Quantum critical behavior of antiferromagnetic itinerant systems with van Hove singularities

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The interplay of magnetic and superconducting fluctuations in two-dimensional systems with van Hove singularities in the electronic spectrum is considered within the functional renormalization-group (fRG) approach. While the fRG flow has to be stopped at a certain minimal temperature $T_{\mathrm{RG}}^{\mathrm{min}}$, we study temperature dependence of magnetic and superconducting susceptibilities below $T_{\mathrm{RG}}^{\mathrm{min}}$ to obtain the crossover temperatures to the regime with strong magnetic and superconducting fluctuations. Near half filling we obtain the largest crossover temperature, corresponding to a regime with strong commensurate magnetic fluctuations, which is replaced by a regime with strong incommensurate fluctuations further away from half filling. With further decreasing density the system undergoes quantum phase transition from incommensurate to paramagnetic phase. Similarly to results of Hertz-Moriya-Millis approach, the temperature dependence of the inverse (incommensurate) magnetic susceptibility at the magnetic quantum-critical point is found almost linear in temperature.

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I. INTRODUCTION

The quantum-critical points (QCP) in itinerant magnets have being investigated during long time. Moriya theory[1] was first attempt to describe thermodynamic properties near QCP. This theory was further developed within Hertz-Millis renormalization-group approach.[2] In more than two dimensions Hertz-Moriya-Millis (HMM) approach predicts that the magnetic transition temperature T_c depends on the distance δ to the QCP as $T_c \sim \delta^{z/(d+z-2)}$. In two-dimensional (2D) systems, the long-range magnetic order at finite temperatures is prohibited according to the Mermin-Wagner theorem but the quantum phase transition is accompanied by vanishing of the temperature of the crossover to the regime with exponentially large correlation length (renormalized-classical regime), $T^* \sim \delta$. The applicability of HMM approach to magnetic systems was recently questioned because of expected strong momenta and frequency dependence of the paramagnon interaction vertices[3] and possible nonanalytical dependence of the magnetic susceptibility[4] which arises due to strong electron-paramagnon interaction.

Itinerant systems with van Hove singularities in the electronic spectrum have strong momentum dependence of interaction vertices due to peculiarity of the electronic dispersion, and, therefore represent an interesting example for studying the quantum-critical behavior. The competition of different kinds of fluctuations, and even long-range orders is important in the presence of van Hove singularities, which makes formulation of effective boson-fermion theories rather complicated. Studying the problem of quantum-critical behavior of these systems in terms of fermionic degrees of freedom may be helpful to obtain concentration dependence of the crossover temperature and provide valuable information about their magnetic properties near quantum-critical points. In particular, fermionic approaches can treat naturally both, (anti-) ferromagnetic and superconducting fluctuations, which were considered to be important near magnetic quantum phase transitions in systems with van Hove singularities in the electronic spectrum.

The simplest mean-field analysis of the Hubbard model is insufficient to study quantum-critical behavior; due to locality of the Coulomb repulsion in this model it is also unable to investigate the range of existence of unconventional (e.g., d- or p-wave) superconducting order and introduction of the nearest-neighbor (nn) interaction is required in this approach.[5] To study the competition of magnetism and superconductivity in the Hubbard model, more sophisticated approaches, e.g., cluster methods[6,7] and functional renormalization-group (fRG) approaches[8–11] were used. The fRG approaches are not limited by the system (cluster) size and offer a possibility to study both, magnetic and superconducting fluctuations, as well as their interplay at weak and intermediate coupling.

The fRG approaches were initially applied to the paramagnetic nonsuperconducting (symmetric) phase of two-dimensional systems to study the dominant type of fluctuations in different regions of the phase diagram.[8–11] Although these approaches suffered from the divergence of vertices and susceptibilities at low-enough temperatures near the magnetic or superconducting instabilities, comparing susceptibilities with respect to different types of order at the lowest accessible temperature provided a possibility to deduce instabilities in different regions of the phase diagram. In fact, the temperature where the vertices and susceptibilities diverge in the one-loop approach can be identified with the above discussed temperature T^* of the crossover to the "strong-coupling" regime with exponentially large magnetic correlation length.

To access the region $T < T^*$, the combination of the fRG and mean-field approach was proposed in Ref. 12, which was also able to study possible coexistence of magnetic and superconducting order at $T=0$ (the magnetic order parameter was assumed to be commensurate). More sophisticated fRG approach in the symmetry-broken phase[13] was developed recently to avoid application of the mean-field approach after the RG flow; the application of this method was however so far restricted by the attractive Hubbard model because of complicated structure of the resulting renormalization-group equations.

In the present paper we use the fRG approach in the symmetric phase[10,11] and perform an accurate analysis of temperature dependence of susceptibilities with respect to both, commensurate and incommensurate magnetic order, as well as superconducting order. We propose continuation method which allows us to study thermodynamic properties both above and below the temperature at which the fRG flow is stopped and extract the crossover temperature T^*. This gives us a possibility to obtain phase diagram, capturing substantial part of the fluctuations of magnetic and superconducting order parameters without introducing symmetry breaking. Contrary to the functional renormalization-group analysis in the symmetry broken phase,[13] the presented method can be easily generalized to study instabilities with different types of the order parameters.

II. METHOD

We consider the 2D t-t' Hubbard model $H_\mu = H - (\mu - 4t')N$ with

$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $t_{ij}=t$ for nn sites i, j, and $t_{ij}=-t'$ for next-nn sites $(t,t'>0)$ on a square lattice; for convenience we have shifted the chemical potential μ by $4t'$. We employ the fRG approach for one-particle irreducible generating functional and choose temperature as a natural cut-off parameter as proposed in Ref. 10. This choice of cutoff allows us to account for excitations with momenta far from and close to the Fermi surface. Neglecting the frequency dependence of interaction vertices, the RG differential equation for the interaction vertex $V_T \equiv V(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)$ has the form[10]

$$\frac{dV_T}{dT} = -V_T \circ \frac{dL_{\rm pp}}{dT} \circ V_T + V_T \circ \frac{dL_{\rm ph}}{dT} \circ V_T, \tag{2}$$

where $\circ$ is a short notation for summations over intermediate momenta and spin, momenta $\mathbf{k}_i$ are supposed to fulfill the momentum-conservation law $\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4$

$$L_{\rm ph,pp}(\mathbf{k},\mathbf{k}') = \frac{f_T(\varepsilon_\mathbf{k}) - f_T(\pm \varepsilon_{\mathbf{k}'})}{\varepsilon_\mathbf{k} \mp \varepsilon_{\mathbf{k}'}} \tag{3}$$

and $f_T(\varepsilon)$ is the Fermi function. The upper signs in Eq. (3) stand for the particle-hole ($L_{\rm ph}$) and the lower signs for the particle-particle ($L_{\rm pp}$) bubbles, respectively. Equation (2) is solved with the initial condition $V_{T_0}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)=U$; the initial temperature is chosen as large as $T_0=10^3 t$. The evolution of the vertices with decreasing temperature determines the temperature dependence of the susceptibilities according to[10]

$$\frac{d\chi_m}{dT} = \sum_{\mathbf{k}'} \mathcal{R}^m_{\mathbf{k}'} \mathcal{R}^m_{\pm\mathbf{k}'+\mathbf{q}_m} \frac{dL_{\rm ph,pp}(\mathbf{k}', \pm\mathbf{k}'+\mathbf{q}_m)}{dT},$$

$$\frac{d\mathcal{R}^m_\mathbf{k}}{dT} = \mp \sum_{\mathbf{k}'} \mathcal{R}^m_{\mathbf{k}'} \Gamma^T_m(\mathbf{k},\mathbf{k}') \frac{dL_{\rm ph,pp}(\mathbf{k}', \pm\mathbf{k}'+\mathbf{q}_m)}{dT}. \tag{4}$$

Here the three-point vertices $\mathcal{R}^m_\mathbf{k}$ describe the propagation of an electron in a static external field, m denotes one of the instabilities: antiferromagnetic (AF) with $\mathbf{q}_m=(\pi,\pi)$, incommensurate magnetic ($\mathbf{Q}$) with the wave vector $\mathbf{q}_m=\mathbf{Q}$, or d-wave superconducting (dSC) with $\mathbf{q}_m=0$ (upper signs and ph correspond to the magnetic instabilities, lower signs and pp to the superconducting instability)

$$\Gamma^T_m(\mathbf{k},\mathbf{k}') = \begin{cases} V_T(\mathbf{k},\mathbf{k}',\mathbf{k}'+\mathbf{q}_m) & m=\text{AF or } \mathbf{Q}, \\ V_T(\mathbf{k},-\mathbf{k}+q_m,\mathbf{k}') & m=\text{dSC}. \end{cases} \tag{5}$$

The initial conditions at T_0 for Eqs. (4) are $\mathcal{R}^m_\mathbf{k}=f_\mathbf{k}$ and $\chi_m=0$, where the function $f_\mathbf{k}$ belongs to one of the irreducible representations of the point group of the square lattice, e.g., $f_\mathbf{k}=1$ for the magnetic instabilities and $f_\mathbf{k}=(\cos k_x - \cos k_y)/A$ for the d-wave superconducting instability, with a normalization coefficient $A=(1/N)\Sigma_\mathbf{k} f^2_\mathbf{k}$. To solve the Eqs. (2) and (4) we discretize the momentum space in $N_p=48$ patches using the same patching scheme as in Ref. 10. This reduces the integrodifferential Eqs. (2) and (4) to a set of 5824 differential equations, which were solved numerically. In the present paper we perform the renormalization-group analysis down to the temperature $T^{\rm min}_{\rm RG}$, at which vertices reach some maximal value (we choose $V_{\rm max}=18t$).

To obtain the behavior of the susceptibilities at $T<T^{\rm min}_{\rm RG}$ we continue analytically obtained temperature dependence of the inverse susceptibilities from the temperature region above (but close to) $T^{\rm min}_{\rm RG}$ by polynomials of fifth to seventh order. We identify the crossover temperature T^*_m to the regime of strong correlations of the order parameter denoted by m from the condition that the continued $\chi^{-1}_m(T^*_m)=0$ (we assume that the inverse susceptibilities are almost analytic functions of temperature in the crossover regime). We have verified that the obtained T^*_m essentially depends on neither the order of polynomial, used for the fitting, nor on the fitting range. Studying the behavior of T^*_m as a function of electron density, interaction strength, etc. allows us to obtain the phase diagram.

III. RESULTS

We consider first small interaction strength $U=2.5t$ and $t'=0.1t$. For this value of t' the ground state was previously found unstable with respect to antiferromagnetic order and/or superconductivity at the fillings close to van Hove band filling.[8–11] Temperature dependences of the inverse antiferromagnetic susceptibility $[\mathbf{Q}=(\pi,\pi)]$ together with the results of analytic continuation for different chemical potentials are shown in Fig. 1. One can see that for large enough chemical potential $\mu>\mu^{\rm AF}_c \approx -0.0375t$ ($\mu=0$ corresponds to van Hove band filling), the inverse antiferromagnetic susceptibility monotonously decreases with decreasing temperature and vanishes at a certain temperature $T^*_{\rm AF}$. The value of $T^*_{\rm AF}$ increases with increasing μ.

Study of susceptibilities at the incommensurate wave vectors (see Fig. 2) shows that close to $\mu^{\rm AF}_c$ (in the range

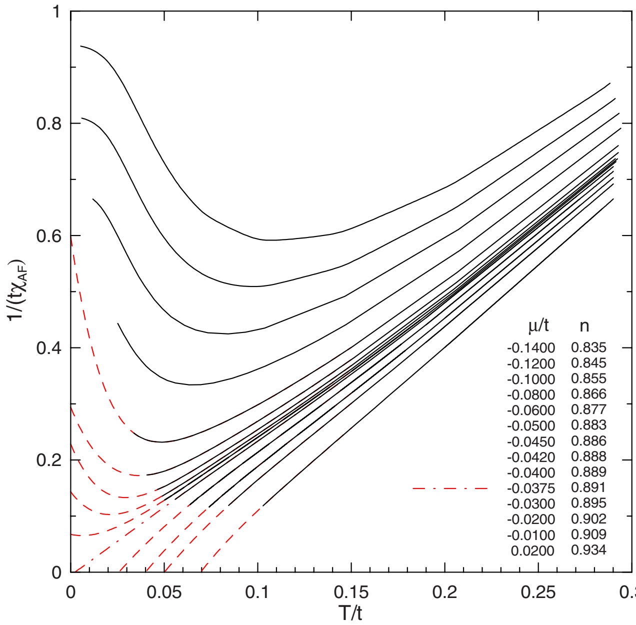

FIG. 1. (Color online) Temperature dependences of the inverse antiferromagnetic susceptibility at $t'/t=0.1$, $U=2.5t$, and different values of the chemical potential (the list of the chemical potentials and fillings corresponds to the curves from top to bottom). Dashed lines show the continuation of the inverse susceptibilities to the temperature region $T<T_{\mathrm{RG}}^{\mathrm{min}}$ by polynomials of 6th order.

$-0.06t<\mu<-0.02t$) we have $T^*_{\mathbf{Q}}>T^*_{\mathrm{AF}}$ for some $\mathbf{Q}=(\pi,\pi-\delta)$. Therefore an instability with respect to incommensurate, rather than a commensurate magnetic order is expected

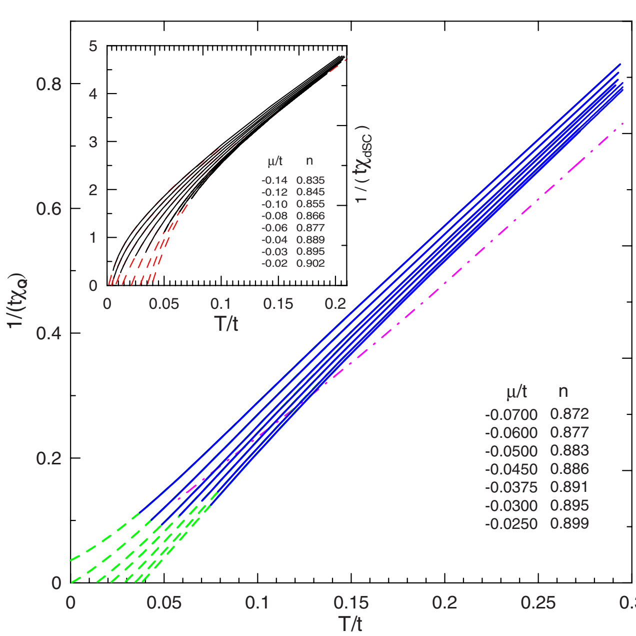

FIG. 2. (Color online) Temperature dependences of the inverse magnetic susceptibility at $t'/t=0.1t$, $U=2.5t$, and the incommensurate wave vector determined by a maximum $T_c^{\mathbf{Q}}$, dashed lines show the continuation to $T<T_{\mathrm{RG}}^{\mathrm{min}}$. Dot-dashed line shows the inverse commensurate susceptibility at $\mu=\mu_c^{\mathrm{AF}}\approx-0.0375t$. The inset shows temperature dependences of the inverse susceptibility with respect to d-wave superconducting pairing at different values of the chemical potential.

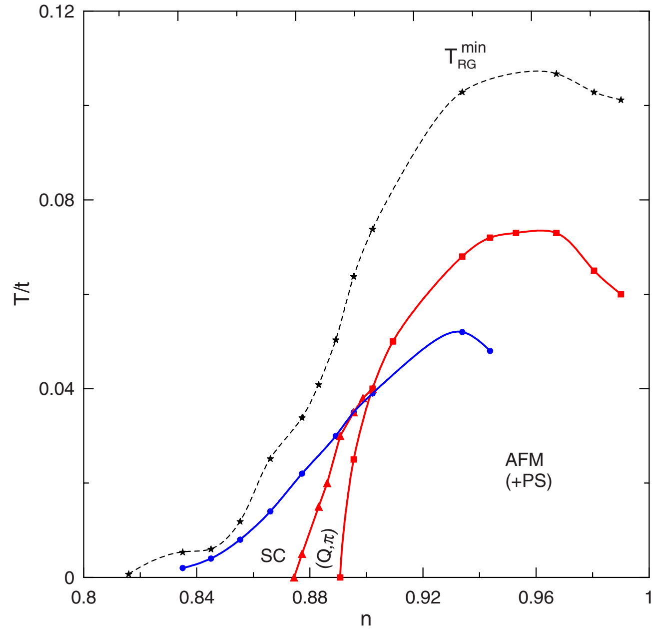

FIG. 3. (Color online) Phase diagram at $t'/t=0.1$ and $U=2.5t$. The temperatures of the crossover into regime with strong antiferromagnetic, incommensurate magnetic, and superconducting fluctuations are marked by squares, triangles, and circles, respectively, PS denotes a possibility of phase separation of the antiferromagnetic phase. Dashed line (stars) show the temperature $T_{\mathrm{RG}}^{\mathrm{min}}$, at which the fRG flow is stopped.

in this interval of μ. At $\mu=\mu_c^{\mathbf{Q}}=-0.06t$ we obtain $T^*_{\mathbf{Q}}=0$, which shows existence of a quantum-critical point below half-filling. Near the quantum-critical point we find $\chi_{\mathbf{Q}}^{-1}\sim T$, which is similar to the result of the Hertz-Moriya-Millis theory.[2,14] The behavior of the inverse susceptibility with respect to the d-wave superconducting order is shown in the inset of Fig. 2. Similarly to the inverse antiferromagnetic susceptibility, it monotonously decreases upon lowering temperature, with a different temperature dependence.

The obtained phase diagram is shown in Fig. 3 and contains regions of strong antiferromagnetic, incommensurate magnetic, and superconducting fluctuations. Away from half-filling the commensurate antiferromagnetic region is expected to be unstable toward phase separation (to hole-rich and hole-poor regions)[15] although this possibility cannot be verified in the present approach. The obtained value of T^*_{dSC} monotonously increases with increasing density for $n\lesssim 0.94$. Deeper in the antiferromagnetic region the superconducting transition temperature is somewhat suppressed. The origin of this suppression comes from the competition between antiferromagnetic and superconducting fluctuations. The coexistence of superconductivity and antiferromagnetism, which is possible in the interval $0.87<n<0.94$, cannot be verified in the present approach.

The region of the incommensurate phase obtained in Fig. 3 is much narrower, than that expected in the mean-field approaches,[16,17] which predict incommensurate instability in the most part of the phase diagram. In fact, accurate mean-field investigations[16,18,19] show, that substantial part of incommensurate state in the mean-field approach is unstable toward phase separation into commensurate and incommen-

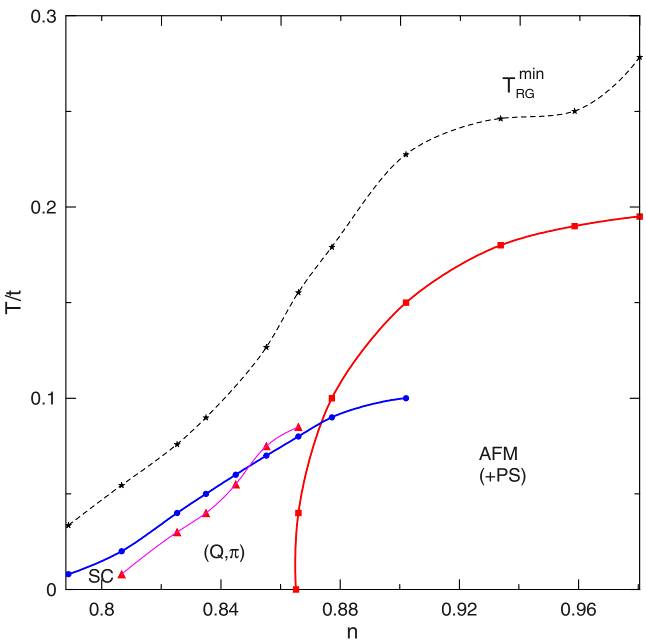

FIG. 4. (Color online) Phase diagram at $t'/t=0.1$ and $U=3.5t$. The notations are the same as in Fig. 3.

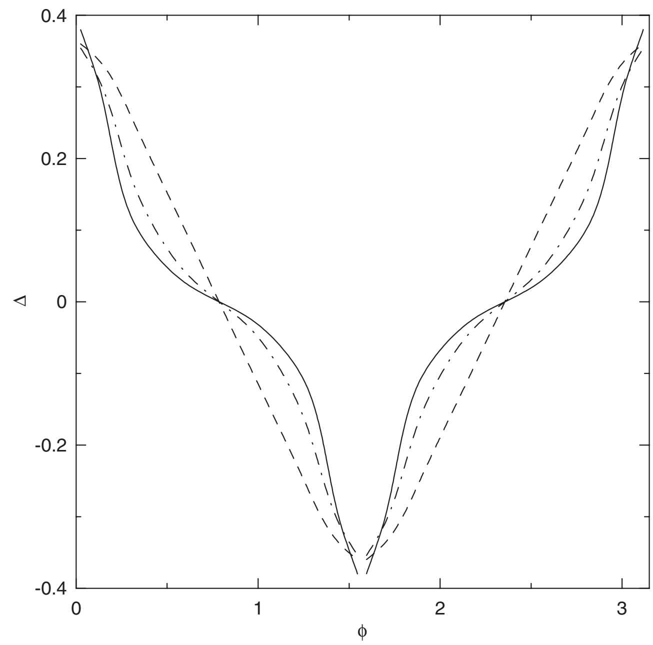

FIG. 5. Angular dependence of the superconducting gap for $U=2.5t$, $n=0.87$ (dot-dashed line) and $U=3.5t$, $n=0.84$ (solid line), $t'/t=0.1$. Dashed line shows the standard $\Delta=(\cos k_x-\cos k_y)/A$ dependence.

surate regions. The presence of incommensurate phases within the renormalization-group approach was noticed previously for $t'=0$ in Ref. 8.

The density dependence of $T^*_{\mathrm{AFM}}(n)$ and $T^*_{\mathrm{dSC}}(n)$, obtained in Fig. 3, is similar to that of the antiferromagnetic and superconducting gap components in the electronic spectrum, $\Delta_{\mathrm{AFM}}(n)$ and $\Delta_{\mathrm{dSC}}(n)$, recently obtained within the combination of functional renormalization-group approach and mean-field theory.[12] Slower decrease in $T^*_{\mathrm{dSC}}(n)$ when going into the antiferromagnetic phase in the present approach is explained by the fact that in the present approach magnetic and superconducting fluctuations are weaker coupled in the absence of spontaneous symmetry breaking since the latter leads to opening a gap in the electronic spectrum at the Fermi surface. Contrary to the study of Ref. 12 we included incommensurate phases in our analysis.

At $U=3.5t$ we obtain similar behavior of the magnetic and superconducting susceptibilities near the quantum-critical point; the resulting phase diagram is shown in Fig. 4. Compared to the case $U=2.5t$, the phase diagram has broader region of the incommensurate phase. The crossover temperature into regime with strong superconducting fluctuations approximately follows that for the incommensurate fluctuations, implying that the superconductivity in this case is possibly caused by incommensurate spin fluctuations. To clarify this point, we plot in Fig. 5 the momentum dependence of the superconducting gap, obtained from the Bethe-Salpeter analysis.[20] We see that the shape of the gap, calculated for $U=3.5t$ shows stronger deviation from the d-wave form, than for $U=2.5t$, which indicates possible role of the incommensurate fluctuations in this case.

IV. CONCLUSION

We have investigated temperature dependence of the commensurate and incommensurate magnetic susceptibilities, as well as the susceptibility with respect to the d-wave pairing in the fRG framework, which allowed us to obtain the phase diagrams of the Hubbard model at different U. We obtain an intermediate region with strong incommensurate fluctuations between the commensurate and paramagnetic regions, the former is characterized by a wave vector $\mathbf{Q}=(\pi,\pi-\delta)$. The size of the incommensurate region increases with increasing interaction strength. The tendency toward incommensurate order near magnetic quantum phase transition comes from the absence of nesting of the Fermi surface at finite t'. The corresponding profile of static noninteracting spin susceptibility $\chi_0(\mathbf{Q})$ is almost flat near $\mathbf{Q}=(\pi,\pi)$ (see, e.g., Ref. 21) showing that one cannot restrict oneself to fluctuations with only one certain $\mathbf{Q}$, as assumed in HMM theory. The obtained size of the incommensurate region is much narrower, than obtained in the mean-field approaches,[16,17] which is explained by existence of a phase separation in these approaches. Near the quantum-critical point the inverse magnetic susceptibility with respect to the preferable order parameter shows in fRG approach almost linear temperature dependence, similar to that in HMM theory. Note that recently the incommensurate magnetic fluctuations were also considered within the renormalization-group approach for fermion-boson model,[22] where similar results were obtained.

While the Mermin-Wagner theorem states no spontaneous breaking of continuos symmetry in two dimensions at finite T, we have obtained finite temperature of vanishing inverse magnetic and superconducting susceptibilities, which is the consequence of the one-loop approximation, considered in Eq. (2). As we argue in Sec. I, the obtained temperatures T^*_m should be considered as a crossover temperature to the regime with strong magnetic fluctuations and exponential increase in the correlation length.

The used method cannot be directly applied to elucidate the type of the order parameter in the ground state since analysis of the temperature region $T<T^*$ necessarily deals with the strong-coupling regime of the fRG flow. To address the problem of the ground-state properties near half-filling, the analysis, which includes treatment of the symmetry-broken phases[12,13] is required. It is remarkable, however, that the filling dependences of the crossover temperatures T_m^* for the antiferromagnetic and superconducting order parameters obtained in the present study are very similar to the filling dependences of the corresponding ground-state order parameters, obtained in the combination of fRG and mean-field approaches.[12]

The patching scheme invoking the projection of the vertices to the Fermi surface, used in the present renormalization-group study, may have some influence on the obtained finite-temperature phase diagram. We expect, however, that this influence does not modify the phase diagram strongly. This is confirmed by the recent two-loop study[23] which necessarily includes corrections to the effect of the projection of vertices and shows that the effects of these corrections and the two-loop corrections to large extent cancel each other.

The nonanalytical corrections to the susceptibility and electron-paramagnon interaction vertices due to peculiar frequency dependence of the electron-paramagnon interaction may become important near quantum phase transition.[3] These corrections are however expected to produce much weaker effect than the effects of the band dispersion considered in the present paper. Investigation of the role of these corrections in the presence of van Hove singularities has to be performed. Application of the method considered in the present paper to ferromagnetic instability and detail comparison of the results of the present approach with the mean-field approach and quasistatic approach of Ref. 18 also has to be performed.

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