Ferromagnetic instability and finite-temperature properties of two-dimensional electron systems with van Hove singularities

A. A. Katanin\textsuperscript{1}, H. Yamase\textsuperscript{2}, and V. Yu. Irkhin\textsuperscript{1}

\textsuperscript{1}Institute of Metal Physics, 620041 Ekaterinburg, Russia
\textsuperscript{2}National Institute for Materials Science, Tsukuba 305-0047, Japan

We study a ferromagnetic tendency in the two-dimensional Hubbard model near van Hove filling by using a functional renormalization-group method. We compute temperature dependences of magnetic susceptibilities including incommensurate magnetism. The ferromagnetic tendency is found to occur in a dome-shaped region around van Hove filling with an asymmetric property: incommensurate magnetism is favored near the edge of the dome above van Hove filling whereas a first-order-like transition to the ferromagnetic ground state is expected below van Hove filling. The dome-shaped phase diagram is well captured in the Stoner theory by invoking a smaller Coulomb interaction. Triplet $p$-wave superconductivity tends to develop at low temperatures inside the dome and extends more than the ferromagnetic region above van Hove filling.

KEYWORDS: ferromagnetism, renormalization group, Stoner theory, incommensurate magnetism, triplet superconductivity, Hubbard model

The stability of itinerant-electron ferromagnetism is an important problem of correlated $d$-electron systems.\textsuperscript{1,2} Stoner proposed a simple approach to treat the ferromagnetic instability, introducing an averaged magnetic field of electrons at each lattice site. His theory is, however, insufficient to describe adequately even magnets with small magnetic moments, especially at finite temperatures. The transition temperatures appear too high in comparison with experimental data and the temperature dependence of the magnetic susceptibility is not described correctly.

Dzyaloshinskii, Kondratenko\textsuperscript{3} and Moriya\textsuperscript{4} proposed the spin-fluctuation theory considering a contribution of paramagnons to thermodynamic properties. They improved the Stoner theory, especially for finite temperature properties of weak and nearly ferromagnetic systems. The condition for ferromagnetic order in the ground state is also corrected by their theory. In the regime of strong Coulomb repulsion the stability of ferromagnetism was considered in the pioneering studies by Nagaoka\textsuperscript{5} and Roth,\textsuperscript{6} which showed the existence of a saturated ferromagnetic region close to half filling and non-saturated ferromagnetism further away from it. The region of the saturated ferromagnetism was investigated in more details within various
approximations in numerous works (see discussion and references in Ref.7).

Two-dimensional systems offer an interesting aspect to study the stability condition of a ferromagnetic ground state and its finite-temperature properties. Because of van Hove singularities in the density of states ferromagnetism can be realized within a one-band model even for moderately small Coulomb repulsion $U$.8) This allows to apply perturbative techniques to this problem to verify and understand results of other approaches. At finite temperatures, the continuous symmetry breaking is absent in two dimensions due to fluctuation effects, resulting in fulfillment of the Mermin-Wagner theorem; the Curie-Weiss law is expected to be accordingly modified.

Another peculiarity of two-dimensional systems is that the ferromagnetic order in two dimensions can be destabilized not only by quantum magnetic fluctuations, e.g., via spin-wave excitations, which are nearly commensurate, but also by incommensurate fluctuations. The importance of incommensurate magnetic fluctuations at weak and moderate Coulomb interaction was recently emphasized within the quasistatic approach,9,10) mean-field theory,11) and a renormalization-group approach.12) These approaches showed that in a large part of the phase diagram spanned by the electron density $n$ and Coulomb interaction $U$ the ferromagnetic order is replaced by an incommensurate one.

Therefore, it is important to consider systematically the effect of commensurate and incommensurate magnetic fluctuations on the ground-state phase diagram and finite temperature properties of ferromagnetism in two dimensions. In an attempt to investigate this problem, we use a functional renormalization-group (fRG) approach in the symmetric phase13–16) and study temperature dependences of magnetic susceptibilities. By extrapolating these results to the limit of zero temperature, one can obtain expected properties such as possible instabilities of the ground state. This procedure was recently applied to studying a possibility of antiferromagnetic and superconducting instabilities near half filling.17)

**Model and method.** We consider the two-dimensional (2D) $t$-$t'$ Hubbard model $H_\mu = H - (\mu - 4t')N$ with

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

where $t_{ij} = t$ for nearest neighbor (nn) sites $i, j$, and $t_{ij} = -t'$ for next-nn sites ($t, t' > 0$) on a square lattice; $c_{i\sigma}^\dagger(c_{i\sigma})$ creates (annihilates) an electron with spin $\sigma$ at $i$ site; $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and $N = \sum_i n_{i\sigma}$. For convenience we have shifted the chemical potential $\mu$ by $4t'$. We choose $t'/t = 0.45$ as a typical value, for which the ferromagnetic instability is favored.15,16,18) We employ the fRG approach for the one-particle irreducible generating functional and choose the
temperature $T$ as a natural cutoff parameter as proposed in Ref.\textsuperscript{15} Neglecting the frequency dependence of interaction vertices, the RG differential equation for the interaction vertex $V_T = V(k_1, k_2, k_3, k_4)$ (with the momenta $k_i$, which are supposed to fulfill the conservation law $k_1 + k_2 = k_3 + k_4$) has the form\textsuperscript{15–17}

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

where $\circ$ is a short notation for summations over intermediate momenta and spins, $L_{ph,pp}$ stand for particle-hole and particle-particle bubbles. The ferromagnetic (FM), triplet $p$-wave superconducting ($p$SC) and incommensurate magnetic ($Q$) susceptibilities can be calculated as

$$\frac{d\chi_m}{dT} = \sum_{k'} R^m_{k', \pm k + q_m} R^m_{k', \pm k + q_m} \frac{dL_{ph,pp}(k'; q_m)}{dT}, \quad (3)$$

$$\frac{dR^m_{k, \pm k - q_m}}{dT} = \pm \sum_{k'} R^m_{k', \pm k + q_m} \Gamma^T_m(k, k') \frac{dL_{ph,pp}(k'; q_m)}{dT},$$

where the three-point vertices $R^m_{k, k'}$ describe the propagation of an electron in a static external field, $m$ denotes a type of instability, $q_{FM, pSC} = 0$ and $q_Q = Q$; upper signs and ph correspond to the magnetic instabilities, lower signs and pp to the superconducting instability;

$$\Gamma^T_m(k, k') = \begin{cases} V(k, k', k' + q_m, k - q_m) & m = FM \text{ or } Q, \\ V(k, -k, k', -k') & m = pSC. \end{cases} \quad (4)$$

Eqs. (2) and (3) are solved with the initial conditions $V_{T_0}(k_1, k_2, k_3, k_4) = U$, $R^m_{k, k' - q_m} = f_k$ and $\chi_m = 0$; the initial temperature is chosen as large as $T_0 = 10^4 t$. The function $f_k$ belongs to one of the irreducible representations of the point group of the square lattice, i.e., $f_k = 1$ for the magnetic instabilities and $f_k = \sin k_{x,y}/A$ for the $p$SC, with $A$ being a normalization coefficient. We also discretize the momentum space in $N_p = 48$ patches using the same patching scheme as in Ref.\textsuperscript{15} This reduces the integro-differential equations (2) and (3) 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 $T_{RG}^{\text{min}}$, where vertices reach a maximal value; we choose $V_{\text{max}} = 18t$. To characterize the strength of fluctuations of the order parameter $m$, we introduce the temperature $T_m$ which is defined by the condition $\chi_m^{-1}(T_m) = 0$. Here $\chi_m^{-1}(T)$ is the inverse susceptibility of the order parameter $m$, analytically extrapolated to the region $T < T_{RG}^{\text{min}}$ (see Ref.\textsuperscript{17} for details). We interpret $T_m$ as a crossover temperature to the regime of strong correlations rather than a phase transition temperature, since the finite temperature transition is prohibited by the Mermin-Wagner theorem, inducing non-analytical corrections to...
susceptibilities, e.g., $\chi_{FM}^{-1}(T) \propto e^{-A_{FM}Q/T}$ at low $T$ as a consequence of an exponentially large correlation length (see, e.g., Ref.19).

To compare the obtained results with the Stoner theory we also study Hamiltonian (1) in the mean-field approximation, by decoupling $n_{i\uparrow}n_{i\downarrow} \to \langle n_{\uparrow} \rangle n_{\downarrow} + n_{\downarrow} \langle n_{\uparrow} \rangle - \langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle$. The second-order transition temperature (Curie temperature) is obtained by the condition $\chi_{FM}^{-1}(T_{C}^{MF}) = 0$. To search for possible first-order transitions, we also compute the Landau free energy as a function of magnetization for fixed chemical potentials.

**Results.** In Fig. 1(a) we present the results of the fRG approach for the inverse magnetic susceptibilities, obtained at $U = 4t$ and different fillings above van Hove filling $n = 0.465$ ($\mu = 0$). Above the crossover temperature the susceptibilities follow approximately the Curie-Weiss law with Curie temperatures replaced by $T_{FM}^{*}$. With increasing $\mu$, the inverse susceptibilities increase, indicating that ferromagnetic fluctuations are weakened. Consequently, the crossover temperature $T_{FM}^{*}$ decreases and vanishes at $\mu \simeq 0.052t$, implying the quantum phase transition from the ferromagnetic to paramagnetic phase. This transition is, however, likely preempted by entering into the phase with strong incommensurate fluctuations, since we confirmed by calculations of $\chi_{Q}$, which yield results similar to Fig. 1(a), that in the range $\mu \in (0.05, 0.055)t$ a condition $T_{Q}^{*} > T_{FM}^{*}$ is fulfilled for some of the vectors $Q = (Q, Q)$ with small $Q$. Therefore, for the ground state above van Hove filling one can expect two successive quantum phase transitions: from the ferromagnetic to an incommensurate and then to the paramagnetic phase with increasing $\mu$. A direct phase transition from the ferromagnetic to paramagnetic phase having strong incommensurate magnetic fluctuations is yet also possible. Further away from van Hove filling we obtain a non-monotonic temperature dependence of the inverse susceptibility with a minimum, which is followed by a maximum for $\mu \in (0.065, 0.085)t$. While the minima of the inverse susceptibility away from van Hove filling are produced by thermal excitations of states near van Hove singularity, an interpretation of the maxima which possibly yield a ‘reappearance’ of magnetic order far away from van Hove filling is not so straightforward. We return to the discussion of this peculiarity below. Even further away from van Hove filling ($\mu > 0.09t$) the flow can be continued down to very low temperatures, such that $T_{RG}^{\min} \approx 0$.

Let us consider now the situation below van Hove filling, which is distinct from the situation above van Hove filling. The obtained temperature dependence of the inverse susceptibilities [see Fig. 1(b)] shows larger bending than that for the Fermi level above van Hove filling; the inverse susceptibilities show deviations from the Curie-Weiss law already at $T > T_{FM}^{*}$. Moreover, the obtained crossover temperature $T_{FM}^{*}$ sharply drops to zero at $\mu \simeq -0.065t$. The
Fig. 1. (Color online) Temperature dependences of the inverse magnetic susceptibility at $U = 4t$ and different values of the chemical potential (marked by numbers) for the Fermi level above (a) and below (b) van Hove energy. Dots denote the temperature $T_{\text{RG}}^{\text{min}}$, at which the fRG flow is stopped; note that $T_{\text{RG}}^{\text{min}} \approx 0$ for $\mu = 0.10t$. Below $T_{\text{RG}}^{\text{min}}$, the susceptibility is analytically extrapolated.

Precise form of the dependence of $T_{\text{FM}}^{*}(\mu)$ in this region depends on the details of analytical extrapolation. One can obtain either discontinuous or sharp continuous transition with vanishing $T_{\text{FM}}^{*}$. Since $T_{\text{FM}}^{*}$ should be interpreted as a crossover temperature characterizing magnetic properties of the ground state in a 2D system, this necessarily implies a sharp change of those around $\mu \approx -0.065t$, in particular a possibility of a first-order phase transition from the ferromagnetic to paramagnetic ground state. Studying the susceptibilities of incommensurate magnetic orders shows that we always obtain $T_{Q}^{*} < T_{\text{FM}}^{*}$ below van Hove filling, i.e., incommensurate magnetic fluctuations are not expected to change our conclusion.

The resulting finite-temperature phase diagram in the $T-\mu$ variables is shown in Fig. 2. $T_{\text{FM}}^{*}$ forms a dome-shaped line, which is asymmetric with respect to the van Hove energy ($\mu = 0$). The incommensurate magnetic tendency occurs near the edge of the dome above the van Hove energy whereas such a feature is not seen below the van Hove energy and instead a first-order-like transition to (commensurate) ferromagnetism is expected as a ground state. In Fig. 2, we also plot $T_{\text{RG}}^{\text{min}}(\mu)$, which is usually interpreted as a crossover temperature to an ordering tendency, by rescaling both temperature and $\mu$ by a factor of $1.6$. The line of $T_{\text{RG}}^{\text{min}}$ almost coincides with that of $T_{\text{FM}}^{*}$, which suggests that our extrapolation procedure to obtain $T_{\text{FM}}^{*}$ is performed in a reasonable way. Employing the same extrapolation procedure for the non-monotonic dependence of the inverse susceptibilities seen in Fig. 1(a) around $\mu \simeq 0.07t$, we obtain the ‘second’, tiny, ferromagnetic region as shown in Fig. 2. We are however not aware of the physical explanation of this possible ‘reappearance’ of ferromagnetic
order, and leave it for future studies.

Since triplet superconductivity is expected around a ferromagnetic state,\textsuperscript{15} we also compute $\chi_{pSC}$ as a function of $T$ in the same fashion of Fig. 1. In Fig. 2 we plot $T_{pSC}^*$, which, similar to previous results,\textsuperscript{15} is smaller than $T_{FM}^*$ around van Hove filling and survives even far above van Hove filling, where $p$-wave superconductivity is therefore expected in the ground state. On the other hand, we do not find an appreciable $T_{pSC}^*$ away from the ferromagnetic phase below van Hove filling. In the region $\mu \in (-0.07, 0.05)t$ the coexistence of ferromagnetism and $p$-wave superconductivity is possible, which is a subject of future studies.

![Phase Diagram](image)

**Fig. 2.** (Color online) Phase diagram obtained in the fRG study for $U = 4t$ in the plane of $\mu$ and $T$. PM denotes the paramagnetic phase.

We now compare the fRG results to those obtained in the Stoner theory, which considers only a (commensurate) ferromagnetic instability. Since the Stoner theory predicts much higher transition temperatures $T_{CMF}^*$ and a much broader concentration range of ferromagnetism, we consider smaller $U = U^{\text{eff}}$, which is chosen such that $\max_{\mu} T_{CMF}^*(\mu; U^{\text{eff}}) = \max_{\mu} T_{FM}^*(\mu; U)$. For $U = 4t$ we obtain $U^{\text{eff}} \simeq 1.7t$. This renormalization of $U$ is due to fluctuations, mainly caused by particle-particle scattering processes, similar to the original idea by Kanamori.\textsuperscript{20} In Fig. 3, we see that not only the height, but also the position and the width of the ferromagnetic region are in good agreement with those in the fRG approach. Furthermore, below van Hove filling, the possibility of the first-order-phase transition as a function of $\mu$ (Fig. 2) within the fRG is also in agreement with the results of ‘renormalized’ Stoner theory, since such a transition is transformed to a phase separation in terms of electronic density.\textsuperscript{10, 21} Above
van Hove filling the renormalized Stoner theory yields a region of phase separation, while the fRG predicts the strong tendency of incommensurate magnetism in the corresponding region. Except for this difference, it is remarkable that the ferromagnetic tendency obtained in the fRG is captured very well in the renormalized Stoner theory with $U^{\text{eff}}$, which is $n$ and $T$-independent.

Considering incommensurate magnetic order in the mean-field theory yields a variety of the ground states in the plane of $n$ and $U$, as revealed in Ref.\cite{11}. In particular, the mean-field theory\cite{11} already predicts incommensurate magnetism above van Hove filling and (commensurate) ferromagnetism roughly below it, for $U = 4t$ the ground state changes at $n = 0.55$ through a second-order transition. Naturally, the mean-field treatment of Ref.\cite{11} predicts magnetic order in a very broad region ($0 < n < 0.9$), which is obviously an overestimation, typical for a mean-field theory. In particular, a broad incommensurate region ($0.55 < n < 0.9$) is replaced by a very narrow region with strong incommensurate fluctuations in the fRG approach. Finally we find that the positions of the quantum phase transitions obtained in the fRG approach show reasonable agreement with the results of $T$-matrix approach\cite{22}. The $T$-matrix approach, however, misses the importance of incommensurate magnetic fluctuations above van Hove filling.

Conclusion. We have studied finite temperature phase diagrams and possible ground-state properties of the one-band Hubbard model at different chemical potentials or fillings. The results are compared to those in the Stoner theory, including a possibility of incommensurate

---

Fig. 3. (Color online) Comparison of the fRG phase diagram in the $n$-$T$ coordinates with the Stoner theory and with the ground-state results of mean-field approach including incommensurate magnetic orders\cite{11} and $T$-matrix approximation\cite{22}. PS denotes a region of phase separation.
magnetic order. We have found that a ferromagnetic tendency occurs in a dome-shaped region around van Hove filling in an asymmetric way: incommensurate magnetism is favored near the edge of the dome above van Hove filling, whereas a first-order-like transition to a (commensurate) ferromagnetic ground state is expected below van Hove filling. The verification of the first-order transition however requires further development of the present fRG approach, e.g., its extension to the symmetry-broken phase. At finite temperatures we observe deviations from the Curie-Weiss behaviour of susceptibilities, which are mostly pronounced below van Hove filling and seen already above the temperature of the crossover to the regime of strong magnetic correlations. In agreement with previous studies, a ferromagnetic tendency is accompanied by development of triplet superconductivity at low temperatures. While our study indicates a pure $p$-wave superconducting state far above van Hove filling, we cannot address whether the ground state is the coexistence of ferromagnetism and triplet superconductivity in a region where a ferromagnetic tendency also occurs. Given that the coexistence is actually observed for various U-based compounds such as UGe$_2$,$^{23}$ URhGe$^{24}$ and UCoGe,$^{25}$ it is an interesting subject to elucidate a possible coexistence of ferromagnetism and $p$-wave superconductivity in the ground state of the Hubbard model near van Hove filling.

Acknowledgements. The authors thank J. Bauer for valuable comments.
References

1) S.V. Vonsovski: Magnetism (Wiley, New York, 1974).
2) V.Yu. Irkhin and Yu.P. Irkhin: Electronic structure, correlation effects and properties of d- and f-metals and their compounds (Cambridge International Science Publishing, 2007).
3) I. E. Dzyaloshinskii and P. S. Kondratenko: Sov. Phys. JETP 43 (1976) 1036.
4) T. Moriya: Spin Fluctuations in Itinerant Electron Magnetism (Springer-Verlag, Berlin, 1985).
5) Y. Nagaoka: Phys. Rev. 147 (1966) 392.
6) L. M. Roth: Phys. Rev. 184 (1969) 451; 186 (1969) 428.
7) M.I. Katsnelson et al., Rev. Mod. Phys. 80 (2008) 315.
8) This also applies to the three-dimensional lattices with the lines of van Hove singularities, leading to divergent density of states, see S. V. Vonsovskii, M. I. Katsnelson, and A. V. Trefilov: Fiz. Metallov. Metalloved. 76 [3] (1993) 4; [4] (1993) 3. We do not however consider this situation in the present paper, since, as a rule, it requires also treatment of multi-band effects.
9) P. A. Igoshev, A. A. Katanin, and V. Yu. Irkhin: Sov. Phys. JETP 105 (2007) 1043.
10) P. A. Igoshev, A. A. Katanin, H. Yamase, and V. Yu. Irkhin: J. Magn. Magn. Mater. 321 (2009) 899.
11) P. A. Igoshev et al.: Phys. Rev. B 81 (2010) 094407.
12) P. A. Igoshev, V. Irkhin, and A. A. Katanin: arXiv: 1012.0125.
13) C. J. Halboth and W. Metzner: Phys. Rev. B 61 (2000) 7364.
14) C. Honerkamp, M. Salmhofer, N. Furukawa, and T. M. Rice: Phys. Rev. B 63 (2001) 035109.
15) C. Honerkamp and M. Salmhofer: Phys. Rev. Lett. 87 (2001) 187004; Phys. Rev. B 64 (2001) 184516.
16) A. A. Katanin and A. P. Kampf: Phys. Rev. B 68 (2003) 195101.
17) A. A. Katanin: Phys. Rev. B 81 (2010) 165118.
18) C. Husemann and M. Salmhofer: Phys. Rev. B 79 (2009) 195125.
19) Y. M. Vilk and A.-M.S. Tremblay: J. Phys. I (France) 7 (1997) 1309.
20) T. Kanamori: Prog. Theor. Phys. 30 (1963) 275.
21) H. Yamase, V. Oganesyan, and W. Metzner: Phys. Rev. B 72 (2005) 35114.
22) R. Hlubina: Phys. Rev. B 59 (1999) 9600.
23) S. S. Saxena et al.: Nature 406 (2000) 587.
24) D. Aoki et al.: Nature 413 (2001) 613.
25) N. T. Huy et al.: Phys. Rev. Lett. 99 (2007) 067007.