Superconducting order parameter symmetry for the extended Hubbard model below $T_c$

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The extended Hubbard model is known to host $s$-wave, $d$-wave and $p$-wave superconducting phases depending on the values of the on-site and nearest-neighbour interactions. By examining the free energy functional of the gap in this model, we find that these symmetries are often dependent on temperature. The critical points of this functional are highly constrained by symmetry and allow us to formulate stringent conditions on the temperature profile of the gap function, applicable to other models as well. We discuss the finite temperature phase diagram of the extended Hubbard model, and point out the existence of first and second order symmetry transitions below $T_c$. Understanding the nature of these transitions may be important for assessing the symmetry of some unconventional superconductors such as UPt$_3$.

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Introduction. – As more and more unconventional superconductors are discovered, the question of the symmetry of the superconducting order parameter has moved to the forefront as one of the most immediate and important questions to answer about any new material, especially given its close connection to the (often unknown) pairing mechanism. Experimentally, it is a difficult question to answer, as the arduous history of the cuprates provides testament for [1]. The resolution of this question has been aided, in part, by phase-sensitive tunnelling measurements, which have been particularly useful in uncovering the gap symmetry of the heavy-fermion compound UPt$_3$ [2]. Like $^3$He, UPt$_3$ has an A and a B phase over different temperature ranges differentiated by different symmetries of the order parameter [3]. A variety of models have been proposed to describe the nature of this gap and its symmetry transition [4]. It is possible that the separation of these phases is due to magnetic moments lifting the degeneracy of the hexagonal lattice, but this is not the only explanation.

As we point out in this paper, many exotic superconducting symmetries can emerge from a normal state that retains the point group symmetry of the lattice. Irrespective of its origin, the lesson to take from UPt$_3$ is that in general, the superconducting order parameter does not necessarily retain a fixed symmetry below $T_c$. Similarly, recent observations in LaAlO$_3$/SrTiO$_3$ suggest that a second component of the gap function develops below $T_c$ [5]. One might consider these to be unusual circumstances. Indeed, LaAlO$_3$/SrTiO$_3$ has strong Rashba coupling; UPt$_3$ has time-reversal symmetry breaking, significant spin-orbit coupling and a complex order parameter in the B phase. However, the purpose of our paper is point out that such exotic conditions are not a requirement for a superconductor to have a rich phase diagram below $T_c$. In fact we illustrate that symmetry transitions occur as a function of temperature in one of the simplest and most studied models for superconductivity, the extended Hubbard model. It is surprising that this possibility has escaped notice until now.

With this expanding collection of unconventional superconductors, one might ask what symmetries can exist in a generic superconductor. The answer is well established within Landau-Ginzburg theory [6]. The gap function is segmented into pieces that transform under irreducible representations of the normal state symmetry group. Any of these individual pieces could form the superconducting state at $T_c$, but cannot be mixed at this temperature. However, at lower temperatures, when the magnitude of the order parameter is no longer small, higher order terms in the Landau free energy become important, and mixing can occur. As we will see, the phases below $T_c$ are simply described by bifurcations of critical points of the free energy. Such mixing and bifurcations have been predicted before in the context of anisotropic tight binding models [7–9]. In this paper, we illustrate these ideas within a case study of the simplest model that has competing symmetry phases: the two-dimensional (2D) extended Hubbard model on a square lattice, relevant for some layered high-temperature superconductors. We will see that even in this very basic model, the temperature-dependent superconducting phase diagram is quite rich.

Mean Field Solution of the Extended Hubbard Model. – We consider the extended Hubbard model on a square lattice with unit lattice spacing, nearest neighbour hopping $t$, on-site interaction $U$, nearest-neighbour interaction $V$, and chemical potential $\mu$

$$H = -t \sum_{\langle i,j \rangle} \langle c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \rangle + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_{i\sigma} n_{j\sigma'} - \mu \sum_i n_{i\sigma},$$

(1)
where \((i,j)\) denotes nearest neighbour sites and \(\sigma\) is a spin index. After Fourier transforming, we restrict our consideration to singlet pairs of zero total momentum. The absence of finite-momentum is expected in an unpolarized system, however triplet \(p\)-wave pairing is allowed in the extended Hubbard model and we avoid it here for the sake of clarity. It is known that \(p\)-wave pairing cannot be stabilized near half-filling, so the following arguments will hold provided the electron density \(n\) (or \(2 - n\)) is not too small [10]. The Hamiltonian in the singlet sector reads (see App. A for details)

\[
H = \frac{1}{N} \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{N^2} \sum_{kk'} V_{kk'} c_{k\uparrow}^\dagger c_{-k'\downarrow} c_{-k'\downarrow} c_{k'\uparrow}.
\]

where \(\xi_k = -2t(\cos k_x + \cos k_y) - \mu\), \(N\) is the total number of sites and

\[
V_{kk'} = U + 4V (s_k s_{k'} + d_k d_{k'}).
\]

Here we have split the interaction into \(s\)-wave, extended \(s\)-wave, and \(d\)-wave parts using the definitions

\[
s_k \equiv \frac{1}{2} (\cos k_x + \cos k_y)
\]

and

\[
d_k \equiv \frac{1}{2} (\cos k_x - \cos k_y),
\]

This interaction is in a simple separable form familiar to BCS lattice models. Mean field theory is employed with the momentum-dependent gap function order parameter

\[
\Delta_k \equiv -\frac{1}{N} \sum_{k'} V_{kk'} (c_{-k'\downarrow} c_{k'\uparrow}).
\]

The mean field Hamiltonian is diagonalized using the usual Bogoliubov transformation to arrive at the self-consistent gap equation

\[
\Delta_k = -\frac{1}{N} \sum_{k'} V_{kk'} \Delta_{k'} g_{k'},
\]

where \(g_{k'} \equiv \frac{1}{2E_{k'}} (1 - 2f_{k'})\), and \(f_{k'}\) is the fermi function evaluated at quasi-particle energy \(E_{k'} = \sqrt{\xi_{k'}^2 + |\Delta_{k'}|^2}\). The \(k\)-dependence determines the appropriate ansatz for the gap function

\[
\Delta_k = \Delta_0 + \Delta_s s_k + \Delta_d d_k.
\]

The three components satisfy the three coupled gap equations

\[
\Delta_0 = -\frac{U}{N} \sum_{k'} g_{k'} (\Delta_0 + \Delta_s s_{k'} + \Delta_d d_{k'}),
\]

\[
\Delta_s = -\frac{4V}{N} \sum_{k'} s_k g_{k'} (\Delta_0 + \Delta_s s_{k'} + \Delta_d d_{k'}),
\]

\[
\Delta_d = -\frac{4V}{N} \sum_{k'} d_{k'} g_k (\Delta_0 + \Delta_s s_{k'} + \Delta_d d_{k'}).
\]

For the sake of generality, we may rewrite the gap function as

\[
\Delta_k = \sum_{\{i\}} \Delta_i x_k^i,
\]

where the basis functions \(x_k^i\) make up the three terms in Eq. (6): \(x_k^0 = 1\), \(x_k^1 = s_k\), \(x_k^2 = d_k\). Such a decomposition can be made for any separable interaction and makes the expressions in the next section valid for many models beyond the extended Hubbard model. Note that \(x_k^0\) and \(x_k^2\) belong to one irreducible representation of the \(D_8\) lattice symmetry group \((A_0)\), while \(x_k^1\) belongs to another \((B_2)\). As a result, Eqs. (7) and (8) decouple from (9) whenever \(\Delta_d = 0\) or \(\Delta_0 = \Delta_s = 0\). We refer to such solutions as pure solutions, and reserve “mixed solutions” for any case where components from two different irreducible representations are non-zero.

**Free Energy.** – This model has three components of the gap function with different symmetries [11]. The natural question to ask is which of these symmetries would be observed for a given value of the parameters \(U\), \(V\) [12] and electron density \(n\)? The answer is whatever minimizes the Helmholtz free energy density. Note that we defined the Hamiltonian in the grand canonical ensemble, but we will work exclusively at fixed electron density. Therefore it is the free energy density \(f = \Omega/N + \mu n\) and not the grand potential density \(\Omega/N\) that must be minimized. Within mean field theory, this value is given by

\[
f_{\text{MF}} = \frac{1}{N} \sum_k \left( \xi_k - E_k + |\Delta_k|^2 g_k \right) + \frac{2k_B T}{N} \sum_k \ln(1 - f_k) + \mu n.
\]

\(f_{\text{MF}}\) gives the correct value of the free energy at the solutions to the gap equation, i.e. the critical points, but it is not the correct functional to minimize in order to obtain the physical state of the system. That functional comes from the finite temperature variational theorem [13]

\[
f \leq f[\Delta_k] = f_{\text{MF}} + \langle H - H_{\text{MF}} \rangle_{\text{MF}}.
\]

Of course, if we know the solutions to the gap equation, we can simply plug them into \(f_{\text{MF}}\) and compare the resulting free energies, but it will prove fruitful to work with the variational free energy \(f[\Delta_k]\). Here, the mean field expectation of an operator \(X\) is given by

\[
\langle X \rangle_{\text{MF}} \equiv \frac{1}{Z_{\text{MF}}} \text{Tr} e^{-\beta H_{\text{MF}}} X.
\]

We must compute

\[
\langle H - H_{\text{MF}} \rangle_{\text{MF}} = \frac{1}{N^2} \sum_{kk'} V_{kk'} \langle c_{k'\uparrow}^\dagger c_{-k'\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \rangle_{\text{MF}}
\]

\[
+ \frac{1}{N} \sum_k |\Delta_k|^2 g_k.
\]

The trace of the quartic term is readily evaluated in the eigenbasis of \(H_{\text{MF}}\) (see App. A):

\[
\langle c_{k'\uparrow}^\dagger c_{k\uparrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow} \rangle_{\text{MF}} = \Delta_k^* \Delta_{k'} g_k g_{k'}.
\]
The free energy functional follows from this
\[
 f[\Delta_k] = \frac{2k_B T}{N} \sum_k \ln(1 - f_k) + \frac{1}{N^2} \sum_{kk'} V_{kk'} \Delta^{*}_k \Delta^{*}_{k'} g_k g_{k'} \\
 + \frac{1}{N} \sum_k (\epsilon_k - E_k + 2|\Delta_k|^2 g_k) + \mu n. \tag{16}
\]

Minimization of the free energy is an important problem that requires strict numerical control. We have made use of the theory of Morse functions [14, 15] to aid our numerical search for the global minimum. These details are included in App. B.

Phase diagram. – By tracking the curvature of the normal state as the temperature is lowered, we are able to identify the number of bifurcations of the gap solutions and therefore the number of critical temperatures. Unlike the d-wave case, the linearized s-wave gap equations can have two eigenvalues in some parts of the parameter space and therefore two critical temperatures. In Fig. 1, we show the phase diagram in the U-V plane based solely on the critical temperatures determined by solving the linearized gap equations. In the positive U regime, there is competing spin-density wave order that we do not consider here [10]. Often, this diagram is taken to give the symmetry of the order parameter below \( T_c \). However, we will see that the true phase diagram is much richer when we take into account the temperature dependence of the gap.

An example of a point in the phase diagram where a mixed solution takes over below \( T_c \) is shown in Fig. 2. By numerically solving the temperature-dependent gap equations (B4), we find that for these parameters, the system starts as a d-wave superconductor at \( T_c^d \), but attains a lower free energy upon the emergence of s-wave components at a lower temperature. Note that the bifurcation rules stated in App. B guarantee that the mixed solution is the only minimum of the three available solutions as long as it exists.

Fig. 3 shows a more unusual situation typical of parameters near the \( T^s_c = T^d_c \) line. Here we see the development of two mixed solutions below \( T_c \). The development of the second mixed solution (mix_s) allows the pure s-wave solution to become a minimum in accordance with the bifurcation rules discussed in App. B. Indeed, in the example shown here it is the global minimum, so that the superconductor undergoes two symmetry transitions below \( T_c \) (d-wave \( \rightarrow \) mix_d \( \rightarrow \) s-wave). The inset of Fig. 3 shows the angular dependence of the gap evaluated on the Fermi surface. In general, mixed gap functions can have zero, two or four nodes depending on the fermi level and the relative magnitude of the \( \Delta_i \)'s. In the particular case shown here, the mixed state is predominantly extended s-wave in that there is no sign change around the Fermi surface. Note that the mixed state is always four-fold degenerate, while here we only show one of the four possible states (the others are found by rotating this by \( \pi/2 \) and multiplying by a sign).

These symmetry transitions have observable conse-
FIG. 3. (a) Temperature dependence of the gap components for all solutions at $U = -4.5$, $V = -5.85$, $n = 0.5$. The solid red line shows $|\Delta_d|/t$ for the $d$-wave solution. The $s$-wave solution (green) and the mixed solutions (purple and blue) have multiple components. In each case, the solid lines show $|\Delta_0|/t$, the dashed lines show $|\Delta_s|/t$ and the dot-dashed line shows $|\Delta_d|/t$. The label mix$_d$ denotes the fact that the mixed solution emerges from the $d$-wave solution, while mix$_s$ means that mixed solution emerges from the $s$-wave solution. (b) Free energy density for the same parameters and solutions. The dashed line indicates the transition temperature between mix$_d$ and pure $s$-wave phases. The insets are polar plots of the gap on the fermi surface (defined by $\xi_k = 0$) before and after the transition.

FIG. 4. Temperature dependence of the specific heat at $U = -4.5$, $V = -5.85$, $n = 0.5$. There is a discontinuity when the mixed state takes over from the $d$-wave state, and a singularity when $s$-wave state takes over from the mixed state. The singularity is a discontinuity in the entropy. Intriguingly, the derivative of the entropy is the same for both states at this temperature, so the singularity appears as a cusp in the specific heat.

FIG. 5. $U$-$V$ phase diagram for different densities showing the wedge of parameter space where there is a different pure symmetry of the gap function at $T = T_c$ and $T = 0$. The dashed lines indicate where $T_{s_c} = T_c^d$ while the solid lines indicate where the free energy densities of $s$ and $d$-wave phases are equal at zero temperature. For a given density, the phase to the upper-left of the wedge is $s$-wave for all temperatures, while to the lower-right it is $d$-wave with a possible transition to a mixed state.

sequences. The specific heat, $c_v = -T \frac{\partial^2 f_{\text{min}}}{\partial T^2}$, will have an additional discontinuity below $T_c$ due to the development of a mixed minimum in the free energy. In the case of a transition to a new pure state, as in Fig. 3, the specific heat will exhibit a singularity consistent with a first-order phase transition. This is shown in Fig. 4 with the parameter values corresponding to Fig. 3. The singularity is infinitesimally thin, but may be broadened by fluctuations and impurities [16].

With these examples, we see that the full temperature-dependent phase diagram is quite complicated. In general, there is an entire wedge near the $T_c^s = T_c^d$ line where the superconductor starts with one pure symmetry at its critical temperature and undergoes a first-order transition to a different pure symmetry at a lower temperature. The dependence on density of this wedge is shown in Fig. 5. Half-filling is a special case that is discussed in App. C.

Conclusion. – In this paper, we have studied the temperature dependence of the symmetry of the superconducting gap in the 2D extended Hubbard model, focusing on the regime of attractive nearest neighbour interaction
We used a mean field approach to determine the gap equations that set the allowed symmetries of the gap.

The precise symmetry of the gap for given parameters \((U,V,n,T)\) is determined by the minimum of the free energy. This can be considered as a critical point of a Morse function in a three-dimensional parameter space. This perspective, outlined in App. B, has conceptual and technical advantages that may translate to other models as well.

We discovered that even within this simple model, there is a rich variety of symmetry phase transitions that occur as a function of temperature, observable through the specific heat. In particular, we note there is a significant piece of the phase diagram where there is a different pure \((s\text{-wave or } d\text{-wave})\) symmetry at \(T = T_c\) and \(T = 0\), with a first order transition at some finite temperature in between. It is interesting that in the region of parameter space where different symmetries are most competitive (have the closest \(T_c\)'s), the mixed solution is not dominant at low temperatures.

A word about the interaction parameter ranges in this paper is warranted. We focused mainly on strong coupling, and found that in this regime, the range of symmetry transitions is significant. Such transitions may also occur at weak coupling, but in this regime the free energies of the \(s\) and \(d\)-wave phases are so similar as to make it difficult to discern the transition. Therefore it would be easiest to observe this phenomenon for large \(|U/t| \sim |V/t|\). One promising avenue to explore this is in the context of ultra-cold atoms, where \(U/t\) is controlled via the optical lattice potential, \(n\) and \(T\) are controlled via evaporative cooling, and \(V\) can be included through dipolar interactions [17, 18].

Lastly, we point out that the phase diagram is highly dependent on the symmetries of the normal state. As shown in App. C, the addition of particle-hole symmetry (half-filling) alters the allowed symmetry phases and transitions below \(T_c\). In the same regard, we expect models with more exotic symmetries of the normal state to have drastically different symmetry transitions below \(T_c\). It would be interesting to consider models with broken inversion or time-reversal symmetry via a Rashba or Zeeman term in the Hamiltonian. Such unconventional symmetries will not only alter the allowed superconducting phases, but may also cause symmetry transitions to become more prolific.

**Appendix A: Mean Field Theory**

The Fourier transform of the extended Hubbard model reads

\[
H = \sum_{k,\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{N} \sum_{kk'q} U_{kk'q} c_{k\sigma}^\dagger c_{k'\sigma} c_{k-k'+q}^\dagger \times c_{k'\sigma}^\dagger c_{k\sigma}
\]

where \(\xi_k = -2t(\cos k_x + \cos k_y) - \mu\), and \(N\) is the total number of sites in the lattice.

From this we identify a reduced Hamiltonian that contains only interactions between Cooper pairs in the singlet channel given by Eq. (2). Our choice of mean field Eq. (4) results in the following mean field Hamiltonian

\[
H_{MF} = \frac{1}{N} \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \frac{1}{N} \sum_{k} \Delta_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger
\]

\[
- \frac{1}{N} \sum_{k} \Delta_k c_{k\uparrow} c_{-k\downarrow} + \frac{1}{N} \sum_{k} \Delta_k (c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)_{MF}
\]

which is diagonalized using the usual Bogoliubov transformation

\[
c_{k\uparrow} = u_k \gamma_{k0} + v_k \gamma_{k1}
\]

\[
c_{-k\downarrow} = -v_k \gamma_{k0} + u_k \gamma_{k1},
\]

where \(|u_k|^2 + |v_k|^2 = 1\) and \(u_k = u_{-k}\), and the \(\gamma_k\) operators have the same anticommutation properties as the \(c_k\) operators. The values of these parameters that diagonalize the Hamiltonian are \(|v_k|^2 = \frac{1}{2} (1 - \frac{\Delta_k}{2E_k})\) and \(u_k v_k^* = -\frac{\Delta_k}{2E_k}\). Eq. (4) then becomes the self-consistent gap equation (5).

Note that within mean field theory we have the identity

\[
\langle \gamma_{k0}^\dagger \gamma_{k0} \gamma_{k'0}^\dagger \gamma_{k'0} \rangle_{MF} = f_k f_{k'},
\]

for \(a, b \in \{0, 1\}\), which is used to derive Eq. (15).

**Appendix B: Critical Points**

The gap equation (5) is reproduced from the solutions to the functional minimization

\[
\frac{\delta f}{\delta \Delta_q} = 0,
\]

while the chemical potential is fixed by the number equation

\[
\frac{\delta f}{\delta \mu} = 0,
\]
which upon using (B1) becomes,
\[ n = 1 - \frac{2}{N} \sum_k \xi_k g_k. \]  
(B3)

The functional minimization of \( f \) can be thought of as a minimization with respect to the \( N \) terms of \( \Delta_k \) (one for each value of \( k \)). However, we can alternatively think of this as a minimization over a three-dimensional parameter space \((\Delta_0, \Delta_s, \Delta_d)\) along with the constraint (10), and the number equation, so that we need only solve
\[ \frac{\partial f}{\partial \Delta_i} = \frac{\partial f}{\partial \mu} = 0. \]  
(B4)

The first derivative is given by
\[ \frac{\partial f}{\partial \Delta_i} = \frac{2}{N} \sum_k x_k^i G_k \left[ \Delta_k^* + \frac{1}{N} \sum_{k'} V_{kk'} \Delta_k \right]. \]  
(B5)

where we have defined \( G_k \equiv g_k + \frac{|\Delta_k|^2}{E_{kk}} \frac{\partial g_k}{\partial E_{kk}} \). Since \( G_k \) is positive definite, this equation simply restates what we already know, the critical points of \( f \) occur at the values of \((\Delta_0, \Delta_s, \Delta_d)\) that satisfy the gap equation. The conceptual advantage of this formulation is that we can now compute a simple Hessian in a low-dimensional parameter space. From here on we focus on real order parameters for simplicity of the argument. In that case, the Hessian elements at the critical points are
\[ H_{ij} = \frac{\partial^2 f}{\partial \Delta_i \partial \Delta_j} \bigg|_{i, p} \]
\[ = \frac{2}{N} \sum_k x_k^i G_k \left[ x_k^j + \frac{1}{N} \sum_{k'} V_{kk'} G_k x_{k'}^j \right], \]  
(B6)

where \( G_k \) is evaluated at the solutions to the gap equation.

It is important to note that the critical points have two symmetries apparent from the gap equation. First, there is inversion symmetry. If \((\Delta_0, \Delta_s, \Delta_d)\) is a critical point, then so is \((-\Delta_0, -\Delta_s, -\Delta_d)\). This is required by antisymmetry of the pair wavefunction. Second, there is mirror symmetry under reflection in the \(\Delta_0-\Delta_s\) plane, since any solution \((\Delta_0, \Delta_s, \Delta_d)\) has a corresponding solution \((\Delta_0, \Delta_s, -\Delta_d)\) upon replacing \(k_x \leftrightarrow k_y, k'_x \leftrightarrow k'_y\). Moreover, the curvature (B6) is a rank-2 tensor under these transformations. That is, under inversion,
\[ H_{ij} \rightarrow \sum_{pq} \delta_{ip} \delta_{jq} H_{pq}, \]  
(B7)

and under reflection in the \(\Delta_0-\Delta_s\) plane,
\[ H_{ij} \rightarrow \sum_{pq} (\delta_{ip} - 2\delta_{id} \delta_{pd})(\delta_{jq} - 2\delta_{jd} \delta_{qd}) H_{pq}. \]  
(B8)

This means that the gradient flow of \( f \) near the critical points respects these symmetries, and the index of any critical points related by these symmetries is the same. The index \( \gamma_i \) of a critical point \( i \) is defined as the number of orthogonal directions along which \( i \) is a maxima of the corresponding function (in this case the free energy). The index plays a large role in the theory of Morse functions [14]. A Morse function is a smooth real function that has no degenerate critical points. For our purposes, the free energy is a Morse function, since the curvature can only vanish on a set of measure zero in the \( T, U, V \) parameter space. As a consequence, the free energy satisfies the following Morse condition (valid for functions \( f((\Delta_i)) \) that increase without bound as the \(|\Delta_i| \) go to infinity):
\[ \sum_{i \in \text{critical points}} (-1)^{\gamma_i} = \chi(M), \]  
(B9)

where \( \chi(M) \) is the Euler characteristic of the domain manifold of \( f \) [15]. We may choose \( M \) to be the three-dimensional space \( \{\Delta_0, \Delta_s, \Delta_d\} \), or any of the pure subsets \( \{\Delta_0, \Delta_s\} \) or \( \{\Delta_d\} \), because any extrema of \( f \) on a pure subset is guaranteed to be a solution to the full gap equation. All of these cases correspond to flat manifolds with \( \chi(M) = 1 \). The combination of symmetries of \( f \) and the Morse condition restrict the possible minima of the free energy in this parameter space.

1. Corollaries of the Morse condition

The simplest question to ask is what can happen at \( T_c \) according to these restrictions. Above \( T_c \) we know the system is in the normal state, there is one critical point, and on any of the above manifolds, Eq. (B9) reads
\[ (-1)^0 = 1. \]  
(B10)

We immediately see that no mixed solution can emerge from this state. This is because mixed solutions are four-fold degenerate by inversion and mirror symmetry, so that the Morse condition reads
\[ (-1)^{\gamma_N} + 4(-1)^{\gamma_m} = 1, \]  
(B11)

denoting the normal index by \( \gamma_N \) and the mixed index by \( \gamma_m \). This equation has no integer solutions. Thus the condition expressed in Ref. [6] that mixed solutions cannot emerge at \( T_c \) is an immediate consequence of the symmetry of the gap equation.

We may also prove the uniqueness (modulo sign) of the pure \( d \)-wave solution. In fact, since the expressions (B5) and (B6) are valid for a generic separable interaction, this will also hold for any single-parameter gap function, including the Hubbard model with only on-site attraction. Existing proofs of the uniqueness the BCS gap solution are quite nontrivial [19]. Here we will see that it is a simple consequence of symmetry and the Morse condition.

**Proof.** For a single component gap \( \Delta_k = \Delta \), with a sep-
arable interaction $V_{kk'} = V x_k x_{k'}$, the Hessian reads

$$H = \frac{2}{N} \sum_k x_k^2 G_k \left( 1 + \frac{V}{N} \sum_{k'} G_{kk'} x_{k'}^2 \right) \quad (B12)$$

$$= \frac{2}{N} \sum_k x_k^2 G_k \left( 1 + \frac{V}{N} \sum_{k'} x_{k'}^2 \left[ g_{kk'} \left| \frac{\Delta_{kk'}}{\partial E_{kk'}} \right| \right] + \left| \frac{\Delta_{kk'}}{E_{kk'}} \right| \right). \quad (B13)$$

The single-component gap equation reads

$$\frac{1}{N} \sum_k x_k^2 g_{kk} = 0 \quad (B14)$$

so that at a critical point

$$H = \frac{2V}{N^2} \sum_{kk'} x_k^2 G_{kk'} x_{k'}^2 \left| \Delta_{kk'} \right| \left| \frac{\partial g_{kk'}}{\partial E_{kk'}} \right| \quad (B15)$$

where its only solutions are $\{\gamma_N = 0, n = 0\}$ and $\{\gamma_N = 1, n = 1\}[20]$. Thus, the single-component BCS gap equation admits one solution modulo sign.

Returning to the extended Hubbard model, this applies to solutions that are pure $d$-wave (in this case, $x_k \to d_k$ and $V \to 4V$ in the arguments above), guaranteeing their uniqueness. In addition, this reasoning guarantees that as long as the $d$-wave solution exists, the normal state must be unstable. At a critical $d$-wave temperature $T_c^d$, two $d$-wave critical points emerge from the normal state critical point as the temperature is lowered. This kind of bifurcation of solutions is completely generic as we now show.

The solutions to the gap equation are continuous functions of $T$, so critical points cannot appear in pairs at arbitrary points in the parameter space but must grow from the normal state or an existing superconducting state as the temperature is lowered. The Morse condition then provides a conservation of indices. For example, a pure state with index $\gamma_p$ that grows from the normal state is two-fold degenerate (baring pathological accidental degeneracies) and therefore must satisfy

$$(-1)^{\gamma_N} + 2n(-1)^0 = 1, \quad (B15)$$

where $\gamma_N$ is the index of the normal state at $T > T_c^d$, and $\gamma_{N_c}$ is the index of the normal state at $T < T_c^d$. The solution is

$$\pm 1 = \mp 1 + 2(\pm 1). \quad (B17)$$

So the normal state bifurcates into two pure states passing its index to the new solutions. The same thing occurs with mixed states which grow out of pure states according to

$$2(-1)^{\gamma_{p_1}} = 2(-1)^{\gamma_{p_2}} + 4(-1)^{\gamma_{p}}, \quad (B18)$$

which is also solved by (B17). A typical evolution of critical points as the temperature is lowered is shown in Fig. 6.

**Appendix C: Half-Filling**

Half-filling is a special case. For $n = 1$, $\mu = 0$, the number equation (B3) ensures that $\frac{1}{N} \sum_k s_k g_k = 0$. As a result, the $\Delta_0$ and $\Delta_s$ gap equations (7), (8) decouple for pure solutions, and the $s$-wave critical points move to the $\Delta_0$ and $\Delta_s$ axes. There are then three pure solutions: on-site $s$-wave, extended $s$-wave and $d$-wave, while the mixed solutions are confined to the $\Delta_0$-$\Delta_s$ and $\Delta_s$-$\Delta_d$ planes. An example of a first-order transition at half-filling is shown in Fig. 7. Note that in this case the mixed state is not involved in the transition. At a critical temperature, the gap function spontaneously generates nodes transitions from an on-site $s$-wave to $d$-wave symmetry.
FIG. 7. (top) Temperature dependence of the gap components for all solutions at $U = -5.5$, $V = -5.5$, $n = 1.0$. The solid red line shows $|\Delta_d|/t$ for the $d$-wave solution. There are now separate on-site $\Delta_0$ and extended $\Delta_s$ s-wave solutions, as well as a mixed solution (blue) confined to the $\Delta_0$-$\Delta_d$ plane. For the mixed solution, the solid line shows $|\Delta_0|/t$, and the dot-dashed line shows $|\Delta_d|/t$. (bottom) Free energy density for the same parameters and solutions. Here we include the normal state free energy (black) for reference.

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Originally, we had imagined altering the values of $U$ and $V$ as a function of temperature, so that the symmetry choice at $T_c$ would almost certainly be overturned as the temperature was lowered. Such temperature-dependent coupling parameters could be argued to occur for a variety of physical reasons. In any event, as we discovered, these transitions occur even if $U$ and $V$ are held constant as a function of temperature as detailed in this paper.

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