# Effect of paramagnetic fluctuations on a Fermi-surface topological transition in two dimensions

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We study the Fermi-surface topological transition of the pocket-opening type in a two-dimensional Fermi liquid. We find that the paramagnetic fluctuations in an interacting Fermi liquid typically drive the transition first order at zero temperature. We first gain insight from a calculation using second-order perturbation theory in the self-energy. This is valid for weak interaction and far from instabilities. We then extend the results to stronger interaction, using the self-consistent fluctuation approximation. Experimental signatures are given in light of our results.

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## I. INTRODUCTION

Fermi-surface reconstruction has been a subject of fundamental interest in the theory of metals for a long time. In noninteracting models, the Lifshitz transition [1] is a well-known example of a Fermi-surface topological transition (FSTT), where the Fermi surface (FS) changes its topology when some external parameter (for example, pressure) is varied. Such FSTTs may change the number of FSs (for example, in a pocket-opening transition) or the nature of a single FS (for example, in a neck-closing transition) [1,2]. An important characteristic of these transitions, however, is that they occur *without* symmetry breaking.

Rather than considering an external agent, one may further ask if such FS deformations can occur as a function of some interaction strength. In this case, one may have symmetry-breaking transitions (Pomeranchuk instabilities [3,4]), as well as non-symmetry-breaking deformations, which were predicted in early works [5,6]. It has since been understood that Pomeranchuk and interaction-driven topological transitions can be put on the same footing [7]. It is then natural to look for a unified theory of the noninteracting Lifshitz FSTTs tuned by an external agent and the FS distortions induced by interactions.

The interest regarding FSTTs in solids has surged recently, with a plethora of both theoretical [4,7–15] and experimental [16,17] works in contexts ranging from nematic phases in cold atoms [8,9] to antiferromagnetic fluctuations in cuprates [15]. In this work, we address the general effects of paramagnetic (PM) fluctuations on a FSTT, specifically asking what the order of the transition is and what the experimental signatures are. The answers to these questions are crucial for the understanding of a number of materials. This study is partially motivated by the layered material $Na_xCoO_2$, which is known both to contain strong PM fluctuations and to have a band structure that admits a FSTT as a function of doping [17].

The fundamental physical feature of the problem is a noninteracting dispersion relation which leads to a large (and, for simplicity, circular) FS in two dimensions (2D) with the chemical potential close to the energy dispersion relation at the center of the band (i.e. $\mu \approx 0$), as shown in Fig. 1, so that in the noninteracting case, a small FS (pocket) may appear as a function of doping. In the following, we will calculate the effect of short-range interactions on this FSTT. We seek to characterize this transition and show its signatures in various physical quantities. Therefore, this paper is organized as follows. We present the model, followed by the second-order perturbation theory, in order to illustrate the equations and the strategy; then we focus on the region of paramagnetic fluctuations. Finally, we discuss experimental consequences and conclusions.

## II. MODEL

The system we consider is a Fermi liquid (FL) with short-range interactions (Hubbard type for simplicity). The Hamiltonian becomes $H = \sum_{\sigma=\uparrow,\downarrow} \int d^2k/(2\pi)^2 [\epsilon(\mathbf{k}) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U n_\uparrow(\mathbf{k}) n_\downarrow(-\mathbf{k})]$, where $\epsilon(\mathbf{k})$ is a model-dependent bare dispersion relation, $c^\dagger_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}$ are the creation and annihilation operators in momentum space, and $n_\sigma(\mathbf{q}) = \int \frac{d^2k}{(2\pi)^2} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma}$ is the density of electrons with spin $\sigma = \uparrow, \downarrow$. As is typical in field theories in 2D, we assume an essential cutoff momentum for the interaction $\Lambda$ [18]. This cutoff can be physically related to any of the usual ultraviolet cutoffs in solid-state models, such as the inverse lattice constant of a lattice model or the inverse screening length of a more realistic short-range potential.

Our results depend only on the behavior of $\epsilon(\mathbf{k})$ close to the two FSs. Therefore, the dispersion close to the center of the FS can be approximated in dimensionless units by $\epsilon_2(\mathbf{k}) = -\frac{k^2}{2}$, while for the large circular FS the dispersion, including the curvature term, is $\epsilon_1(\mathbf{k}) = v_{F1}(|k| - 1) + \frac{(k-1)^2}{2m_1}$ (we use units where $k_{F1} = 1$ at $\mu = 0$ and $m_2 = 1$). Without interactions, the pocket appears continuously by changing the doping (chemical potential $\mu$); the magnitude of its Fermi vector is denoted by $k_{F2}$. With interactions, however, there is competition between the kinetic energy $E_{\text{kin}} \sim k^2_{F2}$ and the interaction contribution

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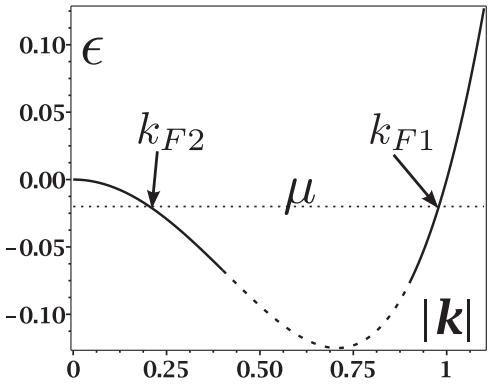


FIG. 1. Schematic representation of the bare dispersion.

to the self-energy; this competition is crucial in determining whether one may add a particle to the small FS or not.

### III. SECOND-ORDER PERTURBATION THEORY

It is instructive to first study the self-energy to second order in perturbation theory (SOPT) far from any symmetry-breaking instabilities and for very weak interaction. We use the developed insight to concentrate on the region of paramagnons near a ferromagnetic (FM) instability, which is the central part of this work.

To first order in perturbation theory, we obtain the Hartree self-energy $\Sigma(k_F,\Omega=0)=Un/2$ (the Fock term is zero), which can be absorbed in $\mu$. Thus, the first nontrivial order is therefore the SOPT:

$$\Sigma(k_F,\omega=0)=U^2\int\frac{d^2q d\omega'}{(2\pi)^3}G(\mathbf{k_F}+\mathbf{q},i\omega')\chi_0(-\mathbf{q},-i\omega'), \tag{1}$$

where $\chi_0$ is the susceptibility of free fermions (frequencies $\omega$ are measured with respect to the chemical potential).

Assuming the onset of a small FS, $\chi_0$ contains contributions from both the large and small FSs. It turns out, however, that the important physics we want to reveal occurs at the small FS, so we initially ignore the large FS and concentrate only on the pocket. The contribution to the susceptibility from the small FS and for $q\gg k_{F2}$ reads

$$\chi_0(\mathbf{q},i\omega)\approx\frac{k_{F2}^2}{\pi\left(q^2+4\frac{\omega^2}{q^2}\right)}, \tag{2}$$

which leads, with logarithmic accuracy, to

$$\Sigma(k_{F2},i\omega=0)\approx\frac{U^2}{8\pi^2}k_{F2}^2\ln\frac{\Lambda}{k_{F2}}+\text{const.} \tag{3}$$

This strong logarithmic dependence on $k_{F2}$ is crucial in the determination of the size of the pocket. Technically, the divergence comes from the integration in Eq. (1) over the region $k_{F2}<q<\Lambda$ where the Green's function can be approximated as $G(\vec{k}_{F2}+\vec{q},\omega)\approx G(\vec{q},\omega)=1/(i\omega+q^2/2)$. We emphasize the momentum region $q\gg k_{F2}$ as this region gives the divergence in self-energy. However, we stress that the approximations make no qualitative difference to the final result, and all plots are obtained via numerical integration with the full $q$ dependence.

For a given chemical potential $\mu$ (we assume the smooth Hartree term is already absorbed) this is given by the solution of the energy balance equation,

$$\mu=\epsilon(k_{F2})+\Sigma(k_{F2},\omega=0)=\frac{k_{F2}^2}{2}\left(\frac{U^2}{4\pi^2}\ln\frac{\Lambda}{k_{F2}}-1\right). \tag{4}$$

Consider $\mu>0$, so that the noninteracting model has all small-momentum states filled and there is no pocket. In the presence of interactions, however, the effective energy of the fermions bends up in the vicinity of $k_{F2}$, with a corresponding maximum $\mu_{\max}=\frac{U^2}{16\pi^2}\Lambda^2e^{-\frac{8\pi^2}{U^2}-1}$ reached when $k_{F2}=\Lambda e^{-\frac{4\pi^2}{U^2}-\frac{1}{2}}$. In addition to the trivial solution without a pocket, there are then two nontrivial solutions of Eq. (7) for $k_{F2}$ in the interval $\mu\in[0,\mu_{\max}]$, as seen in Fig. 2(a). Solving for $k_{F2}$ yields

$$k_{F2}^{(1);(2)}(\mu)=\frac{4\pi\sqrt{\mu}}{U\sqrt{-W_{0;-1}\left(-\frac{16\pi^2\mu e^{\frac{8\pi^2}{U^2}}}{\Lambda^2U^2}\right)}}, \tag{5}$$

where $W_i(z)$ is the product logarithm function [19].

Which of the three solutions for $k_{F2}$ is stable is determined by the grand canonical potential $\Omega$, which we find by integrating $d\Omega=-n\,d\mu$, starting from the point $k_{F2}=0$ where the phases merge. The result is plotted in Fig. 2(b): the trivial phase with $\mu<\mu_{\text{crit}}$ is unstable, and a first-order phase transition to the solution with a larger pocket occurs (indicated by arrow). This happens because at small $k_{F2}$ the logarithm in the $U^2$ term outweighs the free kinetic term. From the expression for $\Omega$ it follows that the position of $\mu_{\text{crit}}$ equally divides the shaded area, a case of Maxwell construction.

Although the above picture of FS reconstruction as a function of interaction $U$ as in Refs. [5,6] is intuitively appealing, in a typical experimental situation one rarely has any strong control over $U$. We therefore imagine returning to the Lifshitz setup, where some external parameter is varied, extending these original ideas to nonzero interaction. With the concrete example of $Na_xCoO_2$ in mind, we examine what happens as a function of doping. To make this picture consistent, however, we must first reinstate the large FS.

It may be intuitively expected that the self-energy of the large FS has no essential dependence on the size of the pocket; however, to check this we evaluate this contribution,

$$\Sigma(k_{F1},\omega=0)\approx\frac{U^2}{8\pi^2}k_{F2}^2\frac{1-v_{F1}m_1}{m_1v_{F1}^2}, \tag{6}$$

which has no logarithmic enhancement. At the level of SOPT, the main role of the large FS is therefore to act as a particle reservoir, with the electron density given by Luttinger's theorem: $n=\frac{1}{2\pi}(k_{F1}^2-k_{F2}^2)$.

We assume that all the nondivergent terms containing $k_{F2}^2$ are effectively included in $\Lambda$ and the small self-energy contributions to the large FS are already included in the bare dispersion parameters. We also assume that the effective

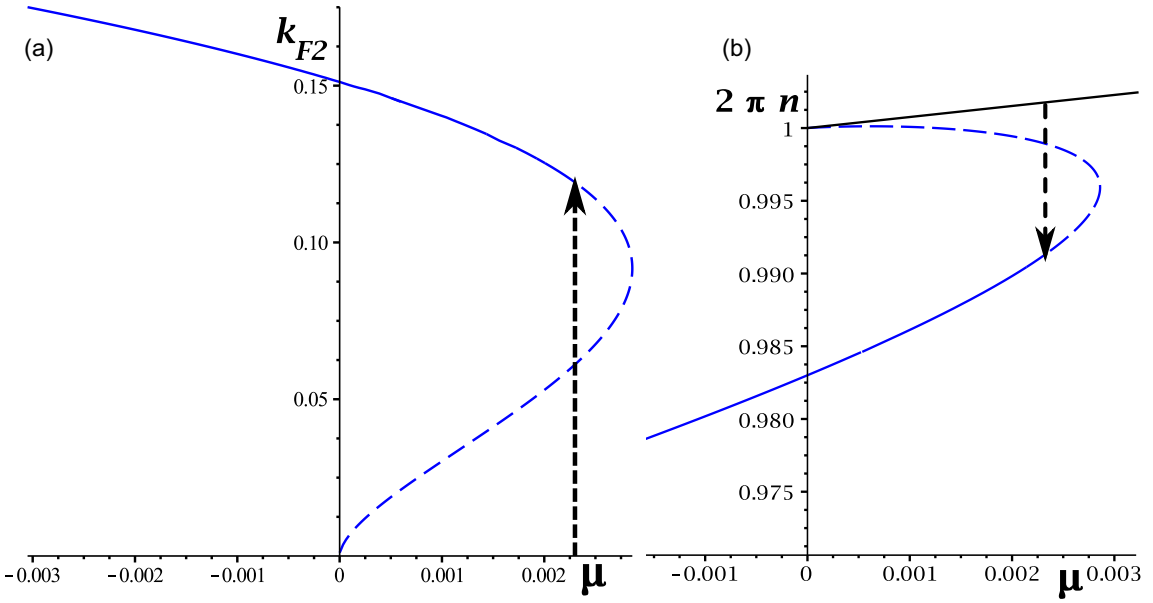


FIG. 2. (Color online) (a) Pocket size $k_{F2}(\mu)$ and (b) electron density $n(\mu)$ for the parameters $U = 4$ (effective $U_{\text{eff}} = 6.3$), $v_{F1} = 2$, $m_1 = 1$, $\Lambda = 1$ (other parameters give qualitatively similar results). For these values the FSTT happens at $\mu = 0.0023$, and electron density jumps by roughly 1%. The dashed arrow indicates the phase transition, which happens when the two shaded domains have equal area, reflecting a Maxwell construction.

chemical potential $\mu$ already includes the Hartree term, as this can play no role at constant density. Then, the chemical balance equation reads

$$\mu = \epsilon(k_{F2}) + \Sigma(k_{F2},\omega = 0) = v_{F1}(k_{F1} - 1). \quad (7)$$

This equation has the solution $k_{F1} = \mu/v_{F1} + 1$, while $k_{F2}$ in given in Eq. (5) and the discussion above. However, one may now view the pocket-opening transition as a function of density (parameterized by $\mu$). Without interactions, the pocket smoothly appears for $\mu < 0$. In the presence of interactions, however, the point of a noninteracting FSTT ($k_{F2} = 0$, $\mu = 0$) is unstable, and when $\mu$ is slightly above zero, there is a first-order phase transition to the branch with larger $k_{F2}$. We see, however, from Eq. (5) that for small $U$, the jump of $k_{F2}$ at the phase transition is exponentially small. We also note that the two phases have a different electron density which decreases abruptly by $\frac{k^2_{F2\ \min}}{2\pi}$ at the FSTT. This implies that if we continuously vary the doping, there is an interval of electron densities where no stable homogeneous phase exists; there would be phase coexistence (phase separation). The physics of such a state is governed by long-range interactions that are not included in the present model. In this situation, we also cannot exclude the possibility of a charge-density-wave phase with broken translational symmetry.

To summarize so far, interactions drive the pocket-opening/pocket-closing first-order FSTT in SOPT, with an exponentially small jump of $k_{F2}$ for small $U$. Going to higher orders in $U$ in general, where a small FS in 2D may have further nonanalyticities due to other fluctuations (see, e.g., Refs. [20,21]), is beyond the scope of the this study. However, by concentrating on the region of large PM fluctuations, we will now show that this jump is enhanced for larger $U$.

## IV. MODERATE U

By increasing the strength of the interaction, approaching but remaining below the Stoner instability, we enter the regime of paramagnons. The summation of ladder and ring diagrams [22] gives the "effective paramagnon" interaction:

$$V(\mathbf{q},i\omega) = \frac{\chi_0(\mathbf{q},i\omega)}{1 - U^2\chi_0^2(\mathbf{q},i\omega)} + \frac{U\chi_0^2(\mathbf{q},i\omega)}{1 - U\chi_0(\mathbf{q},i\omega)}. \quad (8)$$

The self-energy in the paramagnon approximation in the low-temperature limit then reads

$$\Sigma(\mathbf{k},i\Omega_n) = U^2 \int_{-\infty}^{\infty} d\omega \int \frac{d^2q}{(2\pi)^3} G(\mathbf{k}+\mathbf{q},i\Omega_n + i\omega)V(\mathbf{q},i\omega). \quad (9)$$

Further diagrams giving the vertex corrections turn out to cancel those of the quasiparticle weight $Z$ [23,24].

As before, we express the bare susceptibility as a sum of two Lindhard functions that come from the two FSs. Evaluating numerically integral (9) for the real part of the self-energy at the small FS, we find that it can be well fitted by the function

$$\Sigma(k_{F2}) \approx \frac{U_{\text{eff}}^2}{8\pi^2}\left[k_{F2}^2\left(\ln\frac{\Lambda}{k_{F2}} + a_1\right) + \frac{b_1}{v_{F1}}k_{F2}^2 + c_1\right]. \quad (10)$$

Here, $a_1$ slowly increases with $U$ and is close to zero for large $U$, and $b_1 \approx -0.8$. The first two terms come from the contribution of the susceptibility from the small FS, while the $b_1$ term comes from the large FS susceptibility. Aside from the small analytic corrections, $a_1$,$b_1$, the overall form of the self-energy is identical to Eq. (3), with an effective interaction strength $U_{\text{eff}}$. For small $U$, $U_{\text{eff}} = U$, but when $U$ approaches the Stoner instability $U_{\text{Stoner}} = 2\pi/(1 + 1/v_{F1})$, the effective interaction strength greatly increases. This is

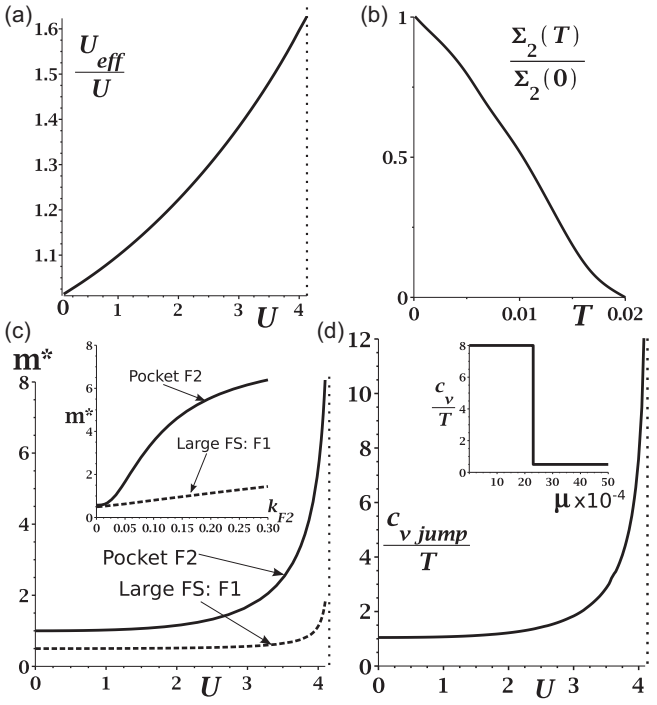


FIG. 3. (a) $U_{\rm eff}/U$ as a function of $U$, defined by Eq. (10). (b) Temperature dependence of $\Sigma(k_{F2})$ for fixed $k_{F2}$. (c) Effective mass at both FSs as a function of $U$ ($k_{F2}=0.2$) and as a function of $k_{F2}$ for $U=4$ in the inset (solid and dashed lines indicate small and large FSs, respectively). (d) Jump in $T$-linear coefficient in $c_v$ due to FSTT for $v_{F1}=2$.

plotted in Fig. 3(a) and can be understood to be the effect of the enhancement of the susceptibility due to PM fluctuations. The large FS now plays a role beyond that of a reservoir: it drives the system closer to the Stoner instability, thus enhancing the PM fluctuations and, consequently, $U_{\rm eff}$. The physics of the first-order Lifshitz transition described previously by SOPT is still valid, with the simple replacement of $U \to U_{\rm eff}$.

It is worth mentioning that while a similar effect of the interactions driving the FSTT first-order has previously been discussed for neck-opening/neck-closing transitions in Refs. [4,8,9], the physical processes in the present case are quite different. In the former, the logarithmic divergence of the single-particle density of states (van Hove singularity) led to a first-order transition that technically originated from the Fock term. In the present study, the large paramagnetic fluctuations lead to the effect.

## V. PROPERTIES

Having shown that the FSTT transition is driven first order by interactions, we now turn to the physical consequences of this calculation. We begin by addressing the question, is the system with the small FS (and large self-energy) a good FL? To answer this question, we consider the frequency and momentum dependence of the retarded self-energy, which reads [25]

$$\mathrm{Im}\Sigma^R(\mathbf{k},\omega) \approx U^2 \int \frac{d^2q}{(2\pi)^2}[\theta(\epsilon(\mathbf{q})) - \theta(\epsilon(\mathbf{q})-\omega)] \times \mathrm{Im}V^R(\mathbf{q}-\mathbf{k},\epsilon(\mathbf{q})-\omega), \quad (11)$$

where $\epsilon(\mathbf{q})$ takes the relevant form of the bare dispersion near each of the two FSs. In SOPT, for the small FS and small momentum transfer (forward scattering) $\mathrm{Im}V^R(q,\omega) = \mathrm{Im}\chi_0^R(q,\omega)$, and it behaves as

$$\mathrm{Im}\chi_0^R(\mathbf{q},\omega) = -\frac{1}{2\pi m}\frac{\omega}{\sqrt{(k_{F2}q)^2-\omega^2}}\theta(k_{F2}q-|\omega|). \quad (12)$$

The computation reveals a logarithmic term coming from the region of forward scattering. A similar one comes from the backscattering region $q \approx 2k_{F2}$. Therefore, when only the small FS is considered, with logarithmic accuracy [25],

$$\mathrm{Im}\Sigma^R(k_{F2},\omega) \approx \frac{U^2}{8\pi^3 k_{F2}^2}\omega^2 \ln\frac{k_{F2}^2}{|\omega|}. \quad (13)$$

In the region of paramagnetic fluctuations, the imaginary part of the self-energy behaves as in SOPT with $U$ replaced by $U_{\rm eff}$, while the real part reads

$$\mathrm{Re}\Sigma^R(k_{F2},\omega>0) = \begin{cases}(1-Z^{-1})\omega, & \omega \lesssim k_{F2}^2 \\ \text{const}, & \omega \gtrsim k_{F2}^2\end{cases} \quad (14)$$

The coefficients are $(-Z^{-1}+1) \approx -\frac{1}{8\pi^2}U^2V(0,0)$, with $V$ given by Eq. (8).

These results show that in the case of small $U$, where the pocket is exponentially small, the pocket is, formally, a good Fermi liquid with large quasiparticle weight $Z$. In addition, $Z$ dictates an evolution from a good Fermi liquid at small $U$ to a bad Fermi liquid close to Stoner instability. For example, for $U=4$, $v_{F1}=2$ (as used in Fig. 2), we obtain $Z^{-1}=16.5$. When $U$ increases, the effective mass

$$m^* \equiv k_F/|v_F^*|, \quad (15)$$

$$v_F^* = Z_{k_F}\left(v_F + \frac{\partial}{\partial k}\mathrm{Re}\Sigma(k,0)\right), \quad (16)$$

diverges as a power law close to the Stoner transition. This can be clearly seen in measurements of the heat capacity, as discussed below, while the small $Z$ in this case leads to an almost smooth spectral function. This makes the pocket almost invisible in angle-resolved photoemission spectroscopy experiments.

The effect of temperature $T$ is summarized in Fig. 3(b), where it is evident that the self-energy $\Sigma_2$ is affected by $T$, and as $T$ is increased, we expect a termination of the first-order jump at a second-order critical end point $T_c$, in a manner analogous to that found in neck-opening/neck-closing Lifshitz transitions [9]. A full discussion of this physics and an accurate estimate of $T_c$ for realistic parameters will be given elsewhere.

The heat capacity at low temperatures can be computed using the FL formula, which for 2D is

$$c_v = \frac{\pi^2}{3}N^*(0)k_B^2T = \frac{\pi T}{3}(m_1^*+m_2^*), \quad (17)$$

where $N^*(0) = k_F/(\pi|v_F^*|)$ is the density of states at the Fermi level. For the noninteracting system when the pocket is continuously open, Eq. (17) leads to a jump in the coefficient of the term proportional to $T$ in $c_v$ at the FSTT. Also, $c_v$ depends only on the pocket's appearance and not on its size, which is indicative of the 2D nature of the pocket. In the presence

of interactions, the PM fluctuations make $m^*$ of the pocket dependent on pocket's size for small $k_{F2}$. This dependence weakens for larger $k_{F2}$ [as seen in Fig. 3(c)], making the doping dependence of $c_v$ remarkably similar to that in the 2D noninteracting case but with the magnitude of the jump at the FSTT dependent on the interaction strength $U$, as seen in Fig. 3(d). In three dimensions, however, a first-order FSTT would have a more obvious experimental signature; a discussion of the three-dimensional FL is given in Ref. [26].

However, for a real layered material such as $Na_xCoO_2$, which has a nonzero interlayer hopping, the situation is different. In this case, the noninteracting Lifshitz transition does not show a jump in $c_v$ as the pocket smoothly opens; instead, it exhibits a square-root singularity as a function of doping (or particle number) [2]. On the other hand, as long as the minimum $k_{F2}^2$ at the transition is larger than the interplane hopping, the theory developed above remains unchanged. The predicted jump in $c_v$ was seen experimentally [17]. Thus, we believe that the present work provides the essential physics behind the FSTT in $Na_xCoO_2$.

Naturally, $c_v$ diverges at the FM (Stoner) transition due to the divergence of $m^*$ for both FSs, as shown in Fig. 3(c). As $U$ increases further, beyond the Stoner instability, the FSTT and the transition to a FM occur together; in this case the FSTT is driven to first order [13] by the magnetic transition.

## VI. CONCLUSIONS

Summarizing, we have studied the effect of the interactions in a topological Fermi-surface deformation (Lifshitz transition) without any symmetry breaking. We found that interactions drive a pocket-opening FSTT first-order in a 2D FL in the region of PM fluctuations. We have presented a robust Maxwell construction for the first-order phase transition between the possible phases of different electron densities. The phases on both sides of the transition remain paramagnetic Fermi liquids, with topologically different FSs and with strongly renormalized parameters. The first-order nature of the transition leads us to think about the possibility of phase separation in the mixed-phase region, the study of which is beyond the scope of the present work. Here, we stress that the continuous Lifshitz transition in the noninteracting case is expected to become first order in the presence of interactions.

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