1 is improved if K_c becomes closer to 2.0. In the numerical calculation we have used the double exponential formula, which is strong in integration where the integrand has a singular point at the upper bound of integration.

IV. APPROXIMATIONS IN THE SCR THEORY

The SCR theory[2] starts from an *exact formula* for the free energy (per unit volume) $f(M,U)$ at temperature $T=\beta^{-1}$ for a given M:

$$f(M,U)=f(M,0)+U(N^2/4-M^2)/V^2+\Delta f(M,U), \tag{4.1}$$

where Δf is given by

$$\Delta f(M,U)=-\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\coth\frac{\beta\omega}{2}\frac{1}{V}\sum_{\mathbf{k}}\int_0^U dU' \times[\mathrm{Im}\chi_{MU'}(\mathbf{k},\omega+i0^+)-\mathrm{Im}\chi_{M0}(\mathbf{k},\omega+i0^+)] \tag{4.2}$$

$$=-\frac{2}{\beta V}\sum_n\sum_{\mathbf{k}}\int_0^U dU' \times[\chi_{MU'}(\mathbf{k},i\omega_n)-\chi_{M0}(\mathbf{k},i\omega_n)], \tag{4.3}$$

where Im represents the imaginary part, and 0^+ a positive infinitesimal quantity. In what follows, we review the SCR theory only for the paramagnetic case. $\chi_{MU'}(\mathbf{k},\omega)$ is the dynamic susceptibility under the magnetic field that stabilizes the value M of the magnetization but the strength of the on-site Coulomb interaction taking the value U'. Note that $\chi_{MU'}$ can be expressed by the fluctuation of the spin by the fluctuation-dissipation theorem so that Δf originates from the spin fluctuation. The first two terms of (4.1) are the free energy of the Stoner theory. Since the inverse of the static susceptibility is given by the second derivative of the free energy with respect to M, for $T>T_c$ $(M=0)$ we obtain

$$\frac{1}{\chi_{0U}(\mathbf{0},0)}=V^2\left.\frac{\partial^2 f(M,U)}{\partial M^2}\right|_{M=0} \tag{4.4}$$

or

$$\frac{\chi_{00}(\mathbf{0},0)}{\chi_{0U}(\mathbf{0},0)}=1-2U\chi_{00}(\mathbf{0},0)+\lambda(T,U), \tag{4.5}$$

where $\lambda(T,U)$ is given by

$$\lambda(T,U)=V^2\chi_{00}(\mathbf{0},0)\left.\frac{\partial^2 f(M,U)}{\partial M^2}\right|_{M=0}. \tag{4.6}$$

In (4.5) the first term terms are the Stoner contribution. Following (4.5) we write the dynamic susceptibility as

$$\frac{\chi_{M0}(\mathbf{k},\omega)}{\chi_{MU}(\mathbf{k},\omega)}=1-2U\chi_{M0}(\mathbf{k},\omega)+\bar{\lambda}(T,U,\mathbf{k},\omega,M). \tag{4.7}$$

If $\bar{\lambda}$ has dependence on T, U, $\mathbf{k}$, ω, and M this expression is still *exact*, that is, Eq. (4.7) is merely a definition of $\bar{\lambda}$. Now we enumerate the approximation used in SCR.

Approximation I. $\bar{\lambda}$ is approximated by λ given in (4.6), which is actually $\bar{\lambda}$ evaluated at $\mathbf{k}=\omega=M=0$. In other words we assume the form

$$\chi_{MU}(\mathbf{k},\omega)=\frac{\chi_{M0}(\mathbf{k},\omega)}{1-2U\chi_{M0}(\mathbf{k},\omega)+\lambda(T,U)} \tag{4.8}$$

with

$$\lambda(T,U)=-V\chi_{00}(\mathbf{0},0)\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\coth\frac{\beta\omega}{2}\times\sum_{\mathbf{k}}\int_0^U dU'\frac{\partial^2}{\partial M^2}[\mathrm{Im}\chi_{MU'}(\mathbf{k},\omega+i0^+)-\mathrm{Im}\chi_{M0}(\mathbf{k},\omega+i0^+)]|_{M=0}. \tag{4.9}$$

Now we have to solve (4.8) and (4.9) self-consistently in terms of $\lambda(T,U)$ to get the static susceptibility given by (4.8) at $\omega=\mathbf{k}=0$ by using known expression for $\chi_{M0}(\mathbf{k},\omega)$. Note here that $\lambda(T,U)$ defined by (4.8) does depend on ω and $\mathbf{k}$ while $\lambda(T,U)$ given by (4.9) does not. In the SCR theory we further make several approximations.

Approximation II. Neglect the U' dependence of $\lambda(T,U')$ when integrating over the variable U' in (4.9).

Approximation III. Neglect $\lambda(T,U')$ compared with 1 in the numerator when we take the derivatives with respect to M in (4.9).

Approximation IV. Rewrite $\coth(\beta\omega/2)$ as $\mathrm{sgn}(\omega)[1-2/(e^{\beta|\omega|}-1)]$ where $\mathrm{sgn}(\omega)$ denotes the sign of ω and then neglect the first term 1. In other words replace $\coth(\beta\omega/2)$ by $\mathrm{sgn}(\omega)[2/(e^{\beta|\omega|}-1)]$.

Approximation V. Replace $\chi_{M0}(\mathbf{k},\omega)$ with several leading terms of the expansion of $\chi_{M0}(\mathbf{k},\omega)$ by powers of $\mathbf{k}$ and $\omega/|\mathbf{k}|$.

Approximation VI. Use the parabolic band with the cutoff momentum.

They think that approximations I–III may be *physically* justified if one assumes that the density of states has a sharp peak at the Fermi surface and that this point may limit the applicability of the theory to the weak ferromagnetism. Approximation IV is not necessarily easy to be justified[17] as well as approximation V.

After collecting all these approximations involved in the SCR theory the author came to the conclusion that it is worthwhile to develop the theory of the ferromagnetism of the itinerant electrons in a systematic, mathematically well-defined manner, for example, by using the inversion method.

V. DISCUSSION

Although we have obtained preferable results for the Curie-Weiss law, the present theory leaves much to be desired if we returned to our original motivation. First, the parameter K_c has to take rather special value to reproduce the linear dependence of $A(\bar{T})$ on $\bar{T}$. This fact suggests that the present theory is subject to the details of the band structure as mentioned before. This sensitivity to the cutoff parameter may be caused by the parabolic band approximation. We give up dealing with the larger momentum region precisely at the cost of calculational simplicity in the approximation. In this respect the study for the case of other more realistic band structures is an interesting future problem.

Second, it is not necessarily easy to justify the interpretation which leads to the neglect of the temperature-independent part of $A(\bar{T})$ although similar approximation has been employed in the literature (for example Refs. 2 and 4). According to Ref. 4, the justification of such an approximation can be stated as follows (although such a process contradicts our original scope); "Since we are mainly interested in the temperature dependence of the physical quantities, the approximation is reasonable if no significant temperature-dependent terms are omitted as a consequence." If we do not make this approximation, $\bar{T}_c$ takes a minus value which forces us to interpret the theory to be no good around the critical point although at least the linear dependence of $A(\bar{T})$ on $\bar{T}$ is reproduced.

Finally, it is not obvious to what degree the approximation of keeping only the first three terms of the inversion series can be justified. Though the inversion method itself is systematic at least formally, it does not guarantee to give a well-controlled approximation. The parameter U/t should be small for the present approximation to be valid, where t is the characteristic order of the hopping term of the Hamiltonian. If it is small, $J^{(n)}(\phi)$ (and $F^{(n)}$) becomes smaller as n gets larger in principle. But it is possible for $F^{(n)}(\phi)$ to become large after $F^{(n)}(\phi)$ is estimated at the desired value of ϕ. Thus the behavior of the higher order of the inversion series of the present model should be studied, for example, by using the formal graph rules for the series that has been already known,[16] which needs a separate study.

We note here that the inversion method has the possibility to be used to justify the paramagnon theories. This is because it can be shown that the result of the inversion method up to the second order coincides with the leading term of the paramagnon theories and that a class of the graphs appearing in the inversion series reproduces the paramagnon theory.[15]

As discussed above, it may be inappropriate to say that only mathematically well-defined approximation is used in order to reproduce the Curie-Weiss law in our theory. But at least our theory does not rely on the equation established through *physical approximation* that is thus hard to be improved. Instead we develop a theory in which we can advance the approximation systematically up to the desired or-

der in principle. In addition, since this framework or the inversion method has a wide applicability, it is very important to give a concrete and nontrivial example of the method, which is what we have done here.

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APPENDIX: FEYNMAN RULES

Although well known, we summarize for clarity the rule to get algebraic expressions from the corresponding Feynman graphs in the imaginary time formalism. First we note the path-integral representation of Ω (see, for example, Appendix D of Ref. 16);

$$\Omega = -\ln\left(\int \mathscr{D}z^* \mathscr{D}z e^{-S[z^*,z,J]} \right), \tag{A1}$$

where z and z^* are Grassmann numbers and $S[z^*,z,J]$ is given by

$$S[z^*,z,J] = \sum_{xx'\sigma} z^*_{x\sigma} G^{-1}_{xx'} z_{x'\sigma} + U \sum_x z^*_{x\uparrow} z_{x\uparrow} z^*_{x\downarrow} z_{x\downarrow} - \sum_{x\sigma} J_{x\sigma} z^*_{x\sigma} z_{x\sigma}, \tag{A2}$$

where x or x' denotes the set $(\tau,\mathbf{r})$ or $(\tau',\mathbf{r}')$, respectively. Σ_x implies $\int d\tau \Sigma_{\mathbf{r}}$ where τ is the imaginary time.

Rule 1. In one specific way (as one likes), assign n labels $x_1, \ldots, x_n$ (internal points) to all the four-point vertices where n is the total number of vertices.

Rule 2. Associate

$y \longrightarrow x$

and

$y \dashrightarrow x$

with $[G^{(0)}_\uparrow]_{xy}$ and $[G^{(0)}_\downarrow]_{xy}$, respectively, and the factor U is assigned to the four-point vertex. No factor is assigned to the external point.

Rule 3. Associate a factor $(-1)^{V+1}(-1)^{L_f}$ for each diagram where V is the number of the factors U in the graph and L_f is the number of Fermion loops.

Rule 4. Associate the inverse of the symmetry factor $1/S$ for the diagram.

Rule 5. Sum (integrate) the product of all factors in 2–4 over the space and imaginary time indices $x_1, \ldots, x_n$.

As is well known, the symmetry factor S for each graph is given by the product of the line symmetry factor and the vertex symmetry factor. The line symmetry factor is 1 in this theory and the rule for the vertex symmetry factor S_V is the following.

Rule S_V. Assign n labels $1, \ldots, n$ to n vertices in one specific but arbitrary way. Count the number of all possible other ways of assigning n labels that give the same topological structure as the first specific way. The number thus obtained plus 1 is S_V. Note that we have to distinguish the spin-up and spin-down propagators and the directions of the arrows when we consider the topological equivalence.

For definiteness we give some examples; the graph in (2.16) or (2.17) has $S=1$ and three graphs in (2.18) have $S=1$, 2, and 1, respectively.

*Present address: Division of Theoretical Studies, Institute for Molecular Science, Nishigonaka 38, Myodaiji, Okazaki, Aichi 444, Japan. Electronic address: okumura@ims.ac.jp

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