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Using a two-orbital model of the superconducting phase of the pnictides, we compute the spectrum of the Leggett mode—a collective excitation of the phase of the superconducting gap known to exist in multigap superconductors—for different possible symmetries of the superconducting order parameter. Specifically, we identify the small regions of parameter space where the Leggett mode lies below the two-particle continuum, and hence should be visible as a sharp resonance peak. We discuss the possible utility of the Leggett mode in distinguishing different momentum dependencies of the superconducting gap. We argue that the observation of a sharp Leggett mode would be consistent with the presence of strong electron-electron correlations in iron-based superconductors. We also emphasize the importance of the orbital character of the Leggett mode, which can result in an experimental observation of the mode in channels other than A_{1g}.

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I. INTRODUCTION

The discovery of high-temperature superconductivity in iron arsenide and related compounds at the beginning of 2008 (Ref. 1) has triggered an enormous interest in the condensed-matter physics community and has stimulated a flurry of experimental activity.[1–9] Upon electron[10] or hole[7] doping of a magnetically ordered parent state, most of the iron-based superconductors exhibit transition temperatures T_c beyond the conventional BCS regime, with some extending up to 56 K,[11] thereby breaking the cuprate monopoly on high-temperature superconductivity. Experimental evidence accompanied by theoretical modeling suggest that the pairing in the iron pnictides is different from the *d*-wave pairing of the cuprates. Nevertheless, they resemble the cuprates in that it is increasingly clear that the magnetism of the parent state (either long-range or fluctuating order) crucially influences the pairing symmetry of the doped system. A conclusive observation of the pairing symmetry still remains elusive with both nodal and nodeless order parameters reported in experiments. This provides a strong incentive to identify new experimental probes potentially sensitive to the symmetry of the superconducting gap.

While a wide range of nodal gap functions were initially predicted,[12–14] the general theoretical view has now converged to favor an extended *s*-wave order parameter (denoted $s^{\pm}$ or $s_{x^2y^2}$) that takes opposite signs on the electron and hole pockets along the multiband Fermi surfaces. The symmetry of this $s_{x^2y^2}$ gap matches that of the iron-pnictide Fermi surface: it is maximal around (0,0), $(\pi,0)$, $(\pi,0)$, and (π,π) the location of the Fermi surfaces in the unfolded one iron per site Brilloiun zone. This sign-alternating nodeless gap is consistent with some experimental data and also has broad theoretical support.[15–23] Indeed, both strong[17,19]-and weak[15,16,18,20–26]-coupling theories of the onset of superconductivity predict an extended *s*-wave order parameter.

Experimentally, however, there is no consensus about the nature of the order parameter with both nodal and nodeless gaps being reported. While most experiments can be explained within the framework of an $s^{\pm}$ gap,[27] several facts, such as the T^3 dependence of the NMR relaxation rate over a significant temperature range,[28–30] residual finite quasiparticle terms in the thermal conductivity,[31,32] as well as the power-law behavior of the penetration depth,[33,34] remain unsettled. Some of the experiments on penetration depth and thermal conductivity could be explained by an $s^{\pm}$ order parameter if there were a large gap anisotropy,[33,34] but this contradicts angle resolved photoemission spectroscopy (ARPES) data, which reveals very isotropic nodeless gaps on the hole Fermi surfaces,[35–37] of magnitudes matching a strong-coupling form $\Delta(k)=\Delta_0\cos(k_x)\cos(k_y)$ (Ref. 17) in the unfolded Brillouin zone.

A possible resolution of this apparent contradiction, consistent with the theoretical prediction of an $s_{\pm}$ order parameter, is that the gap anisotropy is doping dependent and that different experiments are done at different dopings. In the strong-coupling mean-field picture,[17,19] the gap anisotropy is intrinsically doping dependent: the gap has a form $\cos(k_x)\cos(k_y)$ which becomes more anisotropic as the doping is increased. In a weak-coupling expansion of Fermi-surface interactions, the gap anisotropy can arise from the presence of an A_{1g} term $\cos(k_x)+\cos(k_y)$ [which does not break the crystal symmetry but can create nodes on the $(\pi,0)$ and $(0,\pi)$ electron surfaces] in the band interactions[38] upon renormalization.[20] A large gap anisotropy is already present in functional renormalization-group studies of orbital models.[18,24]

In this paper, we analyze another physical phenomenon—the Leggett mode of multiband superconductors—that depends on the strength of the pairing order parameter and could also, in principle, quantitatively distinguish a sign-changing gap from other gap symmetries. Specifically, we investigate to what extent the pairing symmetry of the iron-based superconductors can be deduced by analyzing the behavior of the Leggett mode as a function of doping and the strength of superconducting order parameters. As the iron-based superconductors have multiple orbitals, the superconducting state exhibits a plethora of collective modes beyond the usual Goldstone/Higgs plasmon. Here we use an effective two-orbital model of the superconducting state to study one of these—the Leggett mode associated with antisymmetric phase fluctuations between the two superconducting order parameters. This gapped collective mode can, in the right parameter range, present a sharp collective mode resonance below the two-particle continuum which could, in principle, be detected experimentally.

To determine whether such a collective mode resonance occurs in the pnictide superconductors, we study the gap and dispersion of the Leggett mode as a function of doping and the superconducting order parameters. We show that, for a sign-changing gap function, the Leggett mode can be below the two-particle continuum for a small regime at low doping. In particular, when the band renormalization is large, an undamped Leggett mode can exist in a relatively large parameter region. Thus, the observation of a sharp Leggett mode will validate the presence of strong electron-electron correlations in the iron-based superconductors. Moreover, in our two-orbital model, the Leggett mode is a B_{1g} mode, instead of a pure A_{1g} mode, which is expected in any band-based model. Therefore, the orbital structure of pairing in the iron-based superconductors can be validated by identifying the existence of the Leggett mode in channels other than A_{1g}.

Unfortunately, we find that the Leggett mode cannot qualitatively distinguish between a sign-changing order parameter and other gapped order parameters. However, the sign-changing order parameter will have a degree of anisotropy which depends on doping. For large doping, the sign-changing order parameter on the enlarged Fermi surface will exhibit larger anisotropy. As such, the superconducting gap will be small on some parts of the Fermi surface and the Leggett mode will be overdamped, lying above the two-particle continuum, and hence unobservable. This presents a testable opportunity if, at moderate doping (when the gaps should theoretically be isotropic), the Leggett mode is below the two-particle continuum and hence observable. If so, the observation of a disappearing collective mode provides indirect support for a sign-changing gap function.

II. COMPUTING THE EFFECTIVE ACTION

The Leggett mode is a collective excitation of two-(or multi) band superconductors, associated with antisymmetric phase oscillations between the two bands. It is thus a neutral mode associated with oscillations between the supercurrents of the two bands. Here we present the effective action for this mode derived from a two-orbital model appropriate to the pnictides at temperatures well below the onset of superconductivity. To render our calculations analytically tractable, we focus on a simplified model of the iron-based superconductors that takes into account only the d_{xz}, d_{yz} orbitals. In this case, an intraband order parameter can have its phase fluctuate between the two orbitals in two modes: the usual symmetric combination (Goldstone) and the antisymmetric combination, which is the Leggett mode.

While the conventional Leggett mode involves only the Fermi-surface gaps, our work involves a Leggett mode in the orbital gaps. We consider the orbital basis rather than an effective band basis, because neglecting the orbital structure of the iron-based superconductors is most likely incorrect: it was shown[39] that due to the difference in mirror symmetry eigenvalues of the electron and one of the hole bands at the Γ point in the Brillouin zone (BZ), the spin-density wave (SDW) state is gapless with a Dirac point in both two- and five-orbital models of iron-based superconductors. This highly nontrivial effect, confirmed by experiments,[40] is lost in the effective band-basis picture. Details of the derivation of the Leggett mode effective action in the orbital basis, which differs slightly from the band-basis result of, e.g., Ref. 41, are given in Appendix A.

A. Model Hamiltonian

Using the insight provided by numerical and analytic studies suggesting that the antiferromagnetic exchange coupling between next-nearest-neighbor Fe sites is strong,[12,42] two of us[17] studied a t-J_1-J_2 model without band renormalization and obtained a gap function of the form $\cos(k_x)\cos(k_y)$, which changes sign between the electron and hole pockets of the Fermi surface of the material. It is this type of strong-coupling superconductivity that we will focus on in this paper, but we point out that other weak-coupling approaches exist and give a similar sign-changing order parameter.[15,16,18,20–23]

To calculate the effective action for the phase modes of the superconducting state, we employ a model of the pnictides which incorporates only the d_{xz} and d_{yz} orbitals at each site together with hybridization between the two. Although this description is only truly valid in the case of unphysically large crystal-field splitting, we use this model for its analytic simplicity. We adopt the band structure proposed in Ref. 14, which at first glance captures the essence of the density-functional theory results

$$H_0 = \sum_{k\sigma} \psi^{\dagger}_{k\sigma} T(k) \psi_{k\sigma} + H_{int},$$

$$T(k) = \begin{pmatrix} \epsilon_x(k) & \epsilon_{xy}(k) \\ \epsilon_{xy}(k) & \epsilon_y(k) \end{pmatrix}, \tag{1}$$

where $\psi^{\dagger}_{k,\sigma} = (c^{\dagger}_{d_{xz},k,\sigma}, c^{\dagger}_{d_{yz},k,\sigma})$ is the creation operator for spin σ electrons in the two orbitals and the kinetic terms read

$$\epsilon_x(k) = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y - \mu,$$

$$\epsilon_y(k) = -2t_2 \cos k_x - 2t_1 \cos k_y - 4t_3 \cos k_x \cos k_y - \mu,$$

$$\epsilon_{xy}(k) = -4t_4 \sin k_x \sin k_y. \tag{2}$$

The hoppings have roughly the same magnitude: $t_1 = -1.0$, $t_2 = 1.3$, $t_3 = -0.85$, and $t_4 = -0.85$ in eV. We find that the half filled, two electrons per site configuration is achieved when $\mu = 1.54$ eV.

The missing ingredient in this two-orbital model is the d_{xy} orbital, which can be shown to be important to the detailed physics of the iron-based superconductors.[43] For example, the kinetic model Eq. (1) gets the location of the second hole pocket wrong—it situates it at the (π,π) point in the unfolded BZ whereas local-density approximation calculations show two hole pockets at the Γ point. However, the two-orbital model gets several of the qualitative characteristics of the iron-based superconductors right: it has a nodal SDW instability and a sign-changing s-wave superconducting instability.

To describe the superconducting phase, we use the approach of Ref. 17, adopting a strong-coupling picture in which the interaction Hamiltonian contains antiferromagnetic nearest-neighbor and next-nearest-neighbor couplings between the spins in both identical and opposite orbitals. While not entirely correct at lattice scales, it was shown that this model gives remarkably large overlaps with the interactions obtained through the functional renormalization-group[44] method, and hence can be considered as an effective interaction model for the iron-based superconductors. Furthermore, for our purposes these interactions are important only insofar as they give, after decoupling in the superconducting channel, the sign-changing $\cos(k_x)\cos(k_y)$ superconducting order parameter. In this sense, the interacting spin model we use can be thought of as an effective Ginzburg-Landau description of iron-based superconductors; the precise mechanism driving the transition to the superconducting phase is irrelevant to the effective action we derive here.

Based on the mean-field analysis of Ref. 17, we will assume throughout that the superconducting instability is dominated by the intraorbital interactions so that the gap is diagonal in the orbital basis. Indeed, at the mean-field level, the interorbital pairing is weaker than the intraorbital pairing by a factor of approximately five.[17] In addition there is a large on-site interorbital Hund's rule coupling which will not enter into the present analysis as it does not alter the nature of the order parameter at mean-field level. We will briefly discuss the impacts of this last term together with the antiferromagnetic interorbital interactions, in Sec. II C.

B. Phase-only effective action

To obtain an effective action for the phase of the superconducting gap, we follow the general protocol of Ref. 45; details of this calculation as applied to the orbital basis are given in Appendix A. In essence, one first decouples the interaction terms in the microscopic model using a Hubbard-Stratonovich transformation. This re-expresses operators quadratic in the fermions as interaction terms between a pair of fermions and the superconducting field Φ. Deep in the superconducting region, where fluctuations in the magnitude $\Delta \equiv |\Phi|$ can be neglected, integrating out the fermions then yields an effective action for the phase modes of the system. Since we work with a two-orbital model, there are *a priori* two superconducting gaps, excluding interorbital pairing. Though by symmetry their magnitudes have to be equal, this leads to two independent phase degrees of freedom. As is well known, one of these is a Goldstone mode which, upon including the Coulomb interactions, becomes a plasma mode. The other is the (gapped) Leggett mode, which will be our principle focus here.

For our purposes, the two phase degrees of freedom are most conveniently expressed in the basis

$$\phi \equiv \frac{1}{\sqrt{2}}(\theta_1 + \theta_2) \quad \varphi \equiv \frac{1}{\sqrt{2}}(\theta_1 - \theta_2), \tag{3}$$

where θ_1 and θ_2 are the phases of the gaps in the xz and yz orbitals, respectively. Hence ϕ represents the symmetric phase oscillation while φ represents the (neutral) antisymmetric phase mode. In this basis, we find the effective action to be (see calculation details in Appendix A)

$$\begin{aligned} S_{eff} = \int d\Omega d^2q (\phi(\Omega,q) \quad \varphi(\Omega,q)) \\ \times \begin{pmatrix} N_{\phi\phi}[\Omega^2 - c^2_{\phi\phi,ij}q_iq_j] & c^2_{\phi\varphi,ij}q_iq_j \\ c^2_{\phi\varphi,ij}q_iq_j & N_{\varphi\varphi}[\Omega^2 - \Omega_0^2 - c^2_{\varphi\varphi,ij}q_iq_j] \end{pmatrix} \\ \times \begin{pmatrix} \phi(\Omega,q) \\ \varphi(\Omega,q) \end{pmatrix} \end{aligned} \tag{4}$$

with momentum-independent coefficients given by

$$N_{\phi\phi} = -\int \frac{d^2k}{(2\pi)^2}\left\{\frac{\Delta^2}{4E_+^{(\Delta)3}} + \frac{\Delta^2}{4E_-^{(\Delta)3}}\right\}, \tag{5}$$

$$\begin{aligned} N_{\varphi\varphi} = -\int \frac{d^2k}{(2\pi)^2}\frac{(\epsilon_x - \epsilon_y)^2}{(E_+ - E_-)^2}\left\{\frac{\Delta^2}{4E_+^{(\Delta)3}} + \frac{\Delta^2}{4E_-^{(\Delta)3}}\right\} \\ - \int \frac{d^2k}{(2\pi)^2}\frac{8\Delta^2\epsilon_{xy}^2}{(E_+ - E_-)^2}\frac{E_+^2 + E_-^2 + \Delta^2 + E_+^{(\Delta)}E_-^{(\Delta)} - E_+E_-}{(E_+^{(\Delta)} + E_-^{(\Delta)})^3 E_+^{(\Delta)}E_-^{(\Delta)}}, \end{aligned} \tag{6}$$

$$M = \int \frac{d^2k}{(2\pi)^2}\frac{4\Delta^2\epsilon_{xy}^2}{E_+^{(\Delta)}E_-^{(\Delta)}(E_+^{(\Delta)} + E_-^{(\Delta)})} \tag{7}$$

with $\Omega_0 \equiv \sqrt{\frac{M}{-N_{\varphi\varphi}}}$. Here, $E_\pm$ are the two-band energies $E_\pm = \frac{1}{2}[\epsilon_x + \epsilon_y \pm \sqrt{(\epsilon_x - \epsilon_y)^2 + 4\epsilon_{xy}^2}]$ of the metallic state and $E_\pm^{(\Delta)} = \sqrt{E_\pm^2 + \Delta^2}$ are the quasiparticle energies in the superconducting phase. All ϵ, E, and Δ are evaluated at the momentum k to be integrated over. The above equations represent the main result of the paper.

In Eq. (4), terms linear in q, as well as terms bilinear in q,Ω, all vanish in the limit $T \to 0$. As expected, this effective action Eq. (4) describes one gapless mode, comprised entirely of symmetric phase fluctuations at $q=0$, and one gapped mode. The latter is the Leggett mode; at $q=0$ it consists purely of antisymmetric phase oscillations between the two superconducting gaps. Here we are principally interested in the Leggett mode gap, Ω_0, as this represents the threshold at which the mode becomes experimentally observable. Thus if $\Omega_0 < 2\Delta$, we expect the Leggett mode to appear as a sharp resonance in the spectrum of the pnictide superconductors.

For terms involving q^2, the expressions for the coefficients $c^2_{\alpha\beta,ij}$ are somewhat more complicated and are thus given in Appendix A 1. We note, however, that for $i \neq j$, any coefficient of $q_i q_j$ vanishes due to symmetry. Further, for $i = j$, symmetry of the coefficients under a 90° rotation of the Brillouin zone fully determines their direction dependence in q. Taking these symmetries into account, Eq. (4) has the form

$$S_{eff} = \int d\Omega d^2 q (\phi \quad \varphi) \times \begin{pmatrix} N_{\phi\phi}[\Omega^2 - c_{\phi\phi}^2 q^2] & c_{\phi\varphi}^2 (q_x^2 - q_y^2) \\ c_{\phi\varphi}^2 (q_x^2 - q_y^2) & N_{\varphi\varphi}[\Omega^2 - \Omega_0^2 - c_{\varphi\varphi}^2 q^2] 0 \end{pmatrix} \begin{pmatrix} \phi \\ \varphi \end{pmatrix}. \tag{8}$$

We should note that the Leggett mode gap is proportional to ϵ_{xy}^2–that is, to the off-diagonal kinetic terms in the orbital basis. This is in contrast to the approach of, for example, Ref. 41, in which the superconducting gap is taken to be diagonal in the band basis of the normal state, and it is the interband interactions which couple the phases of the two gaps, and hence generate the Leggett mode. This difference stems from the fact that we take the gap to be diagonal in the orbital basis: $\Delta_\alpha(k) = \langle c_{\alpha\uparrow k} c_{\alpha\downarrow -k} \rangle$, where α indexes the orbitals and assume that the pairing is defined over the whole Brillouin zone. Any model in which the interaction is written in orbital space and which aims to respect the point-group symmetries of the lattice will require this type of orbital-basis formalism.

C. Including Hunds interactions

In light of the fact that our approach is based on an absence of off-diagonal interactions in the superconducting channel (when the orbital basis is used), it is useful to consider in more detail the validity of this assumption in the presence of interorbital couplings. In the pnictides the ferromagnetic Hund's rule interaction

$$H_H = - J_H \sum_r S_{1r} S_{2r} \equiv - J_H \sum_r c_{1r\sigma}^\dagger \sigma_{\sigma,\sigma'} c_{1r\sigma'} c_{2r\gamma}^\dagger \sigma_{\gamma,\gamma'} c_{2r\gamma'} \tag{9}$$

is the principal source of such interactions.

Since spin ordering must be absent in the superconducting phase, generically we may decouple the Hunds interaction in either the particle-particle channel or the particle-hole channel. At lowest loop order, the particle-particle interaction serves only to renormalize the band structure. The particle-hole contribution was, as previously noted, shown to be small by Ref. 17. Neglecting the small interorbital pairing at mean field, we find that the Hunds interaction affects the effective action for the Leggett mode φ only through higher loop corrections in the fermion propagator.

Further, it is straightforward to include the effect of the small interorbital interaction in the superconducting channel. Such a term simply modifies the effective action for the superconducting phase by adding a term $V_{12}(\Delta_1 \Delta_2^* + \Delta_2 \Delta_1^*) \equiv 2|\Delta|^2 V_{12} \cos(\varphi)$. This modifies the gap of the Leggett mode according to

$$\Omega_0^2 \to \Omega_0^2 - \frac{V_{12}}{V_{11}V_{22} - V_{12}^2} \frac{\Delta_0^2}{N_{\varphi\varphi}}. \tag{10}$$

Here $V_{\alpha\beta}$ parametrize the superconducting interaction between orbitals α and β, as described in Eq. (A2), and we have taken $\Delta(k) = \Delta_0 \cos(k_x)\cos(k_y)$. For $0 < V_{12} \ll V_{11}, V_{22}$, the effect of including such a term is always to bring the Leggett mode gap down in energy.

D. Effective action with Coulomb terms

In the above analysis, we ignored the effects of the Coulomb interaction on the phase modes. In a single-band superconductor, including the Coulomb interactions modifies the effective action for the phase θ of the superconducting gap such that at zero temperature θ becomes a plasma mode.[46] (At finite temperatures a second mode, the Carlson-Goldman mode, is known to exist both in one[47]-and two[48]-band superconductors.) We will not examine in detail the plasma mode here; rather we note that including Coulomb interactions does not substantially modify the relevant features of the Leggett mode, as we show below. This is not surprising since the Leggett mode is, at long wavelengths, associated with the neutral antisymmetric phase oscillations, and hence does not couple to the Coulomb interaction.

In the presence of Coulomb interactions, the phase-only effective action has the form

$$S_{eff} = \int d\Omega d^2 k (\phi \quad \varphi) \begin{pmatrix} N_{\phi\phi}\left[\dfrac{\Omega^2}{1 - U(q) N_{\phi\phi}} - c_{\phi\phi}^2 q^2\right] & c_{\phi\varphi}^2 (q_x^2 - q_y^2) \\ c_{\phi\varphi}^2 (q_x^2 - q_y^2) & N_{\varphi\varphi}[\Omega^2 - \Omega_0^2 - c_{\varphi\varphi}^2 q^2] \end{pmatrix} \begin{pmatrix} \phi \\ \varphi \end{pmatrix} + \Delta_\alpha V_{\alpha,\beta}^{-1} \Delta_\beta \tag{11}$$

(For the sake of completeness we derive this result in Appendix B). The dispersion of the symmetric mode ϕ is modified by the denominator of its Ω^2 term; in practice since the Coulomb interaction $U(q)$ is singular as $q \to 0$ this makes the symmetric mode into a plasma mode, exactly as is known to occur in a single-band superconductor.[47]

Equation (11) shows that including Coulomb interactions does not alter the mass gap of the Leggett mode, as the plasma mode does not mix with the Leggett mode φ at $q = 0$. The net effect of the Coulomb terms on $\varphi(\Omega, q)$ will be a modification of the q^2 term in the effective action of the Leggett mode. Integrating out ϕ, we obtain

$$S_{eff}=\int d\Omega d^2k\varphi(q)\varphi(-q)N_{\varphi\varphi}\left\{\Omega^2-\Omega_0^2-c_{\varphi\varphi}^2(q_x^2-q_y^2)\left[1+\frac{c_{\phi\varphi}^4}{c_{\varphi\varphi}^2N_{\varphi\varphi}}\frac{q_x^2-q_y^2}{\frac{\Omega^2}{(1-N_{\phi\phi}U(q))}+q^2c_{\phi\phi}^2}\right]\right\}+\Delta_\alpha V_{\alpha,\beta}^{-1}\Delta_\beta. \quad (12)$$

Hence for small q,Ω, in the presence of Coulomb interactions, provided that $\lim_{q\to 0}\frac{\Omega^2}{q^2[1-N_{\phi\phi}U(q)]}$ is finite, the net effect is a modification of the effective velocity of the mode. The above equation needs to be solved self-consistently to obtain the mode dispersion. However, the limit $q\to 0$, which determines whether the Leggett mode is above or below the particle-particle continuum, is unchanged from the case without the Coulomb interaction.

III. RESULTS

Having established the general form of the effective action of the Leggett mode, we now turn to a quantitative evaluation of the coefficients in Eq. (4). Our principle interest will be what potential information the Leggett mode can give about the form of the superconducting gap—in particular, we address the question of whether it can distinguish between the popular extended *s*-wave gap and other plausible pairing symmetries. Unfortunately, it is clear from our equations that the Leggett mode properties depend on the absolute value of the gap function, thereby preventing any qualitative sensitivity of the mode to a sign change in the gap function. We find that the clearest signature is the lifetime of the Leggett mode as a function of doping—at low dopings we find the Leggett mode to lie below the two-particle continuum; at higher doping the mode is always at higher energies than the two-particle continuum and hence will give at best a very broad resonance.

A. Leggett mode gap

We begin by studying the Leggett mode gap Ω_0 for several different gap functions with the objective of understanding the qualitative differences expected between these in potential experiments. In each case, the mode is expected to be visible if it lies below the two-particle continuum, which is set by 2 min$|\Delta|$ (where the minimum is taken over the Brillouin zone).

At $q=0$ and $T=0$, the symmetric and antisymmetric phase oscillations decouple, and from the effective action Eq. (12) the gap of the Leggett mode φ is given by

$$\Omega_0=\sqrt{-\frac{M}{N_{\varphi\varphi}}}$$

with M and $N_{\varphi\varphi}$ given by Eqs. (5) and (7). Note that $M>0$ and $N_{\varphi\varphi}<0$ so that the Leggett mode gap is well defined. We can evaluate the coefficients $N_{\varphi\varphi}$ and M by integrating the expressions in Eqs. (5) and (7) numerically over the Brillouin zone. We use the values of ϵ_α quoted in Eq. (2).

Figure 1 shows the expected gap of the Leggett mode for extended *s*-wave, standard *s*-wave, *d*-wave, and $\Delta_0 \sin k_x \sin k_y$ gaps, as a function of the filling fraction ν and the maximum gap magnitude Δ_0. The general form of Ω_0 is similar in all four cases: it increases with the superconducting gap Δ_0 and has its lowest values at a filling of approximately $\nu=0.4$. For all four order parameters, we also find the gap of the Leggett mode shows an academically interesting chemical-potential dependence, droping sharply between $\nu=0.4$ and $\nu=0.5$ independent of the momentum dependence of the order parameter.

The qualitative features of these plots can be understood by considering the form of Eqs. (5) and (7). First, we see that Ω_0 increases monotonically with Δ_0, at a slightly less than linear rate. Though naively both M and $N_{\varphi\varphi}$ scale quadratically with Δ_0, $N_{\varphi\varphi}$ has divergences if $E_+^{(\Delta)}$ or $E_-^{(\Delta)}$ vanish; these are cut off by the gap but nevertheless contribute the major part of the integral. Consequently, $N_{\varphi\varphi}$ is well approximated by $N_{\varphi\varphi}\sim V_{FS}/\Delta$ with V_{FS} the volume of the Fermi surface. On the other hand, M vanishes at the Fermi surface in the limit of small Δ, scaling approximately as $M\Delta$ in this region. Hence the quantity $\sqrt{\frac{M}{-N_{\varphi\varphi}}}$ increases with Δ, with a power close to (but slightly less than) 1.

The nonmonotonic dependence on ν, which is similar in all four cases, stems from the dependence of the shape and volume of the Fermi surface on the chemical potential. As stated above, the integral expression for $N_{\varphi\varphi}$ is dominated by contributions near the Fermi surface. M, on the other hand, receives significant contributions from the entire Brillouin zone and is thus much less sensitive to the shape of the Fermi surface.

To illustrate how these effects play out in our two-orbital model, Fig. 2 plots the Fermi surface of the two-orbital model in the normal state for the range of dopings considered here. Between $\nu=0.4$ and $\nu=0.45$, at precisely the locus of the sharp drop in Ω_0 seen above, a new set of Fermi pockets appears at the points $(\pm\pi,0)$ and $(0,\pm\pi)$ as a second pair of bands crosses the Fermi level in the normal state. In the superconducting state this results in more areas where the expressions for $N_{\varphi\varphi}$ are relatively large—in particular, due to the much smaller Fermi velocity near the new branches of the Fermi surface, the area over which $N_{\varphi\varphi}$ is large increases sharply, leading to a sudden reduction in Ω_0. Also worthy of note are the extremal values $(\nu=0.3,\ \nu>0.6)$ at which the Fermi surface intersects with the nodes of the extended *s*-wave gap. These account for the nonmonotonic behavior of Ω_0 observed in both extended *s*-wave and *d*-wave order parameters between $\nu=0.3$ and 0.4, as the cutoff in the normal-state divergences of $N_{\varphi\varphi}$ grows smaller. Though the application of our simple two-orbital model at large fillings is not warranted, and the features discussed in this paragraph are model dependent, we expect them to be accurate for gaps diagonal in the orbital basis

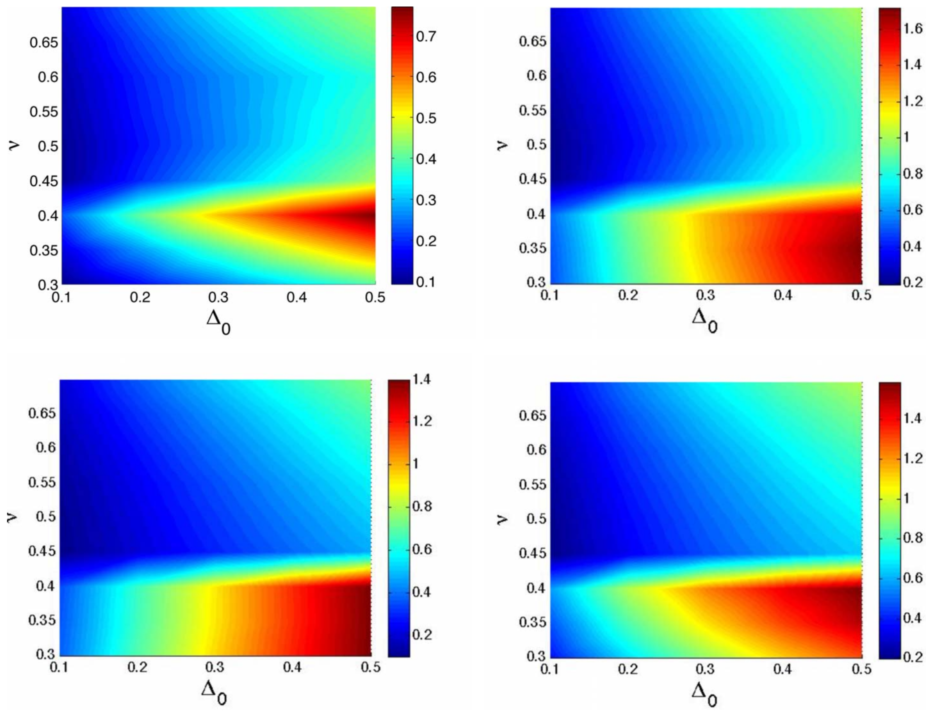

FIG. 1. (Color online) Gap of the Leggett mode for (a) extended s-wave, (b) standard s-wave, (c) $\Delta=\Delta_0 \sin k_x \sin k_y$, and (d) d-wave superconducting gaps. The magnitude of Ω_0 in eV is indicated by the color map to the right of each figure with blue corresponding to regions of smaller Ω_0 and red to regions of larger Ω_0. The vertical axis indicates the filling ν with 1/2 filling corresponding to the undoped case; the horizontal axis is the scale of the maximum magnitude of the gap in eV: we take $\Delta=\Delta_0\Gamma_k$.

inasmuch as the band structure given by the two-orbital model is correct.

B. Observability of the Leggett mode

In order for the Leggett mode to give a sharp resonance in experiments, it should lie below the two-particle continuum. For the d-wave and sine-wave gaps, which are nodal for the iron-based superconductors' Fermi surfaces, this is obviously never the case. For ordinary s-wave and extended s-wave gaps, the position of the Leggett mode at $q=0$ relative to the two-particle continuum depends on the values of ν and Δ_0. Figure 3 plots distance between the gap of the Leggett mode and the minimum energy of the two-particle continuum as a

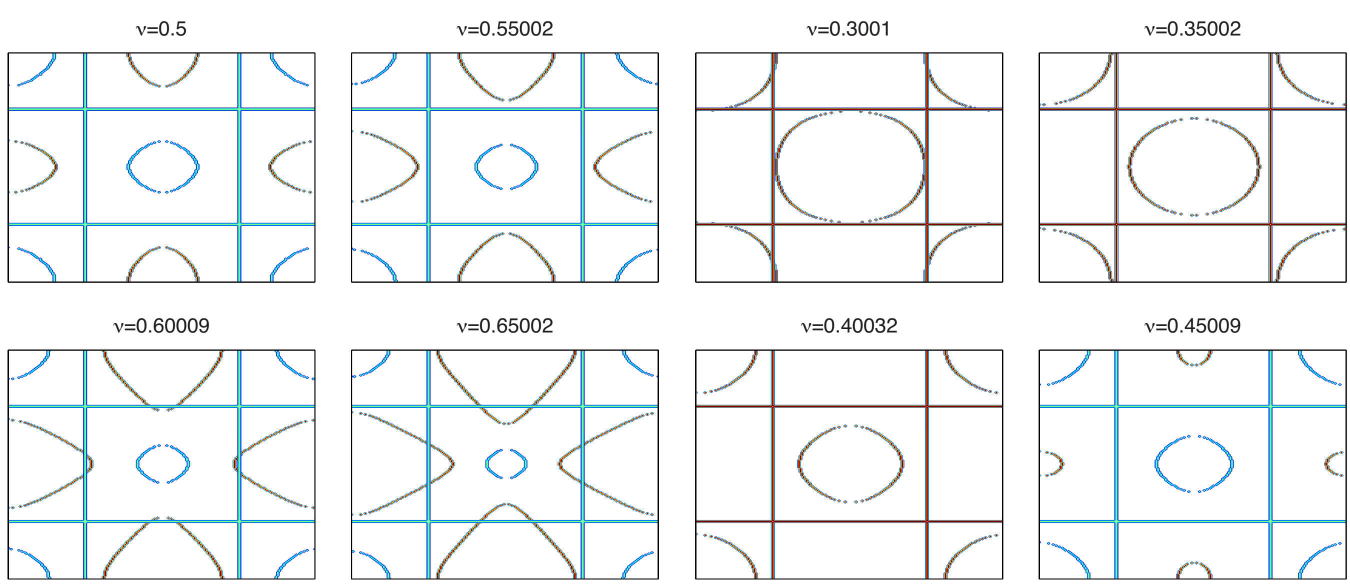

FIG. 2. (Color online) Plots of Fermi surface as a function of chemical potential for $0.3<\nu<0.65$. The relevant filling fractions are shown as ν in the title of the figure. The electron pockets first appear at approximately $\nu=0.4$ and cross the nodal lines at $\nu=0.6$. The nature of the hole pockets does not change substantially over the range shown here.

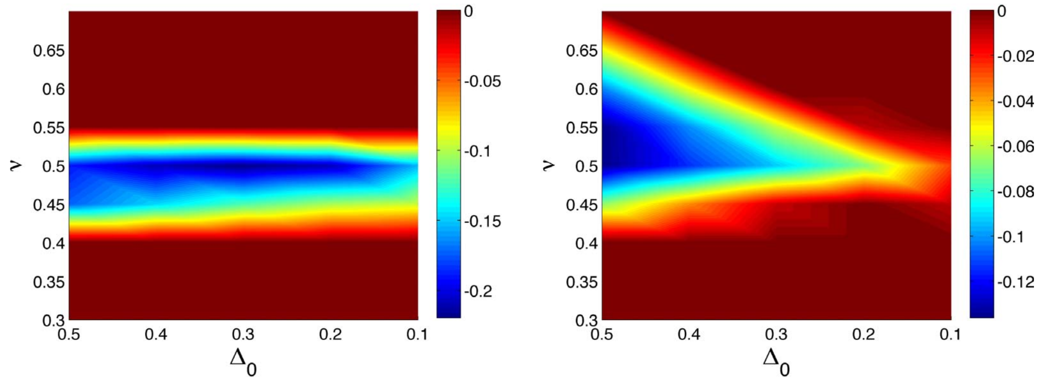

FIG. 3. (Color online) Distance between the Leggett mode and two-particle continuum for (a) extended s-wave and (b) ordinary s-wave gaps, as a function of filling fraction ν and gap magnitude Δ_0 in eV. Dark maroon area indicates regions where the Leggett mode lies above the two-particle continuum. Blue regions indicate maximum distance from the two-particle continuum. The vertical colorbar indicates the energy scale of these differences, as a fraction of the two-particle continuum 2 min Δ_0.

function of Δ_0 for both extended s-wave ($\Gamma_k = \cos k_x \cos k_y$) and standard s-wave ($\Gamma_k = 1$) gaps.

The principle difference between the two nodeless gaps is the range of dopings over which the Leggett mode is expected to be observable. In the pure s-wave case, the two-particle continuum is given by $2\Delta_0$, independent of the shape of the Fermi surface. Hence, as seen in Fig. 3(b), the dominant effect here is that the gap of the Leggett mode scales sublinearly in Δ_0, and hence becomes observable only at large values of the gap. Its separation from the two-particle continuum is extremely small at the small values of Δ_0 expected to occur near half filling. (Away from half filling, the gap of the Leggett mode lies above the two-particle continuum, as shown in the figure, due to the Fermi-surface effects discussed above.) In the extended s-wave case, however, the minimum of the gap also depends on how close the Fermi surface comes to the nodes of the gap function. Hence the dependence on filling fraction here is more pronounced [Fig. 3(a)]; for all values of Δ_0 the Leggett mode sits definitively below the two-particle continuum in the interval $0.45 < \nu < 0.5$. Further from half filling, where the nodes of the extended s-wave gap sit closer to the Fermi surface, the mode is never visible. Ω_0 is smaller overall in the extended s-wave case, compensating for the fact that the minimum of the two-particle continuum is de facto smaller than in the standard s-wave case. Most notably, for the small values of Δ_0 expected near 1/2 filling, we expect the Leggett mode to be below the two-particle continuum in the extended s-wave case

C. Dispersion of the Leggett mode for extended s-wave gap

We now return to the general form of the effective action for the phase degrees of freedom and analyze the structure of its modes at small q. In the absence of the Coulomb interaction, the form of the dispersion is effectively characterized by

$$w^2 = \frac{1}{2}\left[q^2(c_{\phi\phi}^2 + c_{\varphi\varphi}^2) + \Omega_0^2 \pm \sqrt{\{q^2(c_{\varphi\varphi}^2 - c_{\phi\phi}^2) + \Omega_0^2\}^2 + \frac{4c_{\phi\varphi}^4}{N_{\phi\phi}N_{\varphi\varphi}} q^4 \cos^2 2\theta}\right], \quad (13)$$

where θ is the angle in the (k_x, k_y) plane. If $c_{\phi\varphi}$ vanishes, we retrieve the gapless Goldstone mode and the gapped Leggett mode. From Eq. (12), we find that adding the Coulomb term modifies this according to

$$w^2 = \frac{1}{2}[\{c_{\phi\phi}^2[1 - 4N_{\phi\phi}U(q)] + c_{\varphi\varphi}^2\}q^2 + \Omega_0^2] \pm \frac{1}{2}\sqrt{\{q^2\{c_{\varphi\varphi}^2 - c_{\phi\phi}^2[1 - 4N_{\phi\phi}U(q)]\} + \Omega_0^2\}^2 + \frac{4c_{\phi\varphi}^4 q^4[1 - 4N_{\phi\phi}U(q)]}{N_{\phi\phi}N_{\varphi\varphi}}\cos^2(2\theta)}. \quad (14)$$

In this case, taking the negative sign for $U(q) \sim q^{-1}$, (the unscreened Coulomb interaction in two dimensions) results in $\omega^2 < 0$, indicating that the Goldstone mode has been replaced by a plasma mode. The structure of the Leggett mode is, however, largely unchanged by the presence of the Coulomb interaction. In particular, we still have $\lim_{q\to -} \omega(q) = \Omega_0$.

Figure 4(a) plots the dispersion relation $\Omega(k)$ for the low-energy modes for several values of Δ_0, μ. As we have kept only terms to quadratic order in q, Ω, we expect this to be

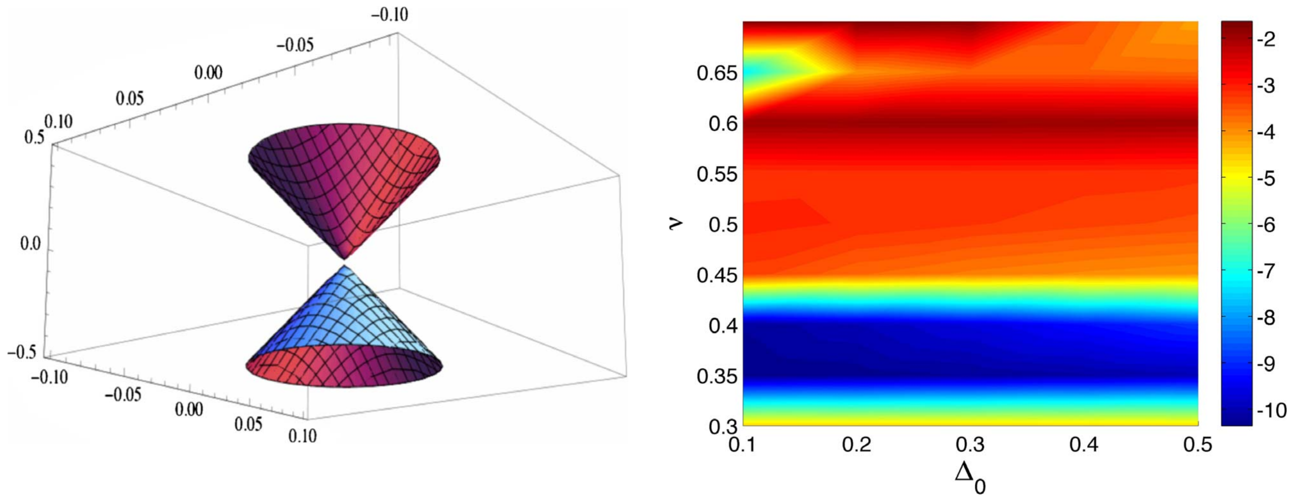

FIG. 4. (Color online) Velocity of the dispersion relations Ω vs q as a function of filling ν and gap magnitude Δ_0 for the extended s-wave gap $\Delta=\Delta_0 \cos k_x \cos k_y$. For small q, the qualitative shape of the dispersion (a) (shown at $\Delta_0=0.1$, $\nu=0.4$) does not depend strongly on either the form of U or the precise choice of Δ_0 and ν. However, the velocity, plotted as a function of Δ_0 and ν in (b), is sharply sensitive to the Leggett gap and chemical potential. In particular, the magnitude of the velocity increases sharply as the filling fraction decreases.

valid for small q and have restricted the range of the plots accordingly. The important feature to note is that the velocity anisotropy, due to the off-diagonal terms $c_{\phi\varphi}(q_x^2-q_y^2)$, is relatively small and the dispersion is approximately rotationally invariant. Because of this, the dispersion relation of the Leggett mode is well characterized by the gap Ω_0 (cf. Sec. III A) and the velocity $v\equiv\lim_{q\to\infty}\omega(q)$. This latter is plotted for the extended s-wave gap in Fig. 4(b).

IV. CONCLUSIONS

We have obtained the fluctuation action for the superconducting phase collective modes of a two-orbital model for iron-based superconductors with particular emphasis on the antisymmetric Leggett mode. By fixing the parameters of the band structure, our calculation has identified the range of doping and superconducting gap magnitude over which the undamped Leggett mode exists below the two-particle continuum. As the Leggett mode's visibility increases with the magnitude of the superconducting gap, this result also suggests that if the bandwidth is narrower, there is a higher possibility of observing the undamped Leggett mode. Therefore, a strong renormalization of bands could enhance the existence of an undamped Leggett mode. Unfortunately, the mode and its dispersion are insensitive to the sign of the order parameter on Fermi surfaces, and the mode does not qualitatively distinguish between the sign-changed s-wave and a normal s-wave superconductors. However, we find that quantitative characteristics of the mode can, in principle, distinguish between such different pairing symmetries. First, we find that the Leggett mode does lie below the two-particle continuum, near half filling and sufficiently deep in the superconducting region, for the extended as well as normal s-wave gap. This is distinct from the case of nodal gaps, where low-energy quasiparticles are always expected to broaden the Leggett mode resonance. Second, we find that the difference in signatures between the two kinds of s-wave pairing symmetry investigated here is subtle, but that the extended s-wave gap is visible over a narrower range in doping, but further below the two-particle continuum over much of its range of detectability. This difference comes from the different doping dependence of the two s-wave gap functions: unlike the normal, sign-unchanging s-wave gap, the $s^{\pm}$ order parameter will most likely change upon doping as the Fermi surfaces become closer to the line of zeroes that a sign-changing gap should have in the Brillouin zone. This gap variation upon doping is present in both strong and weak coupling models.[20] In this situation, the Leggett mode will move from a relatively sharp mode below the two-particle continuum into a strongly damped mode above the two-particle continuum as doping is increased. This quantitative change can, in principle, be observed in experiments.

It has been claimed that the Leggett mode has been observed in MgB_2 by Raman scattering[49] and point-contact transport measurements,[50] although the energies of the Leggett mode measured in the two experiments are different. Reference 51 found that in the weak-coupling treatment of superconductors with an $s_{\pm}$ gap, however, the A_{1g} Leggett mode does not couple to Raman scattering. The analysis carried out here relies heavily on the fact that iron-based superconductors are more strongly coupled than MgB_2, and that the superconducting phase is thus well described by considering the orbital, rather than the band, basis. This leads to a result which differs from that of the weakly coupled approach in two ways. First, the strong-coupling approach suggests that the Leggett mode should be observable in Raman spectra. Second, in the strong-coupling treatment, the different orbital symmetries should be kept explicitly when determining the relevant Raman channels. For our model, the Leggett mode is caused by an oscillation between the condensates involving the scattering of a pair of d_{xz}-orbital electrons into a pair of d_{yz}-orbital electrons. Such a process causes a relative density fluctuation, $\delta n = n_{xz} - n_{yz}$, between two orbitals, which belongs to the B_{1g} irreducible representation of the point group (D_{4h}) of the crystals. Therefore, the Leggett mode is a B_{1g} mode in this orbital-based model and should exist in the B_{1g} channel in Raman-scattering experiments. [Without the orbital characters, the Leggett mode should be a pure A_{1g} mode, as is the case in MgB_2 (Ref. 49)]. Thus, observing the Leggett mode in channels other than A_{1g} should provide important evidence about the orbital structure of condensed pairs in the iron-based superconductors.

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APPENDIX A: CALCULATING THE PHASE-ONLY EFFECTIVE ACTION

We begin by deriving the effective phase-only action for a generic Hamiltonian of the form

$$H = \sum_{\alpha,\beta,r,r'} \sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{\alpha,r,\sigma}[\epsilon(r,r')_{\alpha\beta} - \mu\delta_{\alpha\beta}]c_{\beta,r',\sigma} + V_{\alpha,\beta}(r;r')b^{\dagger}_{\alpha,r}b_{\beta,r'} + ieU(r-r')\rho_r\rho_{r'}. \tag{A1}$$

Here α,β are orbital indices, V is the superconducting interaction [in our model, a spin-spin antiferromagnetic interaction decoupled in the Cooper channel to give us $\cos(k_x)\cos(k_y)$ pairing], and U is the Coulomb interaction. The density is given by $\rho_r = \Sigma_{\alpha\sigma}c^{\dagger}_{\alpha,r,\sigma}c_{\alpha,r,\sigma}$ and the superconducting bilinear is $b^{\dagger}_{\alpha,r} = c^{\dagger}_{\alpha,r,\uparrow}c^{\dagger}_{\alpha,r,\downarrow}$.

We may decouple the two four-fermion interactions by means of two Hubbard-Stratonovich transformations. This decoupling gives the action

$$\begin{aligned} S = \sum_{\alpha,\beta,r,r'} \Bigg\{ & \sum_{\sigma} c^{\dagger}_{\alpha,r,\sigma}[(\partial/\partial_\tau - \mu)\delta_{\alpha,\beta} + \epsilon_{\alpha,\beta}(r,r')]c_{\beta,r',\sigma} \\ & - \delta_{r,r'}[\Phi_{\alpha r}b_{\alpha,r'} + \Phi^{\dagger}_{\alpha r}b^{\dagger}_{\alpha,r'}] - ie\delta_{r,r'}[\chi_r\rho_{r'} + \chi^{*}_r\rho_{r'}] \\ & - \Phi^{\dagger}_{\alpha r}V^{-1}_{\alpha,\beta}(r;r')\Phi_{\beta r'} - \chi_r U(r-r')^{-1}\chi_{r'} \Bigg\}, \end{aligned} \tag{A2}$$

where Φ is the Hubbard-Stratonovich field associated with the superconducting interaction and χ is associated with the Coulomb interaction.

In computing this effective action, we follow the method of Ref. 47 to isolate the action for the phase degrees of freedom. That is, taking $\Phi_{\alpha r} = \Delta_{\alpha r}e^{i\theta_\alpha(r)}$, we perform the gauge transformation

$$c_{\alpha,r,\sigma} \to e^{i\theta_\alpha(r)/2}c_{\alpha,r,\sigma} \tag{A3}$$

to absorb all terms involving the phase of the superconducting order parameter into the first term of Eq. (A2). We then have

$$\begin{aligned} S = \sum_{\alpha,\beta,r,r'} \Bigg\{ & \sum_{\sigma} c^{\dagger}_{\alpha,r,\sigma}e^{-i\theta_\alpha(r)/2}[(\partial/\partial_\tau - \mu)\delta_{\alpha,\beta} + \epsilon_{\alpha,\beta}(r,r')] \\ & \times c_{\beta,r',\sigma}e^{i\theta_\alpha(r')/2} - \delta_{r,r'}[\Delta_{\alpha r}(b_{\alpha,r'} + b^{\dagger}_{\alpha,r'})] \\ & - ie\delta_{r,r'}[\chi_r\rho_{r'} + \chi^{*}_r\rho_{r'}] \\ & - \Phi^{\dagger}_{\alpha r}V^{-1}_{\alpha,\beta}(r;r')\Phi_{\beta r'} - \chi_r U(r-r')^{-1}\chi_{r'} \Bigg\}. \end{aligned} \tag{A4}$$

It is convenient to re-express the kinetic terms as

$$\begin{aligned} \sum_{\alpha,\beta,r,r'} \{ & c^{\dagger}_{\alpha,r,\uparrow}e^{-i\theta_\alpha(r)/2}[(\partial/\partial_\tau - \mu)\delta_{\alpha,\beta} + \epsilon_{\alpha,\beta}(r,r')]c_{\beta,r',\uparrow}e^{i\theta_\beta(r')/2} - c_{\alpha,r,\downarrow}e^{-i\theta_\beta(r')/2}[(-\partial/\partial_\tau - \mu)\delta_{\alpha,\beta} + \epsilon_{\beta,\alpha}(r',r)]c^{\dagger}_{\beta,r',\downarrow}e^{i\theta_\alpha(r)/2} \\ & + \delta_{\alpha,\beta}\delta_{r,r'}e^{-i\theta_\alpha(r)/2}[(\partial/\partial_\tau - \mu) + \epsilon_{\alpha,\beta}(r',r)]e^{i\theta_\beta(r')/2}\}. \end{aligned} \tag{A5}$$

The first two terms can now be combined with the rest of the fermionic action can be expressed in matrix form in the BCS basis. The final line of Eq. (A5) gives a separate contribution to the action, which can be expressed, to quadratic order in $\theta, \partial_r\theta$

$$\int d^2r d\tau \left\{ \frac{i}{2}\frac{\partial}{\partial_\tau}\theta_\beta(r) + \int d^2k \left[\frac{1}{2}\frac{\partial}{\partial_{r_i}}\theta_\beta(r)\frac{\partial}{\partial_{k_i}}\epsilon_{\beta,\beta} - \frac{1}{8}\theta_\beta(r)\frac{\partial^2}{\partial_{r_i}\partial_{r_j}}\theta_\beta(r)\frac{\partial^2}{\partial_{k_i}\partial_{k_j}}\epsilon_{\beta,\beta}(k) \right] \right\}. \tag{A6}$$

The first term is a total derivative and will not contribute to the dynamics of the phase-only effective action. The second term in any case vanishes, as v is odd over the Brillouin zone. Hence only the last term appears in the effective action.

As we are interested in the dynamics of the phase degrees of freedom, we replace $\Delta_{\alpha,r}$ by its mean-field value. For the time being, we drop the Coulomb terms by setting $U=0$, $\chi=0$; these terms are discussed in Sec. II D. We further consider only the slowly varying phase fluctuations. This allows us to expand the exponentials of the fermionic terms in Eq. (A4) using

$$
\begin{aligned}
e^{-i/2[\theta_\alpha(r)-\theta_\alpha(r')]} &\approx 1-\frac{i}{2}[\theta_\alpha(r)-\theta_\alpha(r')] \\
&\quad -\frac{1}{4}[\theta_\alpha(r)-\theta_\alpha(r')]^2 e^{-i/2[\theta_1(r)-\theta_2(r')]} \\
&\approx e^{-i/2\varphi_0}\bigg\{1-\frac{i}{2}[\theta_1(r)-\theta_2(r')-\varphi_0] \\
&\quad -\frac{1}{4}[\theta_\alpha(r)-\theta_\alpha(r')-\varphi_0]^2\bigg\},
\end{aligned}
\tag{A7}
$$

where we have explicitly separated out the possible background expectation value of the phase difference φ_0 between the gaps. In practice $\varphi_0=0$ is set by the mean-field equations.

Defining $\psi_r^\dagger=(c_{1,r,\uparrow}^\dagger,c_{1,r,\downarrow},c_{2,r,\uparrow}^\dagger,c_{2,r,\downarrow})$, we may now express the first two terms in Eq. (A5), after Fourier transforming, as

$$
S_{Fermi}=\int d\omega_1 d\omega_2 \frac{d^2k_1}{4\pi^2}\frac{d^2k_2}{4\pi^2}\psi_{k_1,\omega_1}^\dagger G^{-1}(k_1,k_2,i\omega_1,i\omega_2)\psi_{k_2,\omega_2}
\tag{A8}
$$

with

$$
G^{-1}(k_1,k_2,i\omega_1,i\omega_2)=G_0^{-1}(k_1,\omega_1)\,\delta_{q,0}\delta_{\Omega,0}+\Sigma(k_1,k_2,i\omega_1,i\omega_2),
\tag{A9}
$$

where here $q\equiv k_1-k_2,\Omega\equiv\omega_1-\omega_2$. We have

$$
G_0^{-1}(k,\omega)=\begin{pmatrix} i\omega+\epsilon_x & \Delta_1 & \epsilon_{xy} & 0 \\ \Delta_1 & i\omega-\epsilon_x & 0 & -\epsilon_{xy} \\ \epsilon_{xy} & 0 & i\omega+\epsilon_y & \Delta_2 \\ 0 & -\epsilon_{xy} & \Delta_2 & i\omega-\epsilon_y \end{pmatrix},
\tag{A10}
$$

where $\epsilon_\alpha\equiv\epsilon_\alpha(k)$ is the kinetic energy in the orbital basis and $\Delta_\alpha\equiv\Delta_\alpha(k)$ is the momentum-dependent superconducting gap in each orbital. The second part of Eq. (A9) is given by

$$
\begin{aligned}
\Sigma(k,q,i\omega,i\Omega) &= -\frac{\Omega}{2}\begin{pmatrix}\theta_1\sigma_z & 0\\ 0 & \theta_2\sigma_z\end{pmatrix}+\frac{i}{2}\begin{pmatrix}\theta_1\delta_q(\epsilon_x)\sigma_0 & [\theta\epsilon_{xy}(k_1)-\theta_1\epsilon_{xy}(k_2)]\sigma_0\\ [\theta_1\epsilon_{xy}(k_1)-\theta_2\epsilon_{xy}(k_2)]\sigma_0 & \theta_2\delta_q(\epsilon_y)\sigma_0\end{pmatrix}, \\
&\quad -\frac{1}{8}\sum_{k_3,i\omega_3}\{\theta_1(k_3,i\omega_3)\ \ \theta_2[q-k_3,i(\Omega-\omega_3)]\}\begin{bmatrix}\delta_{q,k_3}^{(2)}(\epsilon_x)\sigma_z & 0\\ 0 & \delta_{q,k_3}^{(2)}(\epsilon_x)\sigma_z\end{bmatrix}\begin{bmatrix}\theta_1(q-k_3,i(\Omega-\omega_3))\\ \theta_2(q-k_3,i(\Omega-\omega_3))\end{bmatrix}, \\
&\quad -\frac{1}{8}\sum_{k_3,i\omega_3}\begin{pmatrix}0 & B(k_1,i\omega_1,k_2,i\omega_2,k_3\,.\,i\omega_3)\sigma_z\\ C(k_1,i\omega_1,k_2,i\omega_2,k_3\,.\,i\omega_3)\sigma_z & 0\end{pmatrix},
\end{aligned}
\tag{A11}
$$

where $\theta_\alpha\equiv\theta_\alpha(q,i\Omega)$, and we have defined the discrete derivatives

$$
\begin{aligned}
\delta_q\epsilon_{\alpha\beta} &= \epsilon_{\alpha\beta}(k_1)-\epsilon_{\alpha\beta}(k_2), \\
\delta_q^{(2)}\epsilon_{\alpha\beta} &= \epsilon_{\alpha\beta}(k_1)-\epsilon_{\alpha\beta}(k_2+k_3)-\epsilon_{\alpha\beta}(k_1-k_3)+\epsilon_{\alpha\beta}(k_2).
\end{aligned}
\tag{A12}
$$

The off-diagonal terms quadratic in the phases are

$$
\begin{aligned}
B(k_1,i\omega_1,k_2,i\omega_2,k_3,i\omega_3) &= \{\theta_2(k_3,i\omega_3)\,\theta_2[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_1)-\theta_2(k_3,i\omega_3)\,\theta_1[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_2+k_3) \\
&\quad -\theta_1(k_3,i\omega_3)\,\theta_2[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_1-k_3)+\theta_1(k_3,i\omega_3)\,\theta_1[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_2)\}, \\
C(k_1,i\omega_1,k_2,i\omega_2,k_3,i\omega_3) &= \{\theta_1(k_3,i\omega_3)\,\theta_1[q-k_3,i(\Omega-\omega_3)]\epsilon_{21}(k_1)-\theta_1(k_3,i\omega_3)\,\theta_2[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_2+k_3) \\
&\quad -\theta_2(k_3,i\omega_3)\,\theta_1[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_1-k_3)+\theta_2(k_3,i\omega_3)\,\theta_2[q-k_3,i(\Omega-\omega_3)]\epsilon_{xy}(k_2)\}.
\end{aligned}
\tag{A13}
$$

Thus in our treatment, the block diagonal terms involve only discrete differences of the band energies, which will become derivatives when the momentum of the phase variables is small. The off-diagonal terms contribute, as well as such differences, a term which is finite at $q=0$ (or $k_1=k_2$). Hence the gap of the Leggett mode is, in the absence of interorbital pairing, generated by the kinetic mixing between the two orbitals.

To obtain the effective action, we integrate out the fermions in Eq. (A8). In practice, we must evaluate the result perturbatively in Σ. Specifically, we have

$$S_{eff} = S_{MF} - Tr\ \ln(1 - G_0\Sigma) \approx S_{MF} + Tr(G_0\Sigma) + \frac{1}{2}Tr(G_0\Sigma G_0\Sigma), \tag{A14}$$

where S_{MF} is the mean-field action, from which we self-consistently determine the values of Δ_1,Δ_2. Here we will evaluate the low-energy, long-wavelength limit of the effective action Eq. (A14) by keeping terms to quadratic order in q,Ω and $\theta_\alpha(q,\Omega)$.

1. Evaluating $TrG_0\Sigma$ and $TrG_0\Sigma G_0\Sigma$

For reference, here we give a more detailed account of the calculation in Sec. II. The separate expressions for the two traces are

$$Tr(G_0\Sigma) = \int \frac{d^2k}{(2\pi)^2}\left\{-\frac{\epsilon_{xy}}{4}[\varphi(q,i\Omega)\varphi(-q,-i\Omega)]\left[1 - \frac{\epsilon_{xy}}{(E_+ - E_-)E_+^{(\Delta)}E_-^{(\Delta)}}[E_-^{(\Delta)}E_+ - E_+^{(\Delta)}E_-]\right]\right\} - \int \frac{d^2k}{(2\pi)^2}\left\{\frac{q_iq_j}{8}[\theta_1(q)\quad \theta_2(q)]\right.$$
$$\times\begin{pmatrix} m_{ij}^{(1)}\left[1 - \frac{E_+(E_+ - \epsilon_y)}{E_+^{(\Delta)}(E_+ - E_-)} + \frac{E_-(E_- - \epsilon_y)}{E_-^{(\Delta)}(E_+ - E_-)}\right] & m_{ij}^{(12)}\frac{\epsilon_{xy}}{(E_+ - E_-)}\left[\frac{E_+}{E_+^{(\Delta)}} - \frac{E_-}{E_-^{(\Delta)}}\right] \\ m_{ij}^{(12)}\frac{\epsilon_{xy}}{(E_+ - E_-)}\left[\frac{E_+}{E_+^{(\Delta)}} - \frac{E_-}{E_-^{(\Delta)}}\right] & m_{ij}^{(2)}\left[1 - \frac{E_+(E_+ - \epsilon_x)}{E_+^{(\Delta)}(E_+ - E_-)} + \frac{E_-(E_- - \epsilon_x)}{E_-^{(\Delta)}(E_+ - E_-)}\right]\end{pmatrix}\left.\begin{bmatrix}\theta_1(-q)\\ \theta_2(-q)\end{bmatrix}\right\}, \tag{A15}$$

where $m_{ij}^{(\alpha)} \equiv \frac{\partial^2\epsilon_\alpha}{\partial k_i \partial k_j}$, and we define $\varphi(q) = \theta_1(q) - \theta_2(q)$. We have dropped the linear term in Ω, because it is a total derivative and hence should not contribute to the action. Here all ϵ, E, and Δ are evaluated at the momentum k to be integrated over. Note that we have also included the quadratic terms in the last line of Eq. (A5).

Evaluating $Tr(G_0\Sigma G_0\Sigma)$ gives

$$\frac{1}{2}Tr(G\Sigma G\Sigma) = -\frac{\Omega^2}{8}[\phi(q)\varphi(q)]\begin{pmatrix} N_{\phi\phi} & 0 \\ 0 & N_{\varphi\varphi}\end{pmatrix}\begin{bmatrix}\phi(-q)\\ \varphi(-q)\end{bmatrix} + \int\frac{d^2k}{(2\pi)^2}\left\{\frac{\epsilon_{xy}^2}{4}\varphi(q)\varphi(-q)\frac{-E_+^{(\Delta)}E_-^{(\Delta)} + \Delta^2 + E_+E_-}{E_+^{(\Delta)}E_-^{(\Delta)}[E_+^{(\Delta)} + E_-^{(\Delta)}]}\right\}$$
$$+ \frac{1}{8}\frac{2q_iq_j}{[E_+^{(\Delta)} + E_-^{(\Delta)}](E_+ - E_-)^2}\left[1 - \frac{\Delta^2 + E_+E_-}{E_+^{(\Delta)}E_-^{(\Delta)}}\right][\phi(q)\varphi(q)]$$
$$\times\left\{\begin{pmatrix} -\left[\epsilon_{xy}^2 + \frac{1}{2}(\epsilon_x - \epsilon_y)^2\right]v_i^{(xy)}v_j^{(xy)} - \epsilon_{xy}^2 v_{i\phi}v_{j\phi} & \frac{\epsilon_{xy}^2}{2}(v_{i\phi}v_{j\varphi} + v_{j\phi}v_{i\varphi}) \\ \frac{\epsilon_{xy}^2}{2}(v_{i\phi}v_{j\varphi} + v_{j\phi}v_{i\varphi}) & \left(\epsilon_{xy}^2 - \frac{1}{2}(\epsilon_x - \epsilon_y)^2\right)v_i^{(xy)}v_j^{(xy)} - \epsilon_{xy}^2 v_{i\varphi}v_{j\varphi}\end{pmatrix}\right.$$
$$+\left.\begin{bmatrix} 0 & -\frac{\epsilon_{xy}(\epsilon_x - \epsilon_y)}{4}[v_i^{(xy)}v_j^{(\phi)} + v_j^{(xy)}v_i^{(\phi)}] \\ -\frac{\epsilon_{xy}(\epsilon_x - \epsilon_y)}{4}(v_i^{(xy)}v_j^{(\phi)} + v_j^{(xy)}v_i^{(\phi)}) & -\frac{\epsilon_{xy}(\epsilon_x - \epsilon_y)}{2}[v_i^{(xy)}v_j^{(\varphi)} + v_j^{(xy)}v_i^{(\varphi)}]\end{bmatrix} + \begin{pmatrix} 0 & \tilde{\Lambda}_{\phi\varphi} \\ \tilde{\Lambda}_{\phi\varphi} & \tilde{\Lambda}_{\varphi\varphi}\end{pmatrix}\right\}\begin{bmatrix}\phi(-q)\\ \varphi(-q)\end{bmatrix}, \tag{A16}$$

where $v_{\phi i} \equiv \partial(\epsilon_x + \epsilon_y)/\partial k_i, v_{\varphi i} \equiv \partial(\epsilon_x - \epsilon_y)/\partial k_i$. Here $\tilde{\Lambda}_{\alpha\beta}$ are terms which come from expanding traces involving B in Eq. (A13) to quadratic order in q.

Combining the mass terms from Eqs. (A15) and (A16) gives the total mass term

$$M = \int\frac{d^2k}{(2\pi)^2}\left\{\frac{4\Delta^2\epsilon_{xy}^2}{E_+^{(\Delta)}E_-^{(\Delta)}(E_+^{(\Delta)} + E_-^{(\Delta)})} - 2\epsilon_{xy}\right\} \equiv \int\frac{d^2k}{(2\pi)^2}\frac{4\Delta^2\epsilon_{xy}^2}{E_+^{(\Delta)}E_-^{(\Delta)}(E_+^{(\Delta)} + E_-^{(\Delta)})}, \tag{A17}$$

where the second equality holds because in practice ϵ_{xy} averages to 0 over the Brillouin zone.

In simplified form, the momentum-dependent terms are

$$\begin{pmatrix} N_{\phi\phi}c^2_{\phi\phi,ij} & c^2_{\phi\varphi,ij} \\ c^2_{\phi\varphi,ij} & N_{\varphi\varphi}c^2_{\varphi\varphi,ij}\end{pmatrix} = \frac{1}{8}\int\frac{d^2k}{(2\pi)^2}\Bigg\{-\frac{1}{(E_+-E_-)}\left[\frac{E_+}{E_+^{(\Delta)}}-\frac{E_-}{E_-^{(\Delta)}}\right]\begin{bmatrix} m^{(xx)}_{ij}\epsilon_x - 2m^{(xy)}_{ij}\epsilon_{xy}+m^{(yy)}_{ij}\epsilon_y & m^{(xx)}_{ij}\epsilon_x - m^{(yy)}_{ij}\epsilon_y \\ m^{(xx)}_{ij}\epsilon_x - m^{(yy)}_{ij}\epsilon_y & m^{(xx)}_{ij}\epsilon_x + 2m^{(xy)}_{ij}\epsilon_{xy}+m^{(yy)}_{ij}\epsilon_y\end{bmatrix}$$
$$+\frac{2}{[E_+^{(\Delta)}+E_-^{(\Delta)}](E_+-E_-)^2}\left[1-\frac{\Delta^2+E_+E_-}{E_+^{(\Delta)}E_-^{(\Delta)}}\right]$$
$$\times\Bigg[\begin{pmatrix} -\left[\epsilon_{xy}^2+\frac{1}{2}(\epsilon_x-\epsilon_y)^2\right]v_i^{(xy)}v_j^{(xy)}-\epsilon_{xy}^2v_{i\phi}v_{j\phi} & \frac{\epsilon_{xy}^2}{2}(v_{i\phi}v_{j\varphi}+v_{j\phi}v_{i\varphi}) \\ \frac{\epsilon_{xy}^2}{2}(v_{i\phi}v_{j\varphi}+v_{j\phi}v_{i\varphi}) & \left[\epsilon_{xy}^2-\frac{1}{2}(\epsilon_x-\epsilon_y)^2\right]v_i^{(xy)}v_j^{(xy)}-\epsilon_{xy}^2v_{i\varphi}v_{j\varphi}\end{pmatrix}$$
$$+\begin{pmatrix} 0 & -\frac{\epsilon_{xy}(\epsilon_x-\epsilon_y)}{4}[v_i^{(xy)}v_j^{(\phi)}+v_j^{(xy)}v_i^{(\phi)}] \\ -\frac{\epsilon_{xy}(\epsilon_x-\epsilon_y)}{4}(v_i^{(xy)}v_j^{(\phi)}+v_j^{(xy)}v_i^{(\phi)}) & -\frac{\epsilon_{xy}(\epsilon_x-\epsilon_y)}{2}[v_i^{(xy)}v_j^{(\varphi)}+v_j^{(xy)}v_i^{(\varphi)}]\end{pmatrix}+\begin{pmatrix} 0 & \tilde{\Lambda}_{\phi\varphi} \\ \tilde{\Lambda}_{\phi\varphi} & \tilde{\Lambda}_{\varphi\varphi}\end{pmatrix}\Bigg]\Bigg\}. \tag{A18}$$

APPENDIX B: EFFECTIVE ACTION WITH COULOMB TERMS

Including terms generated by the Coulomb repulsion modifies the interaction term Σ of the full fermion propagator Eq. (A11) according to[46]

$$\Sigma = \tau_3\otimes 1\left(i\frac{i\Omega\phi}{2}-ie\chi\right)+\tau_3\otimes\tau_3 i\frac{\Omega\varphi}{2}+\Sigma'_{kin}, \tag{B1}$$

where Σ_{kin} involves only spatial derivatives of the phases θ_1 and θ_2. Here χ is the Hubbard-Stratonovich field associated with the Coulomb interaction. The form of the coupling for χ to fermions can be deduced from gauge invariance: the phase θ_i is obviously a gauge-dependent quantity, and the gauge-invariant degrees of freedom are the combinations $\partial_\tau\theta/2 - e\chi - eA_0$ and $\nabla\theta/2 - e/c\mathbf{A}$.[47] Hence the effective action for χ is the same as that for $\partial_\tau\theta/(2e)$. Equation (B1) indicates that χ couples in all cases like the time derivative of the *symmetric* component of the phase fluctuations.

To obtain the full effective action for the phase-only modes in the presence of Coulomb interactions, we first integrate out the fermions, giving an effective action for the three Hubbard-Stratonovich fields ϕ,φ,χ. There are two relevant contributions: from $TrG\Sigma$, we obtain

$$-ie\chi(q)Tr[(\tau_3\otimes 1)G_{k-q}] = -ie\chi(q)\langle\rho_{k-q}\rangle \tag{B2}$$

which cancels the first-order term in χ in the effective action Eq. (A2).

From $TrG\Sigma G\Sigma$, we obtain contributions whose coefficients are *the same* as the contributions from the time derivatives of ϕ. In particular, as the coefficients of the cross terms in q,Ω from traces $G\Sigma G\Sigma$ all vanish, the couplings between χ and ϕ,φ depend only on Ω. Hence the effective action for the fields ϕ,φ,χ has the form

$$S_{eff} = \int d\Omega d^2q(\phi\quad\varphi\quad\chi)\begin{pmatrix} N_{\phi\phi}[\Omega^2-c^2_{\phi\phi}q^2] & c^2_{\phi\varphi}(q_x^2-q_y^2) & -2\Omega N_{\phi\phi} \\ c^2_{\phi\varphi}(q_x^2-q_y^2) & N_{\varphi\varphi}[\Omega^2-\Omega_0^2-c^2_{\varphi\varphi}q^2] & 0 \\ -2\Omega N_{\phi\phi} & 0 & U^{-1}(q)+4N_{\phi\phi}\end{pmatrix}\begin{pmatrix}\phi\\ \varphi\\ \chi\end{pmatrix}+\Delta_\alpha V^{-1}_{\alpha,\beta}\Delta_\beta, \tag{B3}$$

where the coefficients N, c are given in Eqs. (5), (A15), and (A16). The dispersion relation is given by finding the values of q, Ω at which $\mathcal{M}$ is singular. Depending on the values of the parameters, $\mathcal{M}$ may have one or two modes which are finite as $q \to 0$. One of these is the gapped Leggett mode; the other is a soundlike mode (the Carlson-Goldman mode) which we find to be absent at $T=0$, consistent with Ref. 47. The third mode is, of course, the plasma mode, which does not appear in the low-energy spectrum. To study only the phase modes, we may equivalently integrate out χ and ϕ to obtain Eq. (11).

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