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The symplectic- N t - J model and s_{\pm} superconductors

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The possible discovery of s_{\pm} superconducting gaps in the moderately correlated iron-based superconductors has raised the question of how to properly treat s_{\pm} gaps in strongly correlated superconductors. Unlike the d-wave cuprates, the Coulomb repulsion does not vanish by symmetry, and a careful treatment is essential. Thus far, only weak correlation approaches have included this Coulomb pseudopotential, which has motivated us to introduce a symplectic N treatment of the t - J model that incorporates the strong Coulomb repulsion through the complete elimination of on-site pairing. Through a proper extension of time-reversal symmetry to the large N limit, symplectic- N is the first superconducting large N solution of the t - J model. For d-wave superconductors, the previous uncontrolled mean field solutions are reproduced, while for s_{\pm} superconductors, the $SU(2)$ constraint enforcing single occupancy acts as a pair chemical potential adjusting the location of the gap nodes. This adjustment can capture the wide variety of gaps proposed for the iron based superconductors: line and point nodes, as well as two different, but related full gaps on different Fermi surfaces.

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I. INTRODUCTION

The new family of iron-based superconductors¹ has expanded the study of high temperature superconductors from the single band, d-wave cuprate superconductors to include multi-band superconductors with full gaps. Experimental² and numerical³⁻⁵ work suggest a range of correlation strengths between different materials. From the theoretical point of view, weak and strong correlation approaches converge on many of the major features: most importantly, the predominantly s_{\pm} structure of the superconducting gap^{3,6-15}. The real materials are likely in the regime of moderate correlations where both approaches are useful. Unlike the d-wave cuprates, where the strong Coulomb repulsion is eliminated by symmetry, these multi-band s_{\pm} superconductors require a careful treatment of the Coulomb pseudopotential¹⁶. While this has been incorporated into weak coupling approaches^{7,10,12,17}, it has yet to be included in strong correlation treatments based on the t - J model. With this in mind, we introduce the symplectic- N t - J model. The use of a large N limit based on the symplectic group, $SP(N)$ allows a proper treatment of time-reversal in the large- N limit¹⁸⁻²⁰, making this the first superconducting large N treatment of the t - J model. Symplectic- N also replaces the usual $U(1)$ constraint of single-occupancy with a $SU(2)$ constraint that strictly eliminates on-site pairing²⁰. This $SU(2)$ constraint is essential to the treatment of s_{\pm} superconductors, where it acts as a pair chemical potential, adjusting the gap nodes to eliminate the Coulomb repulsion.

This paper is intended as an introduction to the symplectic- N t - J model, illustrating the importance of

the additional constraint with the example of s_{\pm} superconductors, and showing how this model contains a range of gap behaviors reproducing those found in various iron-based materials. We do not attempt to model any material specific properties, merely to qualitatively illustrate the effects of including the Coulomb pseudopotential in a strongly correlated model. We begin by reviewing the Coulomb pseudopotential in section II and demonstrate the lack of superconductivity in the $SU(N)$ t - J model corresponding to the usual slave boson mean field theory. In section III, we introduce symplectic Hubbard operators, which allow us to develop a superconducting large- N treatment of the t - J model. We demonstrate this mean field theory on several examples in section IV, before discussing the range of possible future directions in V.

II. THE COULOMB PSEUDOPOTENTIAL AND THE t - J MODEL

On-site pairing is disfavored by the Coulomb pseudopotential, which will cost a bare amount, $UN(0)$, where U is the on-site Coulomb repulsion and $N(0)$ is the density of states at the Fermi energy. However, in the weak coupling limit, where we assume the pairing is mediated by the exchange of a boson with characteristic frequency ω_B , the time scale of the pairing, ω_B is much longer than that of the Coulomb repulsion. In other words, while the effective electron-electron interaction is attractive, it is also retarded, meaning the electrons like to be in the same place, but at different times, while the Coulomb repulsion is a nearly instantaneous repulsion of two electrons at the same place and time. The Coulomb

pseudopotential is therefore renormalized¹⁶,

$$\mu^* = \frac{N(0)U}{1 + N(0)U \log \frac{E_F}{\omega_B}} \quad (1)$$

to weak coupling. If $T_c \propto \omega_B \exp(-1/\lambda)$, the attractive interaction is replaced by $\lambda \rightarrow \lambda - \mu^*$, which reduces T_c slightly at weak coupling, but does not destroy superconductivity. In BCS superconductivity, the bosons exchanged are phonons, and the Debye frequency, $\omega_D \ll E_F$. However, in more strongly correlated superconductors, the two time scales are of the same order, and the Coulomb pseudopotential can drastically affect the superconductivity. Strongly correlated examples, like the cuprate and heavy fermion superconductors, avoid this problem by developing a d-wave gap, where the pairing with a positive gap is exactly cancelled out by that with a negative gap, as guaranteed by the d-wave symmetry. This choice of gap neutralizes the Coulomb pseudopotential. However, the iron-based superconductors are widely believed to have an s_{\pm} gap, where the amount of cancellation between positive and negative gap regions is not protected by symmetry, and depends strongly on the Fermi surfaces (see Fig. 1). When this cancellation is incomplete, μ^* reduces T_c and it is extremely important to consider this effect when mapping out the phase diagram, as it affects the relative stability of s- and d-wave gaps. These effects have been incorporated in the weakly correlated solutions^{7,10,12,17}, but not yet in the strongly correlated approaches.

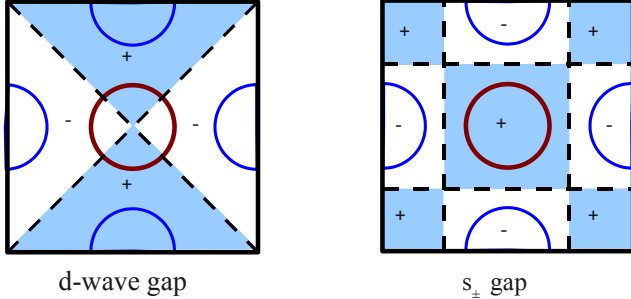


FIG. 1: (Color online) (Left) In the d-wave gap, the cancellation of the superconducting order parameter over the Fermi surface is guaranteed by symmetry, as the positive (blue) regions will exactly cancel the negative (white) regions. (Right) However, in the s_{\pm} superconducting gap, the amount of cancellation is extremely sensitive to the Fermi surface.

Here, we take the strongly correlated limit, $U \rightarrow \infty$ to eliminate double occupancy, which corresponds to taking $\mu^* \rightarrow \infty$. The Heisenberg model describes the insulating half-filled limit of the $t - J$ model, but generally holes ($n < 1$) or electrons ($n > 1$) will hop around in an anti-ferromagnetic background. Doubly occupied states must

be avoided, and the hopping is not that of free electrons. Rather, it is projected hopping, described by the $t - J$ model^{21,22},

$$H = - \sum_{ij} t_{ij} [X_{\sigma 0}(i)X_{0\sigma}(j) + \text{H.c.}] + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j. \quad (2)$$

The Hubbard operators, $X_{ab} = |a\rangle\langle b|$, where $|a\rangle = |0\rangle, |\sigma\rangle$ ensure that only empty sites, or holes can hop (or for $n > 1$ that electrons can only hop from doubly occupied sites to singly occupied sites). Here, $X_{\sigma 0}$ are projected hopping operators

Exact solutions of the $t - J$ model are unavailable, and the typical approach is to write down a mean field solution using the slave boson approach²³⁻²⁵, which divides the electron into charged, but spinless holons and neutral spinons. The most common choice is the $U(1)$ slave boson representation²⁷,

$$X_{\sigma 0} = f_{\sigma}^{\dagger} b, \quad (3)$$

so-called because it is invariant under $U(1)$ gauge transformations. However, mean field solutions do not necessarily satisfy all the conditions on the full model, and may not maintain the $\mu^* \rightarrow \infty$ limit. Large N approaches generate mean-field solutions by extending the $SU(2)$ $t - J$ model to some larger group. When developing a large N treatment of the hopping term, one must take care that the two terms are consistent, or in other words, that the charge fluctuations described by the t term generate the spin fluctuations in the Heisenberg term. The algebra of these operators, given by

$$\{X_{\alpha 0}, X_{0\beta}\} = f_{\alpha}^{\dagger} f_{\beta} + b^{\dagger} b \delta_{\alpha\beta}. \quad (4)$$

extends the algebra of Hubbard operators from $SU(2)$ to $SU(N)$, and we see that two charge fluctuations in sequence give rise to a spin fluctuation described by the $SU(N)$ spin operator, $S_{\alpha\beta} = f_{\alpha}^{\dagger} f_{\beta}$.

The large N limit of the full $SU(N)$ $t - J$ model is:

$$H = - \sum_{\langle ij \rangle} \frac{t_{ij}}{N} f_{i\alpha}^{\dagger} b_i b_j^{\dagger} f_{j\alpha} + \sum_{ij} \frac{J_{ij}}{N} (f_{i\alpha}^{\dagger} f_{j\alpha}) (f_{j\beta}^{\dagger} f_{i\beta}). \quad (5)$$

Decoupling the J term yields a dispersion for the spinons, but not pairing²⁸. There is no superconductivity in this large N limit.

While the large N limit of the $SU(N)$ $t - J$ model contains no superconductivity, $1/N$ corrections do yield an effective attractive electron-electron interaction⁴⁷, $\Gamma \sim 1/N$. The superconducting transition temperature, $T_C \sim e^{-N}$ is then non-perturbative in $1/N$ and far smaller than any finite power of $1/N$ corrections. While the $SU(N)$ expansion can suggest which pairing channels may become attractive, it clearly provides a very poor starting point to study the superconducting state. In the next section, we shall see that the $SU(N)$ large N limit loses the time-reversal symmetry necessary to describe superconductivity, which is not fully restored for any finite expansion in $1/N$.

III. THE SYMPLECTIC- N $t - J$ MODEL

A superconducting large N limit requires a proper definition of time-reversal, as Cooper pairs can only form between time-reversed pairs of electrons. If we attempt to generalize the time-reversal operation, θ from $SU(2)$ to $SU(N)$, the transformation of $SU(N)$ spins becomes $S_{\alpha\beta} \xrightarrow{\theta} \tilde{\alpha}\tilde{\beta}S_{-\beta-\alpha}$, where $\tilde{\alpha} = \text{sgn}(\alpha)$. However, not all $SU(N)$ spins, $S_{\alpha\beta} = f_{\alpha}^{\dagger}f_{\beta}$ invert under this time-reversal operation. In fact, there is no consistent definition of time-reversal in $SU(N)$ for any $N > 2$, which makes it impossible to properly capture singlet superconductivity to any finite order in the $SU(N)$ large N expansion. There is, however, a subset of spins that invert under time-reversal, which generate the group $SP(N)$. It turns out that the inversion of spins under time-reversal is actually equivalent to symplectic symmetry, and the only way to preserve time-reversal in the large N limit is to use symplectic spins^{18,19},

$$S_{\alpha\beta} = f_{\alpha}^{\dagger}f_{\beta} - \tilde{\alpha}\tilde{\beta}f_{-\beta}^{\dagger}f_{-\alpha}, \quad (6)$$

where α ranges from $-N/2$ to $N/2$. Here we use the fermionic representation because we are interested in the doped spin liquid states that become superconductors. Introducing doping means introducing a small number of mobile empty states, and we can represent the Hilbert space with the Hubbard operators, $X_{AB} = |A\rangle\langle B|$, where $|A\rangle = |0\rangle, |\alpha\rangle$, with $|\alpha\rangle$ representing the N possible spin states. When an electron hops on and off a site, it can flip the spin of the site. Mathematically, this action implies that the anticommutator of two Hubbard operators generates a spin operator. In a symplectic- N generalization of the t - J model, anticommuting two such Hubbard operators must generate a symplectic spin, satisfying the relations:

$$\begin{aligned} \{X_{\alpha 0}, X_{0\beta}\} &= X_{\alpha\beta} + X_{00}\delta_{\alpha\beta} \\ &= S_{\alpha\beta} + \left(X_{00} + \frac{X_{\gamma\gamma}}{N}\right)\delta_{\alpha,\beta}, \end{aligned} \quad (7)$$

where the last equality follows from the traceless definition of the symplectic spin operator, $S_{\alpha\beta} = X_{\alpha\beta} - \frac{X_{\gamma\gamma}}{N}\delta_{\alpha\beta}$, and we are using the Einstein summation convention, here and throughout the paper. When we represent the Hubbard operators with slave bosons, the symplectic projected creation operators take the following form²⁰,

$$X_{\alpha 0} = f_{\alpha}^{\dagger}b + \tilde{\alpha}f_{-\alpha}a, \quad (8)$$

dictated by equation (7), and the other two Hubbard operators take the form

$$\begin{aligned} X_{\alpha\beta} &= S_{\alpha\beta} + \delta_{\alpha\beta} \\ X_{00} &= b^{\dagger}b + a^{\dagger}a. \end{aligned} \quad (9)$$

This double slave boson form for Hubbard operators was derived by Wen and Lee²⁴ as a way of extending the local

$SU(2)$ symmetry of spin²⁶ to include charge fluctuations. In our approach, the $SU(2)$ symmetry, $f_{\sigma} \rightarrow \cos\theta f_{\sigma} + \text{sign}(\sigma)\sin\theta f_{-\sigma}$ appears as a consequence of the time-inversion properties of symplectic spins for all even N , which permits us to carry out a large N expansion¹⁸. We can simplify these expressions by introducing Nambu notation, $B^{\dagger} = (b^{\dagger}, a^{\dagger})$ and $\tilde{f}^{\dagger} = (f_{\alpha}^{\dagger}, \tilde{\alpha}f_{-\alpha})$, as $X_{\alpha 0} = \tilde{f}_{\alpha}^{\dagger}B$. The hopping term of symplectic- N $t - J$ model can thus be written,

$$\begin{aligned} H &= -\sum_{ij} \frac{t_{ij}}{N} \left[\left(f_{i\alpha}^{\dagger}b_i + \tilde{\alpha}f_{i-\alpha}a_i \right) \left(f_{j\alpha}b_j^{\dagger} + \tilde{\alpha}f_{j-\alpha}a_j^{\dagger} \right) + \text{H.c.} \right] \\ &= -\sum_{ij} \frac{t_{ij}}{N} \left(\tilde{f}_{i\alpha}^{\dagger}B_iB_j^{\dagger}\tilde{f}_{j\alpha} + \text{H.c.} \right) \end{aligned} \quad (10)$$

Restricting the spin and charge fluctuations to the physical subspace requires that we fix the Casimir of the Hubbard operators²⁹,

$$\mathcal{C} = \vec{S}_j^2 + [X_{0\alpha}, X_{\alpha 0}] - (X_{00} + 1)^2, \quad (11)$$

where $\vec{S}_j^2 = \frac{1}{2} \sum_{\alpha\beta} S_{\alpha\beta}(j)S_{\beta\alpha}(j)$. A detailed calculation (see Appendix) shows that

$$\mathcal{C} = (N/2)^2 - 1 - \vec{\Psi}_j^2, \quad (12)$$

where $\vec{\Psi} \equiv (\Psi^{\dagger}, \Psi, \Psi_3)$ is given by

$$\begin{aligned} \Psi_3 &= n_f + n_b - n_a - \frac{N}{2} \\ \Psi^{\dagger} &= \sum_{\alpha>0} f_{\alpha}^{\dagger}f_{-\alpha}^{\dagger} + b^{\dagger}a \\ \Psi &= \sum_{\alpha>0} f_{-\alpha}f_{\alpha} + a^{\dagger}b. \end{aligned} \quad (13)$$

In the infinite- U limit, the Casimir, \mathcal{C} is set to its maximal value, and we obtain the constraint $\vec{\Psi}_j = 0$. Writing out the condition that $\vec{\Psi}_j$ vanishes, we obtain

$$\begin{aligned} b_j^{\dagger}b_j - a_j^{\dagger}a_j + f_{j\alpha}^{\dagger}f_{j\alpha} &= N/2 \\ b_j^{\dagger}a_j + \sum_{\alpha>0} \tilde{\alpha}f_{j\alpha}^{\dagger}f_{j-\alpha}^{\dagger} &= 0 \\ a_j^{\dagger}b_j + \tilde{\alpha}f_{j-\alpha}f_{j\alpha} &= 0. \end{aligned} \quad (14)$$

The first equation imposes the constraint on no double occupancy. The second terms play the role of a Coulomb pair pseudo-potential, forcing the net s-wave wave pair amplitude to be zero when superconductivity develops. Under the occupancy constraint, there is only a single physical empty state, which is

$$|0\rangle = \left(b^{\dagger} + a^{\dagger}\tilde{\alpha}f_{-\alpha}^{\dagger}f_{\alpha}^{\dagger} \right) |\Omega\rangle, \quad (15)$$

for $N = 2$. The physical interpretation of these terms becomes clearer if we pick a particular gauge. Since we only have two flavors of bosons and N flavors of fermions, the only way the bosons contribute in the large N limit is by

condensing. As the bosons are condensed at all temperatures, Fermi liquids and superconductors are the only possible states; while this situation is clearly unphysical, and will be resolved with $1/N$ corrections, it allows us to fix the gauge in a particularly simple way by setting $a = 0$ and condensing only the b bosons, $b^2 = Nx/2$ because the bosons carry all the charge in the system. The factor of $N/2$ makes the doping extensive in N . The constraint simplifies to,

$$\begin{aligned} f_{j\alpha}^\dagger f_{j\alpha} &= \frac{N(1-x)}{2} \\ \tilde{\alpha} f_{j\alpha}^\dagger f_{j-\alpha}^\dagger &= 0 \\ \tilde{\alpha} f_{j-\alpha} f_{j\alpha} &= 0, \end{aligned} \quad (16)$$

In a mean field theory, these three constraints are enforced by a trio of Lagrange multipliers $\vec{\lambda} = (\lambda_+, \lambda_-, \lambda_3)$ in a constraint term that takes the form

$$H_C = \sum_j \lambda_3 \left[f_{j\alpha}^\dagger f_{j\alpha} - \frac{N(1-x)}{2} \right] + \lambda_+ (\tilde{\alpha} f_{j\alpha}^\dagger f_{j-\alpha}^\dagger) + \text{H.c.} \quad (17)$$

The first constraint is clearly recognizable as imposing Luttinger's theorem. This term is present in the conventional $U(1)$ slave boson approach²³. The second terms impose severe constraints on the pair wavefunction when superconductivity develops, implementing the infinite Coulomb pseudopotential. For d-wave superconductors like the cuprates, which have been the main focus of previous $t - J$ model studies, these constraints are satisfied automatically, and at the mean-field level, there is no difference between the symplectic- N limit and many of the previously considered uncontrolled mean field theories^{23,24,30}. However, for s_\pm pairing, these additional constraints enforce the Coulomb pseudopotential, μ^* and have a large effect on the stability of s_\pm superconductivity.

Once the bosons are condensed, and the Heisenberg term decoupled, the spinon Hamiltonian is quadratic,

$$H = \sum_{ij} \tilde{f}_i^\dagger \left[-\frac{xt_{ij}}{2} \tau_3 + U_{ij} \right] \tilde{f}_j + \frac{N[|\Delta_{ij}|^2 + |\chi_{ij}|^2]}{J_{ij}}, \quad (18)$$

where we have introduced the $SU(2)$ matrix notation,

$$U_{ij} = \begin{bmatrix} -\chi_{ij} & \Delta_{ij} \\ \tilde{\Delta}_{ij} & \tilde{\chi}_{ij} \end{bmatrix}. \quad (19)$$

χ_{ij} generates a dispersion for the spinons, while Δ_{ij} pairs them. The full Hamiltonian is given by $H + H_C$. The physical electron, $c^\dagger \sim \langle b \rangle f^\dagger + \langle a \rangle f$ will either hop coherently, forming a Fermi liquid when Δ is zero, or will superconduct when Δ is nonzero. The mean field phase diagram is obtained by minimizing the free energy with respect to these mean field parameters, χ_{ij} and Δ_{ij} ,

$$\begin{aligned} \chi_{ij} &= \frac{J_{ij}}{N} \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle \\ \Delta_{ij} &= \frac{J_{ij}}{N} \langle \tilde{\alpha} f_{i\alpha}^\dagger f_{j-\alpha}^\dagger \rangle, \end{aligned} \quad (20)$$

and enforcing the constraint on average, $\langle \sum_j f_{j\alpha}^\dagger f_{j\alpha} \rangle = \frac{N(1-x)}{2}$ and $\langle \sum_j \tilde{\alpha} f_{j\alpha}^\dagger f_{j-\alpha}^\dagger \rangle = 0$, where $\langle \dots \rangle$ is the thermal expectation value.

The $J_1 - J_2$ model will have two sets of bond variables, χ_η and Δ_η , where η indicates a link, (ij) . We assume that χ_1 and χ_2 are uniform, and allow Δ_1 and Δ_2 to be either s-wave or d-wave. When these order parameters are Fourier transformed, we find $\chi_{\mathbf{k}} = \chi_1 \gamma_{1\mathbf{k}} + \chi_2 \gamma_{2\mathbf{k}} \equiv 2\chi_1(c_x + c_y) + 4\chi_2 c_x c_y$ and $\Delta_{\mathbf{k}} = \sum_\eta \Delta_\eta \delta_{\eta\mathbf{k}}$ is a combination of s-wave and d-wave pairing on the nearest and next nearest neighbor links,

$$\begin{aligned} \text{extended } s & 2\Delta_{1s}(c_x + c_y) \\ d_{x^2-y^2} & 2\Delta_{1d}(c_x - c_y) \\ s_\pm & 2\Delta_{2s}(c_{x+y} + c_{x-y}) = 4\Delta_{2s}c_x c_y \\ d_{xy} & 2\Delta_{2d}(c_{x+y} - c_{x-y}) = -4\Delta_{2d}s_x s_y \end{aligned} \quad (21)$$

and we define $c_\eta = \cos k_\eta a$, $s_\eta = \sin k_\eta a$. The full Hamiltonian (including the constraint) has the form,

$$\begin{aligned} H &= \sum_{\mathbf{k}} \tilde{f}_{\mathbf{k}}^\dagger \left(-\frac{x\epsilon_{\mathbf{k}}}{2} + U_{\mathbf{k}} + \lambda_3 \tau_3 + \lambda_1 \tau_1 \right) \tilde{f}_{\mathbf{k}} \\ &+ \mathcal{N}_s \sum_\eta \frac{N}{J_\eta} (|\Delta_\eta|^2 + |\chi_\eta|^2) - \frac{N\mathcal{N}_s x \lambda_3}{2} \end{aligned} \quad (22)$$

where $\epsilon_{\mathbf{k}}$ is the Fourier transform of t_{ij} , $U_{\mathbf{k}}$ is the Fourier transform of U_{ij} and $\lambda_1 = \frac{1}{2}(\lambda_+ + \lambda_-)$. (λ_2 is unnecessary if Δ is real). This Hamiltonian can be diagonalized, and the spinons integrated out to yield the free energy,

$$\begin{aligned} F &= -2NT \sum_{\mathbf{k}} \log 2 \cosh \frac{\beta\omega_{\mathbf{k}}}{2} \\ &+ \mathcal{N}_s \sum_\eta \frac{4N}{J_\eta} (|\Delta_\eta|^2 + |\chi_\eta|^2) - \frac{N\mathcal{N}_s x \lambda_3}{2}, \end{aligned} \quad (23)$$

where $\omega_{\mathbf{k}} = \sqrt{\alpha_{\mathbf{k}}^2 + \beta_{\mathbf{k}}^2}$, $\alpha_{\mathbf{k}} = \lambda_3 - \frac{x\epsilon_{\mathbf{k}}}{2} + \chi_{\mathbf{k}}$, and $\beta_{\mathbf{k}} = \lambda_1 + \Delta_{\mathbf{k}}$. Minimizing this free energy leads to the four mean field equations,

$$\begin{aligned} \partial F / \partial \chi_\eta &= \int_{\mathbf{k}} \frac{\tanh \frac{\beta\omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \alpha_{\mathbf{k}} \gamma_{\eta\mathbf{k}} - \frac{4}{J_\eta} = 0 \\ \partial F / \partial \Delta_\eta &= \int_{\mathbf{k}} \frac{\tanh \frac{\beta\omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \beta_{\mathbf{k}} \delta_{\eta\mathbf{k}} - \frac{4}{J_\eta} = 0 \\ \partial F / \partial \lambda_3 &= \int_{\mathbf{k}} \frac{\tanh \frac{\beta\omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \alpha_{\mathbf{k}} - x/2 = 0 \\ \partial F / \partial \lambda_1 &= \int_{\mathbf{k}} \frac{\tanh \frac{\beta\omega_{\mathbf{k}}}{2}}{2\omega_{\mathbf{k}}} \beta_{\mathbf{k}} = 0. \end{aligned} \quad (24)$$

The first three are identical to those for the $U(1)$ slave boson mean field theories²³, but the last enforces the absence of s-wave pairing. λ_1 acts as a pair chemical potential adjusting the regions of negative and positive gap.

IV. SIMPLE EXAMPLES

Now let us see this constraint in action, applied to several simple cases. First, we shall take the simplest

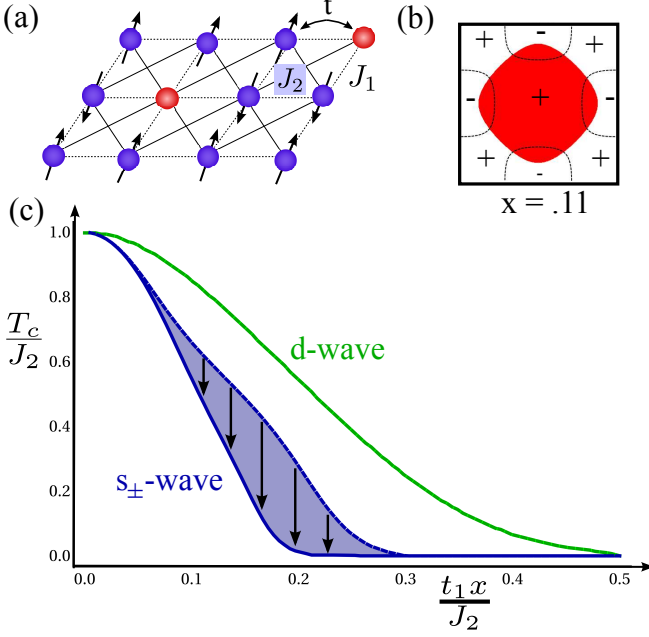


FIG. 2: (Color online) (a) The $t_1 - J_2$ model. (b) The Fermi surface (electrons shown in red) for the $t_1 - J_2$ model at intermediate doping. In the superconducting state, the gap nodes follow the dashed lines, separating regions of positive and negative gap. (c) The superconducting transition temperatures for the $t_1 - J_2$ model both with (solid lines) and without the λ_1 constraint (dashed lines), for s -wave (blue) and d -wave (green) superconductivity. d -wave superconductivity is unaffected by the Coulomb repulsion, while the s -wave transition temperature is decreased.

lattice to exhibit s_{\pm} pairing: the $t_1 - J_2$ model shown in Fig. 2 (a). Here, only the next-nearest exchange coupling, J_2 and nearest neighbor hopping, t_1 are nonzero, which leads to a single electron Fermi surface with the potential for either d_{xy} or s_{\pm} pairing. The dispersion is given by $\epsilon_{\mathbf{k}} = 2t_1(\cos k_x a + \cos k_y a)$. The superconducting transition temperatures can be determined by setting $\Delta_{2s/d} = 0^+$ and solving the mean field equations, (24) for T_c . The results are shown in Fig. 2(c), where we have calculated the transition temperatures as a function of doping, x both with and without the λ_1 constraint. The d -wave transition temperature is unaffected, as $\partial F/\partial \lambda_1 = 0$ by symmetry, but the s -wave T_c is suppressed. Note that the two transition temperatures are identical for $x = 0$. Looking at the gap structure, Figure 2(b), we see that λ_1 has adjusted the gap nodes such that there are equal amounts of positive and negative gap density of states, eliminating the Coulomb repulsion. As there is only one Fermi surface in this example, there are necessarily line nodes even in the s -wave state. The energetic advantage of a fully gapped s -wave Fermi surface is thus lost, so that d -wave superconductivity, which requires no costly adjustment of the nodes, becomes energetically favorable for this lattice.

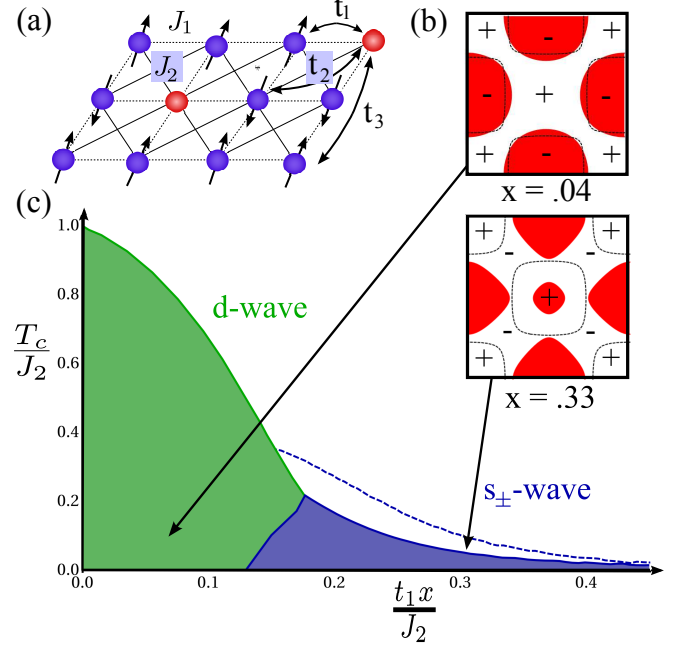


FIG. 3: (Color online) (a) The $t_1 - t_2 - t_3 - J_2$ model. (b) The Fermi surface (electrons shown in red) for the $t_1 - t_2 - t_3 - J_2$ model at both low (single Fermi pocket) and intermediate doping (two Fermi pockets). The gap nodes of the superconducting state are indicated with dashed lines. (c) The doping phase diagram for the $t_1 - t_2 - t_3 - J_2$ model, calculated with the λ_1 constraint (solid lines) and without (dashed lines). There is a quantum phase transition between d -wave pairing (green) and s -wave pairing (blue) as doping increases and the s -wave states become fully gapped.

However, if there are multiple Fermi surfaces, s_{\pm} superconductivity can gap out both surfaces with opposite signs. If we tune the $t_1 - t_2 - t_3$ hoppings, keeping only J_2 , we can obtain such a Fermi surface, which has two electron pockets as shown in Figure 3(a,b). It is of course impossible to reproduce the electron and hole Fermi surfaces of the iron-based superconductors with this single band model, but these two electron pockets capture the essential aspects from the Coulomb pseudopotential point of view. The dispersion is given by

$$\epsilon_{\mathbf{k}} = -2t_1(\cos k_x a + \cos k_y a) - 4t_2 \cos k_x a \cos k_y a - 2t_3(\cos 2k_x a + \cos 2k_y a), \quad (25)$$

where we have taken $t_2 = -3t_1$ and $t_3 = 4t_1$ to get the two electron pockets. Again, we calculate the s -wave and d -wave transition temperatures in the presence of the pseudopotential terms, showing the phase diagram in Figure 3(c). Our one-band approach makes this difficult, as the size of the pockets shrinks with increasing doping. The s -wave order parameter has line nodes for low doping, which recede to point nodes and then vanish as the Fermi surface becomes fully gapped at larger dopings, where the s -wave superconductivity is more favorable than d -wave, causing a d -wave to s -wave quan-

tum phase transition as a function of doping. If we had equally balanced hole and electron pockets at zero doping, s-wave would likely win out over d-wave at all dopings.

V. DISCUSSION

This study of the symplectic- N t - J model illustrates the importance of incorporating the Coulomb pseudopotential into any strongly correlated treatment of s_{\pm} superconductors. The symplectic- N scheme provides the first mean field solution of the $t - J$ model that is both controlled and superconducting. The large- N limit is identical to previous mean-field studies²³, but contains the additional constraint fields λ_{\pm} which enforce the constraint $\tilde{\Psi} = 0$. For d-wave pairing, this constraint is inert, as the s-wave component of the pairing is zero by symmetry, but this constraint plays a very active role for s-wave pairing, acting as a pair chemical potential that adjusts the gap nodes to eliminate any on-site pairing. As such, these models can capture the full variety of gap physics proposed in the iron-based superconductors: from line nodes to point nodes to two different full gaps that are not otherwise expected in a local picture. Properly accounting for the adjustment of the line nodes is essential when comparing the relative energies of d-wave and s-wave pairing states in the model calculations.

However, the large- N limit suffers from an overabundance of coherence, due to the ubiquity of the boson condensation. As such, the only phases captured here are Fermi liquids and superconductors, and studying the effects of $1/N$ corrections is an important future direction. This application is especially relevant to the cuprates, where there have been many interesting, but uncontrolled corrections to the mean field theories, revealing pseudogap-like phases formed by pre-formed pairs and incoherent metallic regions^{24,25}. A controlled $1/N$ study of the phase diagram of the $t - J$ model studying the differences between s-wave and d-wave pairing should be of great interest.

While the $t - J$ models taken in this paper illustrate the basic effect of the Coulomb pseudopotential on strongly correlated superconductors, they are but poor approximations of the real materials, due to the single band approximation. A better theory would involve multiple orbitals per site coupled by a ferromagnetic Hund's coupling, $-|J_H| \vec{S}_{\mu i} \cdot \vec{S}_{\mu' i}$ between spins in different orbitals, $\mu \neq \mu'$ on the same site, as well as more realistic dispersions. Current large- N techniques cannot treat such a ferromagnetic coupling, but future work might introduce add the pair chemical potential, λ_1 to current uncontrolled mean-field approaches^{8,9} or take $J_H \rightarrow \infty$, which may prove more tractable.

Interestingly, while the majority of the iron-based superconductors have at least two electron and hole pockets, there are a handful of "single band" materials: there are the end members KFe_2As_2 ³¹ and $\text{K}_{1-x}\text{Fe}_{2-y}\text{Se}_2$ ³²,

which appear to have only hole³³ or electron pockets³⁴, respectively; and the single layer FeSe , which has a single electron pocket^{35,36}. In this local treatment, KFe_2As_2 's single hole pocket must lead to a nodal d-wave superconductor³⁷, as in the $t - J_2$ example above, where the s_{\pm} transition temperature is always smaller than the d-wave temperature. A d-wave gap is strongly suggested by recent heat conductivity measurements³⁸. On the other hand, $\text{K}_{1-x}\text{Fe}_{2-y}\text{Se}_2$ and single-layer FeSe have electron pockets, which can develop node-less d-wave order, as originally discussed from the weak coupling approach³⁹⁻⁴¹. Including the Coulomb pseudopotential could again become important in this d-wave system if the tetragonal symmetry were broken.

Finally, an intriguing open problem in the iron-based superconductors is the relationship between the local quantum chemistry and the superconducting order⁴². The strong dependence of the superconducting transition temperature on the Fe-As angle^{43,44} suggests that there might be a more local origin of superconductivity, similar to the composite pairs found in heavy fermion materials described by the two-channel Kondo lattice¹⁸. These two origins of s_{\pm} pairing could then work in tandem to raise the superconducting transition temperature⁴⁵, and as such a future generalization of this work to take into account both the local iron chemistry and the staggered tetrahedral structure is highly desirable. Such tandem pairing might explain the robustness of these superconductors to disorder on the magnetic iron site⁴⁶.

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VI. APPENDIX

In this section, we show that the operator combination

$$\mathcal{C} = \frac{1}{2} S_{\alpha\beta} S_{\beta\alpha} + [X_{0\alpha}, X_{\alpha 0}] - (\tilde{X}_{00})^2 \quad (26)$$

commutes with the Hubbard operators, where $\tilde{X}_{00} = X_{00} + 1$. \mathcal{C} is therefore the quadratic casimir of the symplectic supergroup $\text{SP}(N|1)$. We also show that

$$C = (N/2)^2 - 1 - \tilde{\Psi}_j^2 \quad (27)$$

in the symplectic slave boson representation.

The Hubbard operators $X_{0\alpha}$, $X_{\alpha 0}$ and X_{00} , together with the symplectic spin operators, $S_{\alpha\beta} = X_{\alpha\beta} - \frac{1}{N} X_{\lambda\lambda}$, form a closed superalgebra:

$$\begin{aligned} [S_{\alpha\beta}, S_{\gamma\delta}] &= \delta_{\beta\gamma} S_{\alpha\delta} - \delta_{\gamma\beta} S_{\alpha\delta} + \delta_{\beta\delta} \tilde{\gamma} \tilde{\beta} S_{\alpha\tilde{\gamma}} - \delta_{\gamma\tilde{\alpha}} \tilde{\alpha} \tilde{\delta} S_{\tilde{\delta}\beta} \\ [X_{0\alpha}, S_{\beta\gamma}] &= X_{0\gamma} \delta_{\alpha\beta} + \tilde{\alpha} \tilde{\beta} X_{0\tilde{\beta}} \delta_{\alpha\tilde{\gamma}} \\ \{X_{0\alpha}, X_{\beta 0}\} &= S_{\beta\alpha} + \delta_{\alpha\beta} \tilde{X}_{00} \\ \{X_{0\alpha}, X_{0\beta}\} &= 0 \\ [X_{0\alpha}, X_{00}] &= -X_{0\alpha}. \end{aligned} \quad (28)$$

Greek indices indicate spin indices $\alpha \in [\pm 1/2, \pm 3/2, \pm j]$ where $j = N/4$ and N is even. For simplicity, we use the notation $\bar{\alpha} = -\alpha$ and $\tilde{\alpha} = \text{sgn}(\alpha)$. The operator $S_{\alpha\beta} = X_{\alpha\beta} - \frac{1}{N}\delta_{\alpha\beta}X_{\lambda\lambda}$ is the traceless symplectic spin operator, while the subsidiary operator, $\tilde{X}_{00} = X_{00} - \frac{1}{N}\sum_{\alpha}X_{\alpha\alpha}$. This graded Lie algebra defines the properties of the generators of the symplectic supergroup $\text{SP}(N|1)$. This superalgebra is faithfully reproduced by the slave boson representation

$$\begin{aligned} X_{\alpha\beta} &= f_{\alpha}^{\dagger}f_{\beta} + \tilde{\alpha}\tilde{\beta}f_{\bar{\alpha}}f_{\bar{\beta}}^{\dagger} \\ X_{\alpha 0} &= f_{\alpha}^{\dagger}b + \tilde{\alpha}f_{\bar{\alpha}}a \\ X_{0\alpha} &= b^{\dagger}f_{\alpha} + a^{\dagger}\tilde{\alpha}f_{\bar{\alpha}} \\ X_{00} &= b^{\dagger}b + a^{\dagger}a \end{aligned} \quad (29)$$

while the spin and subsidiary operator, \tilde{X}_{00} are given by

$$\begin{aligned} S_{\alpha\beta} &= X_{\alpha\beta} - \frac{1}{N}\delta_{\alpha\beta}X_{\lambda\lambda} = f_{\alpha}^{\dagger}f_{\beta} - \tilde{\alpha}\tilde{\beta}f_{\bar{\beta}}f_{\bar{\alpha}}^{\dagger} \\ \tilde{X}_{00} &= X_{00} + \frac{1}{N}X_{\alpha\alpha} = b^{\dagger}b + a^{\dagger}a + 1. \end{aligned} \quad (30)$$

By inspection, \mathcal{C} contains only rotationally invariant combinations of the Hubbard operators and each term leaves the number of slave bosons unchanged, so that it commutes with $S_{\alpha\beta}$ and X_{00} . We now show by direct evaluation that it also commutes with the fermionic Hubbard operators $X_{0\alpha}$ and $X_{\alpha 0}$

First we evaluate the commutator between $X_{\alpha 0}$ and the spin part of the Casimir,

$$\begin{aligned} [X_{0\alpha}, S_{\beta\gamma}S_{\gamma\beta}] &= [X_{0\alpha}, S_{\beta\gamma}]S_{\gamma\beta} + S_{\beta\gamma}[X_{0\alpha}, S_{\gamma\beta}] \\ &= X_{0\gamma}S_{\gamma\alpha} + X_{0\bar{\beta}}S_{\bar{\alpha}\beta}\text{sgn}(\alpha\beta) \\ &\quad + S_{\beta\alpha}X_{0\beta} + \text{sgn}(\alpha\gamma)S_{\bar{\alpha}\gamma}X_{0\bar{\gamma}} \end{aligned} \quad (31)$$

Using the identity $S_{\alpha\beta} = -\text{sgn}(\alpha\beta)S_{\bar{\beta}\bar{\alpha}}$, we can convert this expression into the form

$$\begin{aligned} [X_{0\alpha}, S_{\beta\gamma}S_{\gamma\beta}] &= X_{0\gamma}S_{\gamma\alpha} + X_{0\bar{\beta}}S_{\bar{\beta}\alpha} + S_{\beta\alpha}X_{0\beta} + S_{\bar{\gamma}\alpha}X_{0\bar{\gamma}} \\ &= 2\{X_{0\beta}, S_{\beta\alpha}\}. \end{aligned} \quad (32)$$

Next we evaluate

$$\begin{aligned} -[X_{0\alpha}, [X_{0\beta}, X_{\beta 0}]] &= -X_{0\beta}\{X_{0\alpha}, X_{\beta 0}\} - \{X_{0\alpha}, X_{\beta 0}\}X_{0\beta} \\ &= -\{X_{0\beta}, S_{\beta\alpha}\} - \{X_{0\alpha}, \tilde{X}_{00}\}. \end{aligned} \quad (33)$$

Finally,

$$\begin{aligned} [X_{0\alpha}, \tilde{X}_{00}^2] &= -[X_{0\alpha}, \tilde{X}_{00}]\tilde{X}_{00} - \tilde{X}_{00}[X_{0\alpha}, \tilde{X}_{00}] \\ &= \{X_{0\alpha}, \tilde{X}_{00}\} \end{aligned} \quad (34)$$

Adding (32), (33) and (34) together gives

$$[X_{0\alpha}, \mathcal{C}] = 0. \quad (35)$$

Since $X_{\alpha 0} = X_{0\alpha}^{\dagger}$ and $\mathcal{C} = \mathcal{C}^{\dagger}$ is Hermitian, it follows that $[X_{\alpha 0}, \mathcal{C}] = 0$. Thus, \mathcal{C} commutes with all Hubbard operators, and is thus a Casimir of the supergroup $\text{SP}(N|1)$ generated by the symplectic operators.

To evaluate the Casimir, we insert the slave boson form of the Hubbard operators. First, evaluating the spin part, we obtain

$$\begin{aligned} S_{\alpha\beta}S_{\beta\alpha} &= 2[f_{\alpha}^{\dagger}f_{\beta}f_{\beta}^{\dagger}f_{\alpha} - f_{\bar{\beta}}^{\dagger}f_{\bar{\alpha}}f_{\bar{\beta}}f_{\alpha}\text{sgn}(\alpha\beta)] \\ &= 2\left[f_{\alpha}^{\dagger}(N - f_{\beta}^{\dagger}f_{\beta})f_{\alpha} + f_{\bar{\beta}}^{\dagger}f_{\bar{\beta}}f_{\bar{\alpha}}f_{\alpha}\text{sgn}(\alpha\beta)\right] \\ &= 2\left[n_f(N + 2 - n_f) - 4\Psi_f^{\dagger}\Psi_f\right] \end{aligned} \quad (36)$$

where $\Psi_f^{\dagger} = \sum_{\alpha>0}\tilde{\alpha}f_{\bar{\alpha}}^{\dagger}f_{\alpha}^{\dagger}$, while

$$[X_{0\alpha}, X_{\alpha 0}] = (N - 2n_f)(n_b - n_a) - N. \quad (37)$$

Combining the various terms in the Casimir, we obtain

$$\begin{aligned} \mathcal{C} &= n_f(N + 2 - n_f) - (N - 2n_f)(n_b - n_a) - N \\ &\quad - 4(\Psi_f^{\dagger} + b^{\dagger}a)(\Psi_f + a^{\dagger}b) + 4b^{\dagger}aa^{\dagger}b - (\tilde{X}_{00})^2. \end{aligned} \quad (38)$$

By regrouping terms, we obtain

$$\begin{aligned} \mathcal{C} &= -(n_f + n_b - n_a - \frac{N}{2})^2 + (n_b - n_a)^2 + \left(\frac{N}{2}\right)^2 \\ &\quad + 2(n_f + n_b - n_a - \frac{N}{2}) - 2(n_b - n_a) \\ &\quad - \Psi^{\dagger}\Psi + 4b^{\dagger}aa^{\dagger}b - (\tilde{X}_{00})^2. \end{aligned} \quad (39)$$

We now introduce the triad of operators

$$\begin{aligned} \Psi_3 &= n_f + n_b - n_a - \frac{N}{2} \\ \Psi^{\dagger} &= \Psi_f^{\dagger} + b^{\dagger}a \\ \Psi &= \Psi_f + a^{\dagger}b \end{aligned} \quad (40)$$

where $[\Psi^{\dagger}, \Psi] = \Psi_3$. Alternatively $\frac{1}{2}(\Psi_1 + i\Psi_2) = \Psi^{\dagger}$ and $\frac{1}{2}(\Psi_1 - i\Psi_2) = \Psi$. The Casimir can then be simplified to

$$\begin{aligned} \mathcal{C} &= -(\Psi_3)^2 + (n_b + n_a + 1)^2 + (N/2)^2 - 1 \\ &\quad - (\Psi_1^2 + \Psi_2^2) - (n_b + n_a + 1)^2 \end{aligned} \quad (41)$$

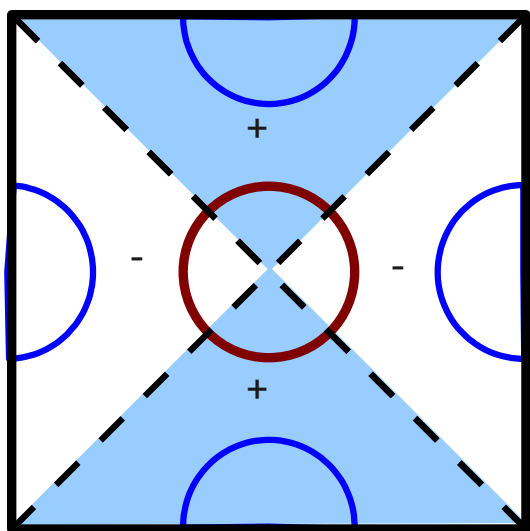
The terms involving n_b and n_a completely cancel out, leaving $\mathcal{C} = \left(\frac{N}{2}\right)^2 - 1 - (\vec{\Psi}^2)$.

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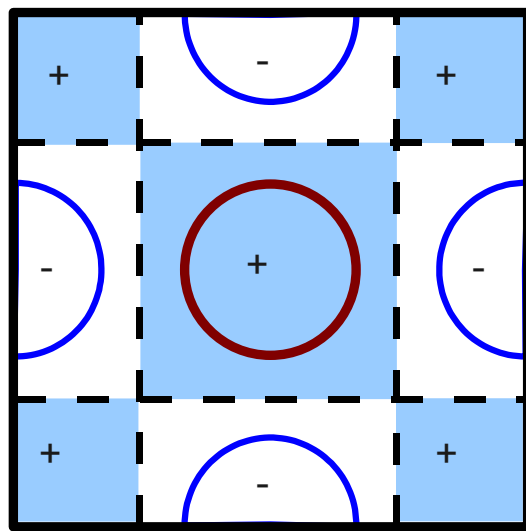
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d-wave gap



s_{\pm} gap

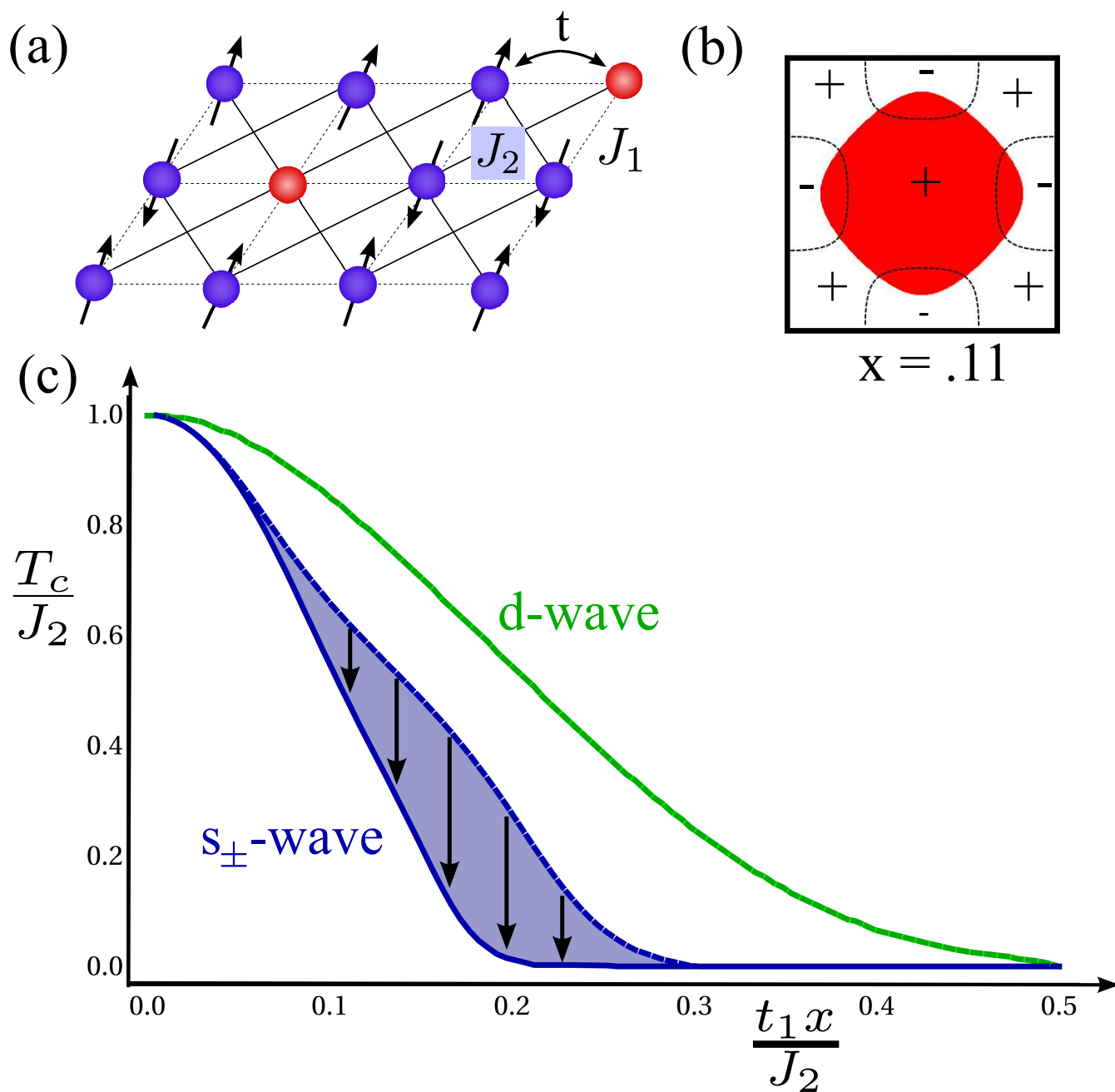


Figure 2 BR12062 18Sep2012

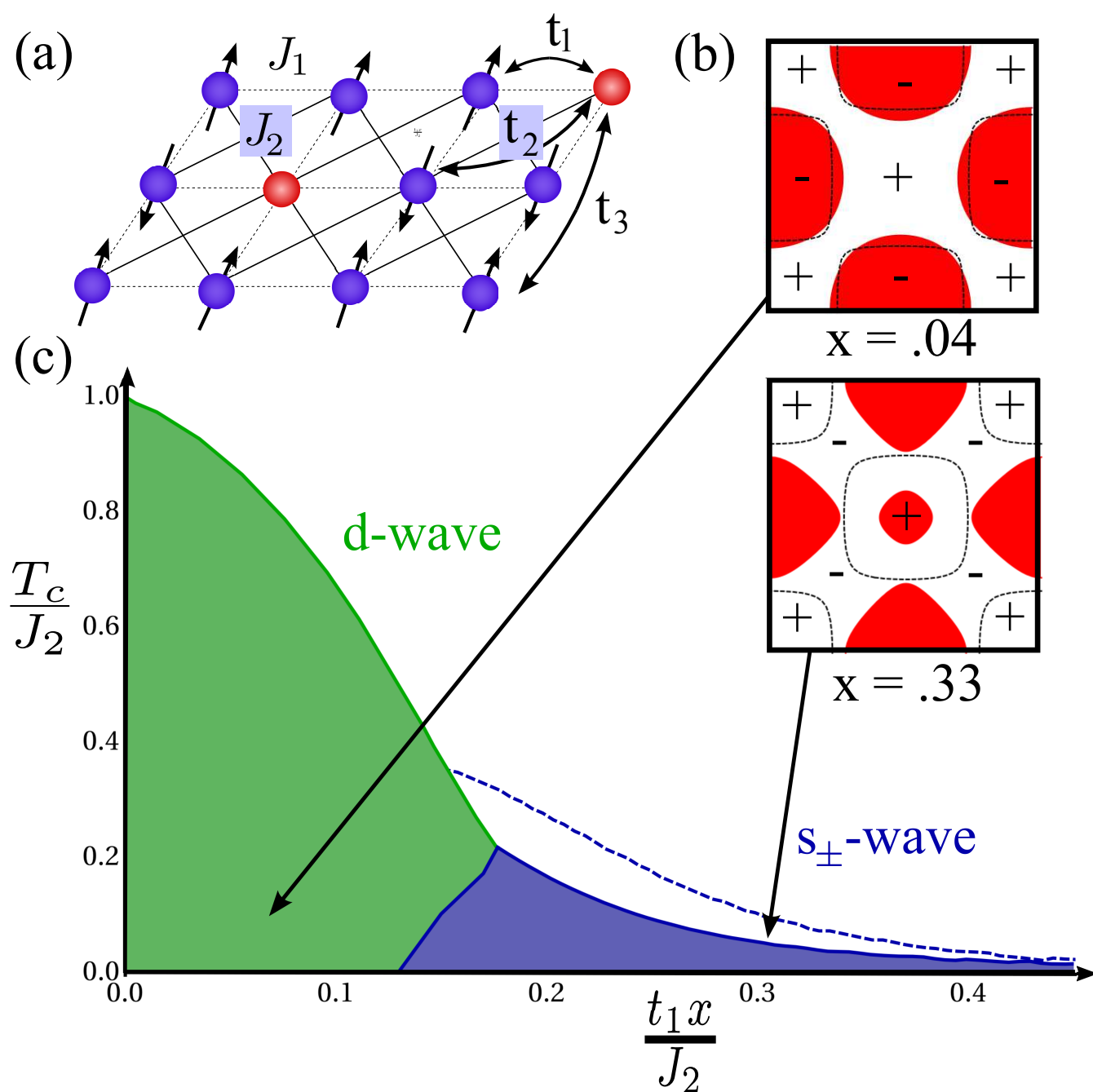


Figure 3 BR12062 18Sep2012