

DYNAMICAL MAGNETIC SUSCEPTIBILITY OF THE PERIODIC ANDERSON MODEL IN THE CHAOTIC PHASE APPROXIMATION

© V. V. Val'kov*[†] and D. M. Dzebisashvili*

Using the diagram technique in the atomic representation in the generalized chaotic phase approximation, we solve the problem of calculating the dynamical magnetic susceptibility of the periodic Anderson model in the strong electron correlation regime. We express the dynamical magnetic susceptibility in terms of four Matsubara Green's functions describing partial contributions, which are calculated based on exact solutions of integral equations.

Keywords: periodic Anderson model, generalized chaotic phase approximation, dynamical magnetic susceptibility

1. Introduction

The periodic Anderson model (PAM) is most often used to interpret physical properties of strongly correlated systems (SCS) such as heavy-fermion intermetallics, compounds with mixed valencies, and Kondo insulators. It is fundamentally important when taking fluctuation processes described by the PAM into account to calculate the dynamical magnetic susceptibility (DMS) and clarify its features. In this respect, we recall that the specific temperature dependence of the static magnetic susceptibility is among those experimental factors that allow segregating heavy-fermion compounds (together with Kondo insulators) into a special class of SCS. The features of the frequency dependence of DMS are essential when interpreting experimental data using electron spin resonance [1], [2]. Moreover, it is well known that acquiring theoretical knowledge on those SCS properties that cannot be described by the mean field approximation requires calculating dynamical spin and charge fluctuations. As an example, we note that taking the dynamics of magnetic fluctuations of a localized f subsystem into account turned out to be very important for developing the theory of the s -wave superconductivity phase in skutterudite $\text{LaFe}_4\text{P}_{12}$ [3]. We stress that according to contemporary views on SCS, the spin-fluctuation mechanism of Cooper instability plays the leading role in forming the superconducting phase with an anisotropic order parameter [4]. Finally, we note that analyzing the poles of the DMS allows determining the boundaries of magnetic structure stability domains and constructing phase diagrams of the systems under consideration.

Two factors underlie the method for calculating the DMS in the PAM that we propose here. The first factor is related to the observation that in the regime of an infinite Coulomb repulsion U of two electrons from an f center, the diagram series for the Green's function in the Hubbard model are topologically equivalent to the series for the f -electron functions in the PAM. This equivalence was first established in [5] and then in [6], [7]. The second factor is that the proposed method for calculating the DMS in the framework of the Hubbard operator diagram technique (HDT) [8], [9] was developed for the Hubbard model

*Institute of Physics, Siberian Branch, RAS, Krasnoyarsk, Russia; Siberia Federal University, Krasnoyarsk, Russia, e-mail: vvv@iph.krasn.ru, ddm@iph.krasn.ru.

[†]Siberia State Aerocosmic University, Krasnoyarsk, Russia.

Translated from *Teoreticheskaya i Matematicheskaya Fizika*, Vol. 164, No. 2, pp. 309–320, August, 2010. Original article submitted November 30, 2009; revised February 18, 2010.

at $U = \infty$. In those papers, the series for the spin Green's functions was summed in the generalized chaotic phase approximation (GCPA). In the diagram language, this approximation corresponds to taking all ring diagrams into account. We note that the effectiveness of the chaotic phase approximation was previously demonstrated when constructing the magnetic dielectric theory (see, e.g., [10]) in the framework of the equation-of-motion method for two-time retarded Green's functions.

The abovementioned equivalence of the diagram series for the Green's function in the Hubbard model and for the Green's function for the localized electrons in the PAM [5]–[7] ensures the direct applicability of the ideas in [8], [9] for calculating the f-electron susceptibility in the PAM. In addition to the Green's functions of localized electrons, we calculate the spin Green's functions of the collectivized subsystem and also the mixed Green's functions.

2. The PAM Hamiltonian in the strong electron correlation regime

The PAM Hamiltonian was first proposed in [11] as a generalization of the single-impurity Anderson model [12] to the system of regularly distributed f centers. This model was studied theoretically based on the atomic representation using the HDT and the generating functional method [5], [6], [13]. In the strong electron correlation regime corresponding to a large value of the one-site Coulomb repulsion, we can exclude states with two f electrons localized at the same site from the basis of one-ion states. Using the atomic representation, we can take the above basis reduction into account naturally and then write the PAM Hamiltonian in the form

$$\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_0 + \widehat{\mathcal{H}}_{\text{int}},$$

where

$$\widehat{\mathcal{H}}_0 = \sum_{\vec{k}\sigma} \xi_{\vec{k}\sigma} c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} + \sum_{f\sigma} \widetilde{E}_{\sigma} X_f^{\sigma\sigma}, \quad \widehat{\mathcal{H}}_{\text{int}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}f\sigma} \{V_{\vec{k}} e^{-i\vec{k}\vec{R}_f} c_{\vec{k}\sigma}^{\dagger} X_f^{0\sigma} + \text{c.c.}\}. \quad (1)$$

In the expression for $\widehat{\mathcal{H}}_0$, the first sum describes the ensemble of noninteracting conductivity electrons placed in the external magnetic field H , which removes the degeneracy of the seed energy spectrum ε_k with respect to the value of the projection of the spin momentum $\sigma = \pm 1/2$: $\xi_{\vec{k}\sigma} = \varepsilon_{\vec{k}} - 2\sigma\mu_{\text{B}}H - \mu$, where μ_{B} is the Bohr magneton. The chemical potential μ participates in this expression because we must average over the grand canonical ensemble in what follows. The secondary quantization operators $c_{\vec{k}\sigma}^{\dagger}$ and $c_{\vec{k}\sigma}$ respectively create and annihilate a conductivity electron in the state with the quasimomentum \vec{k} and the spin projection σ . The second term in the Hamiltonian $\widehat{\mathcal{H}}_0$ takes the presence of localized f-electron states with the initial energy E_0 into account. In the magnetic field, the energy of these states contains the Zeeman correction depending on the g -factor: $\widetilde{E}_{\sigma} = E_0 - \sigma h - \mu$, where $h = g\mu_{\text{B}}H$. We use the Hubbard operators in the atomic representation to describe f-ion states: $X_f^{m,n} = |m\rangle\langle n|$. The vector $|n\rangle$ describes the state without electrons for $n = 0$ and the one-electron state with the spin projection σ for $n = \sigma$ ($\sigma = \uparrow, \downarrow$). We forbid the appearance of double-electron states $n = 2$, as noted above. The interaction operator $\widehat{\mathcal{H}}_{\text{int}}$ in (1) is responsible for hybridization processes between collectivized and localized electrons. The matrix element $V_{\vec{k}}$ determines the intensity of these processes. The nondiagonal Hubbard operator $X_f^{0\sigma} = |0\rangle\langle\sigma|$ describes changing the f-ion valency.

3. Spin Green's function of localized electrons

To calculate the DMS of a localized subsystem, we introduce the spin Green's function

$$D_{dd}^{+-}(x-x') = -\langle T_{\tau} \widetilde{X}^{\uparrow\downarrow}(x) \widetilde{X}^{\downarrow\uparrow}(x') \rangle. \quad (2)$$

In this definition, we use the four-dimensional coordinates $x = (\vec{R}_f, \tau)$ and $x' = (\vec{R}_{f'}, \tau')$ for brevity, the Hubbard operators in the Heisenberg representation are $\tilde{X}^\alpha(x) = e^{\tau\widehat{\mathcal{H}}} X_f^\alpha e^{-\tau\widehat{\mathcal{H}}}$, and the angle brackets denote the thermodynamic average with the density matrix $e^{-\beta\widehat{\mathcal{H}}} / \text{Sp}\{e^{-\beta\widehat{\mathcal{H}}}\}$ determined by Hamiltonian (1). As is known [14], in the passage to the interaction representation ($X^\alpha(x) = e^{\tau\widehat{\mathcal{H}}_0} X_f^\alpha e^{-\tau\widehat{\mathcal{H}}_0}$), the scattering matrix

$$S(\beta) = T_\tau e^{-\int_0^\beta d\tau \widehat{\mathcal{H}}_{\text{int}}(\tau)} \quad (3)$$

arises, and Green's function (2) becomes

$$D_{dd}^{+-}(x-x') = -\frac{\langle T_\tau X^{\uparrow\downarrow}(x) X^{\downarrow\uparrow}(x') S(\beta) \rangle_0}{\langle S(\beta) \rangle_0}. \quad (4)$$

The average $\langle \cdot \rangle_0$ is here taken with the density matrix $e^{-\beta\widehat{\mathcal{H}}_0} / \text{Sp}\{e^{-\beta\widehat{\mathcal{H}}_0}\}$ determined by the free-particle Hamiltonian $\widehat{\mathcal{H}}_0$. In formula (3), the operator $\widehat{\mathcal{H}}_{\text{int}}(\tau)$ is also taken in the interaction representation, and the exponent is

$$-\int_0^\beta d\tau \widehat{\mathcal{H}}_{\text{int}}(\tau) = -\int_0^\beta d\tau \frac{1}{\sqrt{N}} \sum_{\vec{p}, f, \sigma} (V_{\vec{p}} e^{-i\vec{p}\vec{R}_f} c_{\vec{p}\sigma}^+(\tau) X_f^{0\sigma}(\tau) + \text{c.c.}). \quad (5)$$

As shown in [5]–[7], we can explicitly pair the secondary-quantized Fermi operators in expression (4). Indeed, we expand the S -matrix in powers of the hybridization interaction and take into account that only expansion terms of even orders contribute. This follows because all means must contain equal numbers of creation and annihilation operators in the normally ordered phase. For the same reason, raising expression (5) to an even power $2n$, we obtain $(2n)!/(n!)^2$ nonzero terms. Pairing all c operators with the c^+ operators, we obtain the new effective scattering matrix

$$\tilde{S}(\beta) = T_\tau e^{-\int dx dx' \sum_\sigma t_\sigma(x-x') X^{\sigma 0}(x) X^{0\sigma}(x')} \quad (6)$$

with the effective integral of localized electron hopping

$$t_\sigma(x-x') = \frac{1}{N} \sum_{\vec{k}} |V_{\vec{k}}|^2 e^{i\vec{k}(\vec{R}_f - \vec{R}_{f'})} G_{\vec{k}\sigma}^{(0)}(\tau - \tau'), \quad (7)$$

which has the Fourier transform

$$t_\sigma(k) = |V_{\vec{k}}|^2 G_{\vec{k}\sigma}^{(0)}(\omega_n). \quad (8)$$

In these terms, the initial propagator of collectivized electrons has the standard form

$$G_{\vec{k}\sigma}^{(0)}(\omega_n) \equiv G_{\vec{k}\sigma}^{(0)} = (i\omega_n - \xi_{\vec{k}\sigma})^{-1}, \quad (9)$$

where $\omega_n = (2n+1)\pi T$, $n = 0, \pm 1, \pm 2, \dots$, is the Matsubara frequency. The c -operator pairing behavior in the expression for the Green's function D_{dd}^{+-} therefore formally corresponds to replacing the scattering matrix $S(\beta) \rightarrow \tilde{S}(\beta)$, and instead of formula (4), we hence obtain the representation

$$D_{dd}^{+-}(x-x') = -\frac{\langle T_\tau X^{\uparrow\downarrow}(x) X^{\downarrow\uparrow}(x') \tilde{S}(\beta) \rangle_0}{\langle \tilde{S}(\beta) \rangle_0}. \quad (10)$$

We note that in this model, the c -operator pairing procedure for all the Green's functions defined on X operators alone means merely replacing $S(\beta) \rightarrow \tilde{S}(\beta)$. If c operators participate in defining the Green's

function, then in addition to changing the S -matrix, we must change the structure of the Green's functions, as is shown in subsequent sections.

Analyzing formulas (6) and (10), we see that the dynamics of electrons of a localized subsystem can be described in the framework of the effective Hubbard model with tunneling integral (7). By virtue of this, we calculate the dynamical susceptibility of the localized subsystem using the results in [8], [9], where the HDT method was used in the GCPA to calculate the spin Green's function for the Hubbard model.

We define the prevalence order of Hubbard operators by the root vector $0\uparrow > 0\downarrow > \uparrow\downarrow$ and introduce the graphic notation

$$\begin{aligned} G_{\uparrow}(x-x') &\Rightarrow x \text{ --- } \blacktriangleleft \text{---} x', & t_{\uparrow}(x-y) &\Rightarrow x \text{ wavy } \blacktriangleleft y, \\ G_{\downarrow}(x-x') &\Rightarrow x \text{ --- } \blacktriangleright \text{---} x', & t_{\downarrow}(x-y) &\Rightarrow x \text{ wavy } \blacktriangleright y. \end{aligned} \quad (11)$$

We here define the fermionic Green's function $G_{\sigma}(x-x')$ such that its Fourier transform satisfies the relation

$$G_{\sigma}(k)P_{\sigma}(k) = \int d(x-x') e^{-ik(x-x')} (-) \langle T_{\tau} \tilde{X}^{0\sigma}(x) \tilde{X}^{\sigma 0}(x') \rangle, \quad (12)$$

where $P_{\sigma}(k)$ is the end factor [15]–[17]. In this notation, we write the diagram series for D_{dd}^{+-} in the form

$$\begin{aligned} D_{dd}^{+-} &= \text{---} \text{---} \odot + \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \blacksquare \text{---} \text{---} + \\ &+ \text{---} \text{---} \blacktriangleleft \text{---} \text{---} \odot + \text{---} \text{---} \blacktriangleright \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \blacktriangleleft \text{---} \text{---} \blacktriangleleft \text{---} \text{---} \text{---} \text{---} . \end{aligned} \quad (13)$$

The spin Green's function, represented here by the double dashed line and denoted by $G_{\uparrow\downarrow}$ in what follows, satisfies the Dyson equation

$$\text{---} \text{---} \text{---} \text{---} = \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} . \quad (14)$$

The thin dashed line corresponds to the initial spin Green's function $g_{\uparrow\downarrow}^{(0)}$ determined from the equation

$$g_{\uparrow\downarrow}^{(0)}(x-x') B^{\uparrow\downarrow} = -\langle T_{\tau} X^{\uparrow\downarrow}(x) X^{\downarrow\uparrow}(x') \rangle_0, \quad (15)$$

where $B^{\uparrow\downarrow} = \langle X^{\uparrow\uparrow} - X^{\downarrow\downarrow} \rangle_0$ is the end factor P_{σ} in the zeroth approximation. In the momentum representation, we have

$$g_{\uparrow\downarrow}^{(0)}(q) = (i\omega_m - h)^{-1}, \quad q = (\vec{q}, \omega_m), \quad \omega_m = 2m\pi T, \quad m = 0, \pm 1, \pm 2, \dots, \quad (16)$$

and correspondingly

$$G_{\uparrow\downarrow}(q) = (i\omega_m - h - \Sigma(q))^{-1}, \quad (17)$$

where $\Sigma(q)$ is the mass operator for the magnon Green's function.

We calculate the four-leg subdiagram $\Gamma(k_1 - q, k_1; k_2 + q, k_2)$ (the black square in diagram (13)) using the GCPA [8], [9], [17]. In this approximation, it satisfies the graphic equation

$$\begin{aligned} \text{---} \text{---} \blacksquare \text{---} \text{---} &= \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} + \\ &+ \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} . \end{aligned} \quad (18)$$

In its analytic form, this equation is

$$\begin{aligned} \Gamma(k_1 - q, k_1; k_2 + q, k_2) &= t_\uparrow(k_1 - q) + t_\downarrow(k_2 + q) + \\ &+ \frac{T}{N} \sum_{k_3} (t_\downarrow(k_3) + t_\uparrow(k_1 - q)) G_\uparrow(k_3 - q) G_\downarrow(k_3) \Gamma(k_3 - q, k_3; k_2 + q, k_2). \end{aligned} \quad (19)$$

Analogously to [8], [9], [17], its solution can be written as

$$\begin{aligned} \Gamma(k_1 - q, k_1; k_2 + q, k_2) &= \frac{1}{d_\perp(q)} [\Phi(q) + t_\uparrow(k_1 - q)(1 - Q(q)) + \\ &+ t_\downarrow(k_2 + q)(1 - \Lambda(q)) + t_\uparrow(k_1 - q)t_\downarrow(k_2 + q)\Pi(q)], \end{aligned} \quad (20)$$

where

$$d_\perp(q) = (1 - Q(q))(1 - \Lambda(q)) - \Pi(q)\Phi(q), \quad (21)$$

$$\begin{pmatrix} \Pi(q) \\ Q(q) \\ \Lambda(q) \\ \Phi(q) \end{pmatrix} = \frac{T}{N} \sum_{k_1} \begin{pmatrix} 1 \\ t_\downarrow(k_1) \\ t_\uparrow(k_1 - q) \\ t_\downarrow(k_1)t_\uparrow(k_1 - q) \end{pmatrix} G_\uparrow(k_1 - q) G_\downarrow(k_1). \quad (22)$$

The diagram expansion for the three-leg subdiagrams $\gamma_\Lambda(k_1 - q, k_1; q)$ and $\gamma_\Pi(q; k_2 + q, k_2)$ in diagram (13) implies that these amplitudes can be expressed in terms of four-leg subdiagram (18):

$$\begin{aligned} & \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3}, \\ & \text{Diagram 4} = \text{Diagram 5} + \text{Diagram 6}. \end{aligned} \quad (23)$$

Using solution (20), we find

$$\begin{aligned} \gamma_\Lambda(k_1 - q, k_1; q) &= \frac{t_\uparrow(k_1 - q)(1 - Q(q)) + \Phi(q)}{d_\perp(q)}, \\ \gamma_\Pi(q; k_2 + q, k_2) &= \frac{t_\downarrow(k_2 + q)(1 - \Lambda(q)) + \Phi(q)}{d_\perp(q)} B_0. \end{aligned} \quad (24)$$

The quantity B_0 , denoted by a small double circle in diagram (23), is determined by the expression

$$B_0 = \langle X^{\uparrow\uparrow} - X^{\downarrow\downarrow} \rangle_0 - f(\tilde{E}_\uparrow) + f(\tilde{E}_\downarrow).$$

The graphic representation for the mass operator Σ in Eq. (14) in this approximation is

$$\text{Diagram 7} = \text{Diagram 8} + \text{Diagram 9} + \text{Diagram 10}. \quad (25)$$

Setting analytic expressions into correspondence with graphs (25), we obtain the mass operator representation

$$\Sigma(q) = \frac{B_0 \Phi(q)}{d_{\perp}(q)} + \delta\mu(h), \quad \delta\mu(h) = \frac{T}{N} \sum_{k_1} [t_{\downarrow}(k_1)G_{\downarrow}(k_1) - t_{\uparrow}(k_1)G_{\uparrow}(k_1)]. \quad (26)$$

Taking the above equations for the four- and three-leg subdiagrams in diagram (13) into account, we find the analytic expression for the Green's function D_{dd}^{+-} , which is known to be related to the DMS of the localized subsystem (after analytic continuation),

$$D_{dd}^{+-}(q) = \frac{\Pi(q) + B_0 \tilde{D}^{(0)}(\omega_m)}{d_{\perp}(q) - \Phi(q)B_0 \tilde{D}^{(0)}(\omega_m)}, \quad (27)$$

where $\tilde{D}^{(0)}(\omega_m) = (i\omega_m - h - \delta\mu(h))^{-1}$. Although the structure of expression (27) formally coincides with that obtained in [8] for the t -model transversal dynamical susceptibility, we must remember that the specific dependences on k and ω_m of the functions in these expressions differ. Moreover, the complete solution of the magnetic susceptibility problem requires calculating three new functions, which were not considered in [8]. We present the solution of this part of the problem in the subsequent sections.

4. Mixed spin Green's functions of localized and collectivized electrons

The complete Matsubara DMS is given by the expression

$$\chi_{\perp}(\tau - \tau') = \langle T_{\tau} \tilde{M}_f^+(\tau) \tilde{M}_f^-(\tau') \rangle,$$

where $M_f^+ = g\mu_B X_f^{\uparrow\downarrow} + 2\mu_B \sigma_f^+$, $M_f^- = g\mu_B X_f^{\downarrow\uparrow} + 2\mu_B \sigma_f^-$, and σ_f^{\pm} is the conductivity electron spin flip operator. Obviously, in addition to the already found D_{dd}^{+-} , calculating χ_{\perp} requires knowing the mixed Green's functions D_{dc}^{+-} and D_{cd}^{+-} defined on the operators $X^{\sigma\bar{\sigma}}$ and σ^{\mp} and also the spin Green's function of the collectivized electrons. In this section, we calculate the first two functions.

The function D_{dc}^{+-} is determined by the expression

$$D_{dc}^{+-}(x - x') = -\langle T_{\tau} \tilde{X}^{\uparrow\downarrow}(x) \tilde{\sigma}^-(x') \rangle. \quad (28)$$

Passing to the interaction representation and taking the relation between the operator $\sigma^-(x')$ and the secondary-quantized operators

$$\sigma^-(x') = \frac{1}{N} \sum_{\bar{k}\bar{k}'} e^{-i\bar{R}_{f'}(\bar{k}-\bar{k}')} c_{\bar{k}\downarrow}^+(\tau') c_{\bar{k}'\uparrow}(\tau') \quad (29)$$

into account, we obtain

$$D_{dc}^{+-}(x - x') = \frac{1}{N} \sum_{\bar{k}\bar{k}'} e^{-i\bar{R}_{f'}(\bar{k}-\bar{k}')} \frac{-\langle T_{\tau} X^{\uparrow\downarrow}(x) c_{\bar{k}\downarrow}^+(\tau') c_{\bar{k}'\uparrow}(\tau') S(\beta) \rangle_0}{\langle S(\beta) \rangle_0}. \quad (30)$$

Pairing the c operators in the obtained expression, we can easily see that as in calculating D_{dd}^{+-} , we obtain the expression for effective S -matrix (6) with effective interaction (7). Because two of the c operators are external, the result of passing to effective interactions does not result in merely replacing $S(\beta) \rightarrow \tilde{S}(\beta)$,

as was the case for the function D_{dd}^{+-} , and additional sums appear. We thus obtain the expression for the Fourier transform of the mixed Green's function D_{dc}^{+-} :

$$D_{dc}^{+-}(q) = \frac{T}{N} \sum_{k_1} V_{\vec{k}_1} G_{k_1 \uparrow}^{(0)} V_{\vec{k}_1 + \vec{q}}^* G_{k_1 + q, \downarrow}^{(0)} F_{\Pi}(q; k_1 + q, k_1). \quad (31)$$

The function $F_{\Pi}(q; k_1 + q, k_1)$ here is the Fourier transform of the two-particle Green's function

$$F_{\Pi}(x; x_n, y_n) = -\langle T_{\tau} X^{\uparrow \downarrow}(x) X^{\downarrow 0}(x_n) X^{0 \uparrow}(y_n) \tilde{S}(\beta) \rangle_{0c}, \quad (32)$$

which is defined by the relation

$$\int dx dx_n dy_n e^{-iqx + ipx_n - ik_1 y_n} F_{\Pi}(x; x_n, y_n) = \frac{N}{T} \delta(k_1 + q - p) F_{\Pi}(q; p, k_1). \quad (33)$$

The subscript c on the right angle bracket in (32) indicates that only connected diagrams are taken into account when calculating this mean by the Wick theorem. We write the graphic series for the function F_{Π} :

$$F_{\Pi} = \text{[Diagrams]} \quad (34)$$

Comparing this expression with Eq. (13), we observe that the analytic contribution of the first six diagrams in (34) is the product of the functions D_{dd}^{+-} and G_{\uparrow} and the remaining four diagrams are expressed in terms of the already known four- and three-leg subdiagrams. Following the HDT rules, we obtain

$$\begin{aligned} F_{\Pi}(q; k_1 + q, k_1) &= D_{dd}^{+-}(q) G_{\uparrow}(k_1) + G_{\uparrow}(k_1) G_{\downarrow}(k_1 + q) F^{0\downarrow} \times \\ &\times \left\{ 1 + G_{\uparrow \downarrow}(q) \gamma_{\Pi}(q; k_1 + q, k_1) + \frac{T}{N} \sum_{k_2} G_{\uparrow}(k_2) G_{\downarrow}(k_2 + q) \times \right. \\ &\times \left. [\Gamma(k_2, k_2 + q; k_1 + q, k_1) + \gamma_{\Lambda}(k_2, k_2 + q; q) G_{\uparrow \downarrow}(q) \gamma_{\Pi}(q; k_1 + q, k_1)] \right\}. \end{aligned} \quad (35)$$

Substituting this relation in Eq. (31), we obtain the desired expression for the mixed Green's function:

$$D_{dc}^{+-}(q) = \frac{(\chi_{1,\downarrow}(q) + \chi_{3,\downarrow}(q) F^{0\downarrow}) [\Pi(q) + B_0 \tilde{D}^{(0)}(\omega_m)] + \chi_{2,\downarrow}(q) F^{0\downarrow} (1 - Q(q))}{d_{\perp}(q) - \Phi(q) B_0 \tilde{D}^{(0)}(\omega_m)}. \quad (36)$$

The new functions χ introduced here are defined by the equations

$$\begin{pmatrix} \chi_{1,\sigma}(q) \\ \chi_{2,\sigma}(q) \\ \chi_{3,\sigma}(q) \end{pmatrix} = \frac{T}{N} \sum_{k_1} V_{\vec{k}_1 - \vec{q}} G_{k_1 - q, \sigma}^{(0)} V_{\vec{k}_1}^* G_{k_1 \sigma}^{(0)} G_{\bar{\sigma}}(k_1 - q) \begin{pmatrix} 1 \\ G_{\sigma}(k_1) \\ G_{\sigma}(k_1) t_{\sigma}(k_1) \end{pmatrix}. \quad (37)$$

We can analogously calculate the second mixed Green's function

$$D_{cd}^{+-}(x-x') = -\langle T_\tau \tilde{\sigma}^+(x) \tilde{X}^{\downarrow\uparrow}(x') \rangle, \quad \sigma^+(x) = \frac{1}{N} \sum_{\vec{k}\vec{k}'} e^{-i\vec{R}_f(\vec{k}-\vec{k}')} c_{\vec{k}\uparrow}^+(\tau) c_{\vec{k}'\downarrow}(\tau). \quad (38)$$

But a simpler way to derive it is to note that the function $D_{dc}^{+-}(x-x')$ becomes $D_{cd}^{+-}(x'-x)$, or $D_{dc}^{+-}(q) \rightarrow D_{cd}^{+-}(-q)$ in the momentum representation, after the change of variable $h \rightarrow -h$ ($\sigma \rightarrow -\sigma$). Because $B_0 \rightarrow -B_0$, $\tilde{D}^{(0)}(\omega_m) \rightarrow -\tilde{D}^{(0)}(\omega_m)$, $Q(q) \leftrightarrow \Lambda(q)$, and $\Pi(q)$ and $\Phi(q)$ remain unchanged under this substitution, we find from expression (36) that

$$D_{cd}^{+-}(q) = \frac{(\chi_{1,\uparrow}(-q) + \chi_{3,\uparrow}(-q)F^{0\uparrow})[\Pi(q) + B_0\tilde{D}^{(0)}(\omega_m)] + \chi_{2,\uparrow}(-q)F^{0\uparrow}(1 - \Lambda(q))}{d_\perp(q) - \Phi(q)B_0\tilde{D}^{(0)}(\omega_m)}. \quad (39)$$

5. The DMS of collectivized electrons in the PAM

The spin Green's function determining the magnetic susceptibility in the conductivity electron subsystem is introduced standardly,

$$D_{cc}^{+-}(x-x') = -\langle T_\tau \tilde{\sigma}^+(x) \tilde{\sigma}^-(x') \rangle. \quad (40)$$

In the interaction representation with (29) taken into account, this function has the form

$$D_{cc}^{+-}(x-x') = \frac{1}{N^2} \sum_{\vec{p}_1 \dots \vec{p}_4} e^{-i(\vec{p}_1 - \vec{p}_2)\vec{R}_f} e^{-i(\vec{p}_3 - \vec{p}_4)\vec{R}_{f'}} \times \\ \times \frac{-1}{\langle S(\beta) \rangle_0} \langle T_\tau c_{\vec{p}_1\uparrow}^+(\tau) c_{\vec{p}_2\downarrow}(\tau) c_{\vec{p}_3\downarrow}^+(\tau') c_{\vec{p}_4\uparrow}(\tau') S(\beta) \rangle_0. \quad (41)$$

The c -operator pairings result in the structure of the expressions for the Fourier transform of the Green's function D_{cc}^{+-} :

$$D_{cc}^{+-}(q) = \frac{T}{N} \sum_{k_1} G_{k_1-q,\uparrow}^{(0)} G_{k_1\downarrow}^{(0)} [1 + t_\downarrow(k_1)D_\downarrow(k_1) + t_\uparrow(k_1-q)D_\uparrow(k_1-q)] + \\ + \left(\frac{T}{N}\right)^2 \sum_{k_1, k_2} V_{\vec{k}_1 - \vec{q}}^* G_{k_1-q,\uparrow}^{(0)} V_{\vec{k}_1} G_{k_1\downarrow}^{(0)} V_{\vec{k}_2 + \vec{q}}^* G_{k_2+q,\downarrow}^{(0)} V_{\vec{k}_2} G_{k_2\uparrow}^{(0)} F(k_1-q, k_1; k_2+q, k_2). \quad (42)$$

Here, $D_\sigma(k) = G_\sigma(k)F^{0\sigma}$ in our approximation, and the Fourier transform $F(k_1, k_2; k_3, k_4)$ of the two-particle Green's function

$$F(x_l, y_l; x_n, y_n) = -\langle T_\tau X^{\uparrow 0}(x_l) X^{0\downarrow}(y_l) X^{\downarrow 0}(x_n) X^{0\uparrow}(y_n) \tilde{S}(\beta) \rangle_{0c} \quad (43)$$

is determined by the relation

$$\int dx_l dy_l dx_n dy_n e^{ik_1 x_l - ik_2 y_l + ik_3 x_n - ik_4 y_n} F_\Lambda(x_l, y_l; x_n, y_n) = \\ = \frac{N}{T} \delta(k_1 - k_2 + k_3 - k_4) F(k_1, k_2; k_3, k_4). \quad (44)$$

The function $F(k_1 - q, k_1; k_2 + q, k_2)$ in the graphical representation is

$$F = \text{[Diagrams]} \quad (45)$$

Taking expression (13) into account, we find that the analytic contribution of the first six diagrams of this series is

$$G_{\downarrow}(k_1)D_{dd}^{+-}(q)G_{\uparrow}(k_2). \quad (46)$$

Taking (34) into account, we find that the contribution of the four diagrams in the third line of (45) is

$$G_{\downarrow}(k_1)(F_{\Pi}(q; k_2 + q, k_2) - D_{dd}^{+-}(q)G_{\uparrow}(k_2)). \quad (47)$$

Analogously, for the four diagrams in the fourth line of (45), we obtain

$$(F_{\Lambda}(k_1 - q, k_1; q) - G_{\downarrow}(k_1)D_{dd}^{+-}(q))G_{\uparrow}(k_2). \quad (48)$$

We calculate the contribution to F of the three last diagrams using the known expressions for the three- and four-leg subdiagrams. Collecting all the terms of series (45) and combining like terms, we obtain the expression for the two-particle Green's function $F(k_1 - q, k_1; k_2 + q, k_2)$:

$$\begin{aligned} F(k_1 - q, k_1; k_2 + q, k_2) = & \\ & = \left(\frac{T}{N}\right)\delta(k_1 - q - k_2)D_{\uparrow}(k_1 - q)D_{\downarrow}(k_2 + q) + \\ & + \frac{G_{\downarrow}(k_1)G_{\uparrow}(k_2)}{d_{\downarrow}(q) - \Phi(q)B_0\tilde{D}^{(0)}(\omega_m)} \{D_{\downarrow}(k_2 + q)(1 - Q(q)) + D_{\uparrow}(k_1 - q)(1 - \Lambda(q)) + \\ & + [\Pi(q) + B_0\tilde{D}^{(0)}(\omega_m)][1 + D_{\uparrow}(k_1 - q)t_{\uparrow}(k_1 - q)][1 + D_{\downarrow}(k_2 + q)t_{\downarrow}(k_2 + q)] + \\ & + D_{\uparrow}(k_1 - q)D_{\downarrow}(k_2 + q)[\Phi(q) + t_{\uparrow}(k_1 - q)(1 - Q(q)) + t_{\downarrow}(k_2 + q)(1 - \Lambda(q))]\}. \end{aligned} \quad (49)$$

Substituting expression (49) in formula (42), we obtain the expression for the desired Green's function

$$\begin{aligned}
D_{cc}^{+-}(q) = & \frac{T}{N} \sum_{k_1} G_{k_1-q,\uparrow}^{(0)} G_{k_1\downarrow}^{(0)} [1 + t_{\downarrow}(k_1)D_{\downarrow}(k_1)] \cdot [1 + t_{\uparrow}(k_1 - q)D_{\uparrow}(k_1 - q)] + \\
& + \left(\frac{T}{N}\right)^2 \sum_{k_1, k_2} V_{k_1-q}^* G_{k_1-q,\uparrow}^{(0)} V_{k_1} G_{k_1\downarrow}^{(0)} V_{k_2+q}^* G_{k_2+q,\downarrow}^{(0)} V_{k_2} G_{k_2\uparrow}^{(0)} \frac{G_{\downarrow}(k_1)G_{\uparrow}(k_2)}{d_{\perp}(q) - \Phi(q)B_0\tilde{D}^{(0)}(\omega_m)} \times \\
& \times \{D_{\downarrow}(k_2 + q)(1 - Q(q)) + D_{\uparrow}(k_1 - q)(1 - \Lambda(q)) + \\
& + [\Pi(q) + B_0\tilde{D}^{(0)}(\omega_m)][1 + D_{\uparrow}(k_1 - q)t_{\uparrow}(k_1 - q)][1 + D_{\downarrow}(k_2 + q)t_{\downarrow}(k_2 + q)] + \\
& + D_{\uparrow}(k_1 - q)D_{\downarrow}(k_2 + q)[\Phi(q) + t_{\uparrow}(k_1 - q)(1 - Q(q)) + t_{\downarrow}(k_2 + q)(1 - \Lambda(q))]\}, \quad (50)
\end{aligned}$$

using which we can study the collectivized electron magnetic susceptibility in the PAM in the regime $U = \infty$.

6. Conclusion

Formulas (27), (36), (39), and (50) solve the considered problem of finding the DMS $\chi(\vec{k}, i\omega_n)$ because $\chi(\vec{k}, i\omega_n)$, as mentioned above, can be expressed in terms of the functions $D_{dd}^{+-}(q)$, $D_{dc}^{+-}(q)$, $D_{cd}^{+-}(q)$, and $D_{cc}^{+-}(q)$. We obtain the specific frequency dependences of $\chi(\vec{k}, i\omega_n)$ on the real axis by analytic continuation from the imaginary frequency axis to the complex plane. The obtained expressions for the partial contributions, which determine susceptibilities for both the localized and collectivized subsystems, then allow obtaining the full DMS even in the case where the localized state g -factor takes arbitrary values.

Acknowledgments. This work was supported in part by the the Presidium of the Russian Academy of Sciences (Program “Quantum Physics of Condensed Matter”), the Siberian Branch of the Russian Academy of Sciences (Interdisciplinary Integration Project No. 53), by the Federal Target Program (“Scientific and Scientific-Pedagogical Resources of Innovated Russia in Years 2009–2013”), and the Russian Foundation for Basic Research (Grant No. 10-02-00251).

REFERENCES

1. P. Schlottmann, *Phys. Rev. B*, **79**, 045104 (2009).
2. E. Abrahams and P. Wolfle, *Phys. Rev. B*, **78**, 104423 (2008).
3. V. V. Val'kov and D. M. Dzebisashvili, *JETP*, **107**, 679–691 (2008).
4. Y. Yanase, T. Jujo, T. Nomura, H. Ikeda, T. Hotta, and K. Yamada, *Phys. Rep.*, **387**, 1–149 (2003); arXiv:cond-mat/0309094v1 (2003).
5. V. A. Moskalenko, *Theor. Math. Phys.*, **110**, 243–255 (1997).
6. Yu. A. Izyumov, N. I. Chashchin, and D. S. Alekseev, *Theory of Strongly Correlated Systems: The Generating Functional Method* [in Russian], RKhD, Izhevsk (2006).
7. V. V. Val'kov and D. M. Dzebisashvili, *JETP Lett.*, **84**, 217–221 (2006).
8. Yu. A. Izyumov and B. M. Letfulov, *J. Phys.: Cond. Mat.*, **2**, 8905–8923 (1990).
9. Yu. A. Izyumov, B. M. Letfulov, E. V. Shipitsyn, M. Bartkowiak, and K. A. Chao, *Phys. Rev. B*, **46**, 15697–15711 (1992).
10. S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* [in Russian], Nauka, Moscow (1975); English transl. prev. ed., Plenum, New York (1967).
11. D. A. Smith, *J. Phys. C*, **1**, 1263–1278 (1968).
12. P. W. Anderson, *Phys. Rev.*, **124**, 41–53 (1961).
13. A. F. Barabanov, K. A. Kikoin, and L. A. Maksimov, *Theor. Math. Phys.*, **25**, 997–1003 (1975).

14. A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* [in Russian], Fizmatlit, Moscow (1962); English transl., Prentice-Hall, Englewood Cliffs, N. J. (1963).
15. R. O. Zaitsev, *Sov. Phys. JETP*, **41**, 100–103 (1975).
16. R. O. Zaitsev, *JETP*, **43**, 574–579 (1976).
17. Yu. A. Izyumov, M. I. Katsnel'son, and Yu. N. Skryabin, *Itinerant Electron Magnetism* [in Russian], Fizmatlit, Moscow (1994).