Weak-coupling approach to interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model

Shuntaro Yoda* and Kosaku Yamada
Department of Physics, Kyoto University, Kyoto 606-8502, Japan
(Received 5 October 1998; revised manuscript received 30 November 1998)

We investigate the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model on the triangular lattice in the weak-coupling regime within the second-order perturbation theory. In systems without frustration, at the filling equal to or close to half-filling, the direction of the deformation of the Fermi surface is the direction toward the Fermi surface at half-filling with the smaller transfer amplitude set to zero, whose nesting vector is commensurate with the underlying lattice. On the other hand, in systems with frustration, the Fermi surface is not deformed by the interaction because of the frustration.
[S0163-1829(99)11435-8]

I. INTRODUCTION

The form of the Fermi surface is a characteristic feature of a metal. Whether the metal is weakly correlated or strongly correlated, generally, the Fermi surface can be determined experimentally by the angle-resolved photoemission spectroscopy and/or the de Haas–van Alphen measurement. These experimental results are compared with band-structure calculations, although the effect of the electron correlation to the Fermi surface beyond the band-structure calculation remains unclear.

So far, the problem of the deformation of the Fermi surface induced by the electron-electron interaction in the two-dimensional Hubbard model has been studied only for the square lattice. Halboth and Metzner[1] calculated for the square lattice with only the nearest-neighbor transfer amplitude within the second-order perturbation theory. Zlatić, Entel, and Grabowski[2] calculated for the square lattice with the anisotropic transfer amplitude in the x and y directions, which is also within the second-order perturbation theory. Both have shown that close to half-filling the interaction enhances the anisotropy of the Fermi surface. The square lattice has no frustration for the antiferromagnetic spin ordering; therefore, at half-filling, we have the antiferromagnetic ground state if the system is insulating. In contrast, in the case of a lattice with frustration for the antiferromagnetic spin ordering, e.g., the triangular lattice, the antiferromagnetic ground state is unfavorable. Then, for the triangular lattice, how is the deformation of the Fermi surface?

In this paper, we investigate the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model on the triangular lattice in the weak-coupling regime within the second-order perturbation theory. We present the formulation of this problem in Sec. II and the results of our numerical calculation in Sec. III. Then, we make some discussion in Sec. IV and finally the conclusion is given in Sec. V.

II. FORMULATION

We consider the two-dimensional Hubbard model on the triangular lattice. The Hamiltonian is given by

$$H = H_0 + H_1, \tag{1}$$

$$H_0 = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}, \tag{2}$$

$$H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{3}$$

where t_{ij} is the transfer amplitude between site i and site j, $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) is the annihilation (creation) operator for the electron of spin σ at site i, U is the on-site Coulomb interaction, and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. We take the transfer amplitude such as

$$t_{ij} = \begin{cases} t & \text{for the nearest neighbor } i,j \text{ in the first and second directions,} \\ t_3 & \text{for the nearest neighbor } i,j \text{ in the third direction,} \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

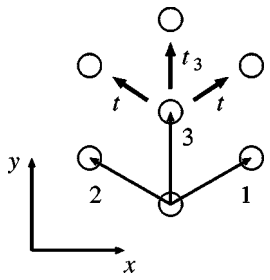

FIG. 1. The triangular lattice and the transfer amplitude.

Here, the first, second, and third directions are the directions shown in Fig. 1. We set a different transfer amplitude in one direction, namely, in the third direction intentionally in order to control frustration systematically. We take the lattice spacing as the unit of length. The noninteracting dispersion of the band ε_k is given by

$$\varepsilon_k = -\left(4t\cos\frac{\sqrt{3}}{2}k_x\cos\frac{1}{2}k_y + 2t_3\cos k_y\right), \tag{5}$$

where k is the momentum.

Our analysis is based on the formalism of the Green's function.[3] The noninteracting (mean-field) one-particle Green's function $G_k^{(0)}(i\omega_n)$ is given by

$$G_k^{(0)}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_k - Un/2 + \mu}, \tag{6}$$

where $\omega_n = (2n+1)\pi T$ is the fermionic Matsubara frequency at temperature T, n is the filling of the band, and μ is the chemical potential. Generally, the one-particle spectrum of the system is given by the pole of the one-particle Green's function. The one-particle spectrum of the noninteracting system is nothing but the noninteracting dispersion of the band ε_k. The Fermi surface of the noninteracting system is calculated from ε_k. We introduce the polar coordinates (k,ϕ) in the momentum space to describe the deformation of the Fermi surface. The angle ϕ is to be measured from the k_x axis. We denote the Fermi momentum of the noninteracting system by $k_{\mathrm{F}}^{(0)}$, which is a function of the angle ϕ.

Now we consider the interacting system. We make the perturbation expansion of the self-energy with respect to U around the nonmagnetic mean-field solution, where the Hartree term is already taken into account. Hence, it is enough to take only the second-order term, is the lowest order that causes the deformation of the Fermi surface. Here we consider only the paramagnetic state. The self-energy $\Sigma_k(i\omega_n)$ is given by

$$\Sigma_k(i\omega_n) = -U^2\frac{T}{N}\sum_{q\nu_n} G_{k-q}^{(0)}(i\omega_n - i\nu_n)\frac{T}{N}\sum_{k_1,\omega_{1n}} G_{k_1}^{(0)}(i\omega_{1n})G_{k_1+q}^{(0)}(i\omega_{1n}+i\nu_n), \tag{7}$$

where q is the momentum, $\nu_n = 2n\pi T$ is the bosonic Matsubara frequency, and N is the number of the lattice sites. The corresponding diagram is shown in Fig. 2. The interacting one-particle Green's function $G_k(i\omega_n)$ is given by the following Dyson equation,

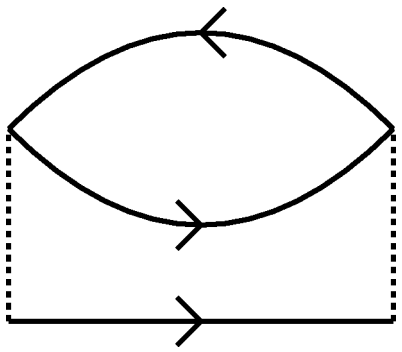

FIG. 2. The diagram of the second-order self-energy. The solid and dotted lines denote the noninteracting Green's function $G^{(0)}$ and the Coulomb interaction U, respectively.

$$G_k(i\omega_n)^{-1} = G_k^{(0)}(i\omega_n)^{-1} - \Sigma_k(i\omega_n). \tag{8}$$

The one-particle spectrum of the interacting system, namely, the dispersion of the renormalized quasiparticle $\omega = E_k$ is given by the pole of the interacting one-particle Green's function and is determined by the following equation:

$$\mathrm{Re}[G_k^{\mathrm{R}}(\omega)^{-1}] = \omega - \varepsilon_k - Un/2 - \mathrm{Re}\,\Sigma_k^{\mathrm{R}}(\omega) + \mu = 0, \tag{9}$$

where $G_k^{\mathrm{R}}(\omega)$ and $\Sigma_k^{\mathrm{R}}(\omega)$ are the analytic continuations of $G_k(i\omega_n)$ and $\Sigma_k(i\omega_n)$, respectively, in the upper half complex plane with respect to the frequency. By expanding $\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(\omega)$ with respect to ω and taking the terms up to the first order, we obtain

$$\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(\omega) = \mathrm{Re}\,\Sigma_k^{\mathrm{R}}(0) + \left.\frac{\partial\,\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(\omega)}{\partial\omega}\right|_{\omega=0}\omega, \tag{10}$$

which is a good approximation for the Fermi liquid. By substituting Eq. (10) for Eq. (9), we obtain

$$E_k = z_k[\varepsilon_k + Un/2 + \mathrm{Re}\,\Sigma_k^{\mathrm{R}}(0) - \mu], \tag{11}$$

where z_k is the so-called renormalization factor and is given by

$$z_k = \left[1 - \left.\frac{\partial\,\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(\omega)}{\partial\omega}\right|_{\omega=0}\right]^{-1}. \tag{12}$$

The Fermi surface of the interacting system is calculated from E_k in such a manner that the volume enclosed by the Fermi surface must be the same as that of the noninteracting system (the Luttinger's theorem).[4] Equivalently, the interacting Fermi surface is determined as the root of the equation $E_k = 0$. Therefore, according to Eq. (11), the renormalization factor z_k makes no contribution to the deformation of the Fermi surface, and hence, the deformation of the Fermi surface is caused by the energy shift resulting from $\mathrm{Re}\Sigma_k^{\mathrm{R}}(0)$. We denote the Fermi momentum of the interacting system by k_F, which is a function of the angle ϕ. We define the shift of the Fermi surface in the radial direction δk_F as

$$\delta k_F = k_F - k_F^{(0)}, \tag{13}$$

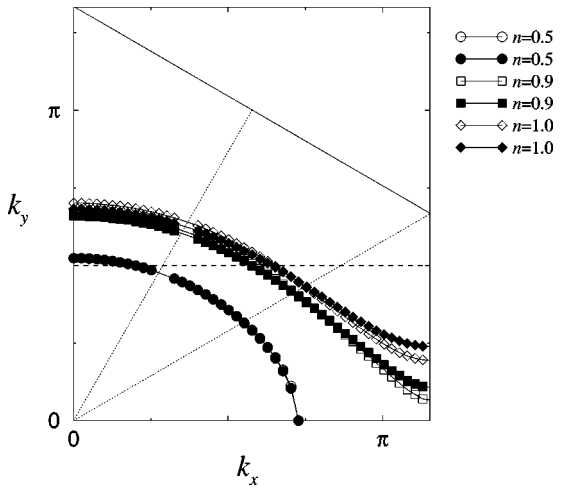

FIG. 3. The noninteracting and interacting Fermi surfaces at various fillings n with $t=0.5$, $t_3=1.0$, and $U=4.0$. The empty and solid symbols denote the noninteracting and interacting Fermi surfaces, respectively. The dashed line is the Fermi surface at half-filling with $t=0$.

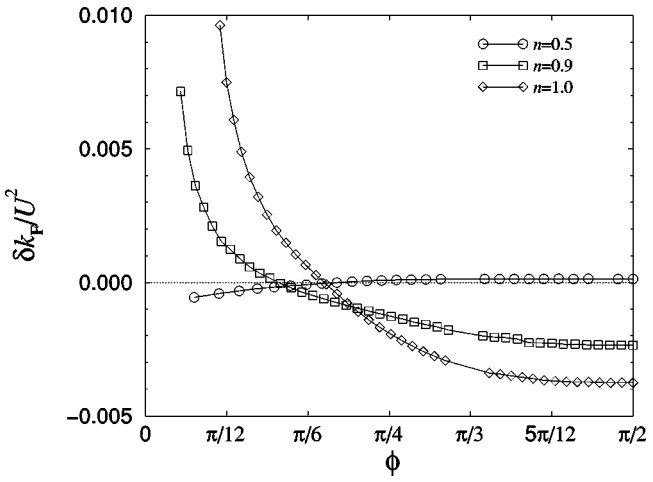

FIG. 4. The angle dependence of the shift of the Fermi surface $\delta k_F/U^2$ at various fillings n with $t=0.5$, $t_3=1.0$, and $U=4.0$.

which is also a function of the angle ϕ. If we expand k_F in the powers of U, the first-order term of U vanishes, then δk_F starts with the second-order term of U. Therefore, in the weak-coupling limit of $U\to 0$, δk_F is proportional to U^2.

Strictly speaking, the Fermi surface of the interacting system must be determined self-consistently from the point of view of the adiabatic continuation, which is the basic concept of the Fermi liquid.[5] In this paper, however, we determine the Fermi surface from the Green's function, which is not self-consistently calculated.

III. CALCULATED RESULTS

We numerically calculate the self-energy directly based on the expression of Eq. (7). These integrals are of the form of the convolution; hence we can carry out the summation of both the momenta and the Matsubara frequencies with use of the algorithm of the fast Fourier transformation.[6] For the momentum, we divide the first Brillouin zone into the mesh of 64×64. On the other hand, for the frequency, we set a sufficiently large cutoff frequency $\omega_c=100$ and divide the range from $-\omega_c$ to ω_c by $n_c=1024$, then the temperature T is given by

$$T=\frac{2\omega_c}{\pi n_c}. \tag{14}$$

Throughout our calculation, we have $T=0.06217$, which is a low enough temperature. For the analytic continuation in the upper half complex plane with respect to the frequency, we make use of the method of the Padé approximant.[7,8] We fix $U=4.0$ throughout our calculation.

In the first place, we show the result for the case without frustration for the antiferromagnetic spin ordering. First, the case of $t<t_3$. We take $t=0.5$ and $t_3=1.0$. The noninteracting and interacting Fermi surfaces at various fillings n are shown in Fig. 3. In order to describe the deformation in a quantitative manner, we show the ϕ dependence of the shift of the Fermi surface $\delta k_F/U^2$ in Fig. 4.

At the filling equal to or close to half-filling, the direction of the deformation is the direction to enhance the anisotropy of the Fermi surface, in other words, the direction toward the Fermi surface at half-filling with $t=0$, whose nesting vector is $Q=(0,\pi)$, which is the wave vector of the antiferromagnetic spin ordering for the triangular lattice with $t=0$. The form of the interacting Fermi surface is determined by the competition between the self-energy $\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(0)$ and the noninteracting dispersion of the band ε_k. Therefore, in this case, $\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(0)$ is more anisotropic than ε_k, which enhances the anisotropy of the Fermi surface. Then, why is the self-energy $\mathrm{Re}\,\Sigma_k^{\mathrm{R}}(0)$ more anisotropic than the original noninteracting dispersion of the band ε_k? The physical interpretation is as follows. When the electrons are easier to move in the third direction than in the first and second directions ($t_3>t$) in the noninteracting system, the effective interaction (the dimensionless coupling constant) is larger in the first and second directions than in the third direction ($U/t>U/t_3$); hence as a result of the many-body effect, the electrons become still harder to move in the first and second directions than in the third direction, which makes the self-energy more anisotropic and enhances the anisotropy of the Fermi surface.

On the other hand, at the small filling, the direction of the deformation is the direction to compensate the anisotropy of the Fermi surface, in other words, the direction toward a circle, although the magnitude of the deformation is smaller than the case of the filling equal to or close to half-filling. The physical interpretation is as follows. When $t_3>t$, the energy cost by the interaction is larger in the third direction than in the first and second directions, which makes the self-energy less anisotropic and compensates the anisotropy of the Fermi surface.

Next, oppositely, the case of $t>t_3$. We take $t=1.0$ and $t_3=0.5$. The noninteracting and interacting Fermi surfaces at various fillings n are shown in Fig. 5, and the ϕ dependence of the shift of the Fermi surface $\delta k_F/U^2$ is shown in Fig. 6. At the filling equal to or close to half-filling, the direction of the deformation is the direction to enhance the anisotropy of the Fermi surface, in other words, the direction toward the Fermi surface at half-filling with $t_3=0$, whose nesting vec-

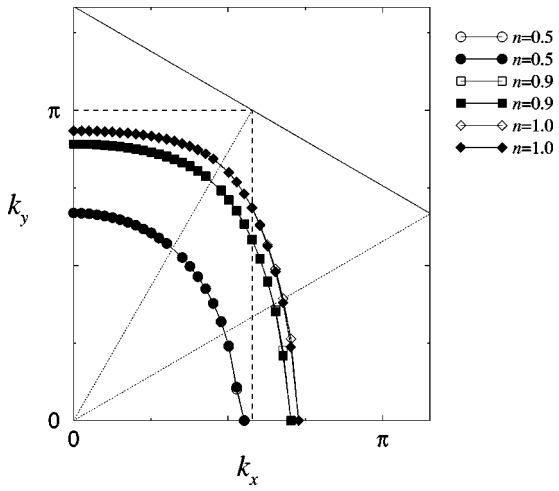

FIG. 5. The noninteracting and interacting Fermi surfaces at various fillings n with $t=1.0$, $t_3=0.5$, and $U=4.0$. The empty and solid symbols denote the noninteracting and interacting Fermi surfaces, respectively. The dashed line is the Fermi surface at half-filling with $t_3=0$.

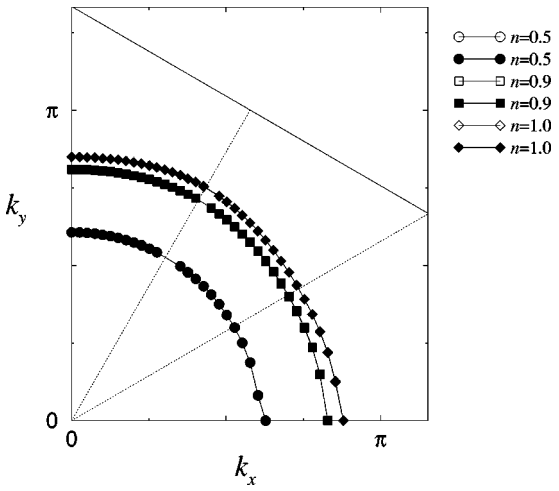

FIG. 7. The noninteracting and interacting Fermi surfaces at various fillings n with $t=t_3=1.0$ and $U=4.0$. The empty and solid symbols denote the noninteracting and interacting Fermi surfaces, respectively.

tors are $Q=(2\pi/\sqrt{3},0),(0,2\pi)$, which are the wave vectors of the antiferromagnetic spin ordering for the triangular lattice with $t_3=0$. On the other hand, at the small filling, the direction of the deformation is the direction to compensate the anisotropy of the Fermi surface.

Finally, we show the result for the case with frustration for the antiferromagnetic spin ordering. We take $t=t_3=1.0$. The noninteracting and interacting Fermi surfaces at various fillings n are shown in Fig. 7, and the ϕ dependence of the shift of the Fermi surface $\delta k_F/U^2$ is shown in Fig. 8. In the case with frustration, no deformation of the Fermi surface is found in the weak-coupling regime.

IV. DISCUSSION

Now, let us reconsider the results for the square lattice with various transfer amplitudes, which have already been obtained by Halboth and Metzner[1] and Zlatić, Entel, and Grabowski.[2] We can express their results in a universal way.

As for the result by Halboth and Metzner[1] for the case with only the nearest-neighbor transfer amplitude t, the direction to enhance the anisotropy of the Fermi surface is nothing but the direction toward the Fermi surface at half-filling, whose nesting vector is $Q=(\pi,\pi)$. This result is not changed by introducing the next-nearest-neighbor transfer amplitude t'. When $t>|t'|$, irrespective of the sign of t', at the filling equal to or close to half-filling, the direction of the deformation is the direction to enhance the anisotropy of the Fermi surface, in other words, the direction toward the Fermi surface at half-filling with $t'=0$, whose nesting vector is $Q=(\pi,\pi)$, which is the wave vector of the antiferromagnetic spin ordering for the square lattice with $t'=0$. This result has been confirmed by the present authors.

As for the result by Zlatić, Entel, and Grabowski[2] for the case with the anisotropic transfer amplitude, namely, the nearest-neighbor transfer amplitude in the x direction t_x and in the y direction t_y, when $t_x>t_y$, the direction to enhance the anisotropy of the Fermi surface is nothing but the direc-

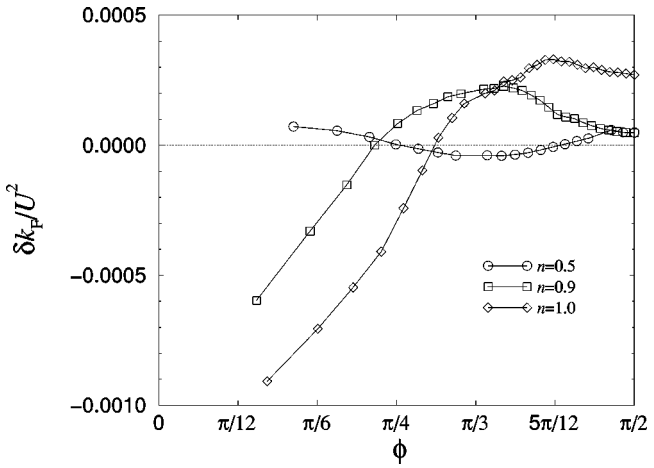

FIG. 6. The angle dependence of the shift of the Fermi surface $\delta k_F/U^2$ at various fillings n with $t=1.0$, $t_3=0.5$, and $U=4.0$.

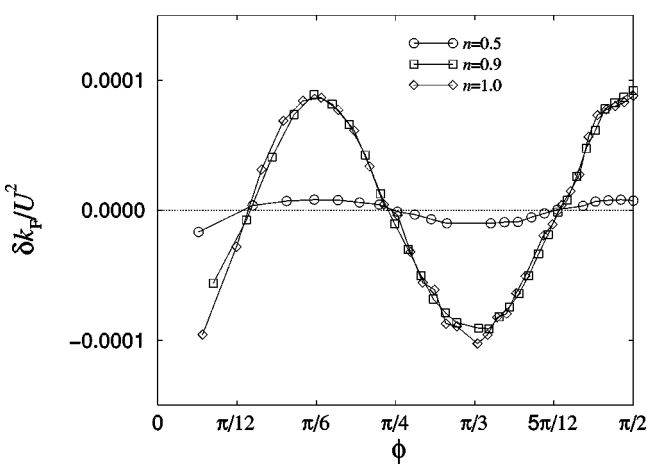

FIG. 8. The angle dependence of the shift of the Fermi surface $\delta k_F/U^2$ at various fillings n with $t=t_3=1.0$ and $U=4.0$.

tion toward the Fermi surface at half-filling with $t_y=0$, whose nesting vector is $Q=(\pi,0)$, which is the wave vector of the antiferromagnetic spin ordering for the square lattice with $t_y=0$.

Unifying these results for the square lattice and our result for the triangular lattice, in the case of the lattice and transfer amplitude without frustration for the antiferromagnetic spin ordering, at the filling equal to or close to half-filling, the direction of the deformation of the Fermi surface is the direction toward the Fermi surface at half-filling with the smaller transfer amplitude set to zero, whose nesting vector is commensurate with the underlying lattice. The interaction has tendency to deform the Fermi surface toward the stronger nesting only for systems without frustration. This statement will be valid generally for all the systems without frustration for the antiferromagnetic spin ordering. This is a universal feature of correlated electron systems, irrespective of microscopic models.

V. CONCLUSION

We have investigated the interaction-induced deformation of the Fermi surface in the two-dimensional Hubbard model on the triangular lattice in the weak-coupling regime within the second-order perturbation theory. Generally in systems without frustration for the antiferromagnetic spin ordering, at the filling equal to or close to half-filling, the direction of the deformation of the Fermi surface is the direction to enhance the anisotropy of the Fermi surface, in other words, the direction toward the Fermi surface at half-filling with the smaller transfer amplitude set to zero, whose nesting vector is commensurate with the underlying lattice. And, at the small filling, the direction of the deformation of the Fermi surface is the direction to compensate the anisotropy of the Fermi surface, in other words, the direction toward a circle. On the other hand, generally in systems with frustration, the Fermi surface is not deformed by the interaction because of the frustration.

*Electronic address: yoda@ton.scphys.kyoto-u.ac.jp

[1] C. J. Halboth and W. Metzner, Z. Phys. B **102**, 501 (1997).
[2] V. Zlatić, P. Entel, and S. Grabowski, Europhys. Lett. **34**, 693 (1996).
[3] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1977).
[4] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).
[5] P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).
[6] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge University Press, New York, 1992), p. 496.
[7] R. W. Haymaker and L. Schlessinger, in *The Padé Approximant in Theoretical Physics*, edited by G. A. Baker, Jr. and J. L. Gammel (Academic Press, New York, 1970), Chap. 11.
[8] H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. **29**, 179 (1977).