Comment on "Quasiparticle Spectra around a Single Vortex in a d-Wave Superconductor"

In a recent Letter [1] Morita, Kohmoto, and Maki (MKM) analyzed the structure of quasiparticle states around a single vortex in a $d_{x^2-y^2}$ superconductor using an approximate version of Bogoliubov–de Gennes (BdG) theory with a model d-wave gap function. Their principal result is the existence of a bound state within the core region at finite energy with full rotational symmetry, which they assert explains the recent scanning tunneling microscopy results on $YBa_2Cu_3O_{7-\delta}$ single crystals [2]. Here, we argue that the approximate BdG equations used by MKM are fundamentally inadequate for the description of a d-wave vortex and that the obtained circular symmetry of the local density of states (LDOS) is an unphysical artifact of this approximation.

BdG equations for a d-wave superconductor differ from the conventional ones by the nonlocality of the off-diagonal term $\int d\mathbf{x}'\,\tilde{\Delta}(\mathbf{x},\mathbf{x}')v(\mathbf{x}')$. MKM approximate this term by a local term $\Delta(\mathbf{k};\mathbf{R})v(\mathbf{R})$ and claim that this is accurate to $O(1/k_F\xi)$, quoting the derivation given by Bruder [3]. A key step in Bruder's calculation is factoring out the rapid k_F oscillation in $v(\mathbf{x})$ by introducing a slowly varying envelope function $\tilde{v}_{\mathbf{k}}(\mathbf{x})$

$$v(\mathbf{x}) = e^{ik_F\hat{\mathbf{k}}\cdot\mathbf{x}}\overline{v}_{\mathbf{k}}(\mathbf{x})\,. \tag{1}$$

$v(\mathbf{x})$ is then substituted in the off-diagonal matrix element and, after transforming to the center of mass frame, both Δ and $\overline{v}$ are Taylor-expanded in the relative coordinate. The leading term in the expansion is that used by MKM and corrections are indeed formally $O(1/k_F\xi)$. Since one cannot expand the rapidly varying function $v(\mathbf{x})$ directly, this manipulation rests heavily on the ansatz (1). An implicit assumption made in (1) is that the wave vector $\mathbf{k}$ is a good quantum number. This is approximately correct in the simple planar scattering situations considered by Bruder [3]. However, $\mathbf{k}$ is certainly *not* a good quantum number near the vortex core; the appropriate ansatz in this situation would involve a sum over $\hat{\mathbf{k}}$ in Eq. (1). One then obtains the leading off-diagonal term of the form $\sum_{\hat{\mathbf{k}}} e^{ik_F\hat{\mathbf{k}}\cdot\mathbf{R}}\Delta(\mathbf{k};\mathbf{R})\overline{v}_{\mathbf{k}}(\mathbf{R})$, indicating that all the plane wave states are mixed together by the nontrivial structure of the gap. This, in turn, results in coupling of the various angular momentum channels and the loss of rotational symmetry. MKM improperly neglect the summation over $\hat{\mathbf{k}}$ in the ansatz (1) for the wave functions.

Inadequacy of MKM's approximation becomes even more transparent when analyzing its implications for the physical quantities, such as the LDOS. A brief examination of the (standard) BdG equations for a d-wave vortex reveals that both the quasiparticle amplitudes and the self-consistent gap function will necessarily exhibit a fourfold anisotropy. This qualitative conclusion is corroborated by the numerical results within the Eilenberger [4] and the lattice BdG [5] formalisms. Anisotropic wave functions are also found near a strongly scattering nonmagnetic impurity [6]. These anisotropies are the salient feature of unconventional superconductivity resulting from an intricate interplay between the center of mass and the relative coordinate in the off-diagonal part of the BdG Hamiltonian. The fact that such anisotropies have not yet been observed experimentally [2] is indeed puzzling and apparently inconsistent with the above theoretical work. However, reconciliation between the theory and the experiment cannot be brought about by simply ignoring the symmetry breaking interactions as is done by MKM.

A brief inspection of MKM Eqs. (1) and (2) reveals that they, in fact, describe a set of decoupled s-wave vortices with the gap functions of various amplitudes (but identical profiles) scaled by the factor $\cos[2\theta(\hat{\mathbf{k}})]$. Each of these vortices possesses a set of bound states [7] with the energy spacing $\Delta^2(\mathbf{k};\infty)/E_F$, contributing sharp peaks in the LDOS. The finding of MKM of the broad peak in the LDOS in the vicinity of the core is a trivial consequence of superimposing the peaks corresponding to the lowest bound states belonging to these s-wave vortices. The full rotational symmetry of the LDOS in MKM's result also directly follows from this observation. Clearly, such calculation does not resolve the interesting question of the existence and the structure of the quasiparticle bound states in d-wave vortices. We expect that the nature of such states will be qualitatively different from the conventional picture of Caroli, de Gennes, and Matricon [7]. However, this structure can emerge only from a solution, numerical or analytical, which preserves complexity and richness of the original BdG theory.

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[1] Y. Morita, M. Kohmoto, and K. Maki, Phys. Rev. Lett. **78**, 4841 (1997).
[2] I. Maggio-Aprile, *et al.*, Phys. Rev. Lett. **75**, 2754 (1995).
[3] C. Bruder, Phys. Rev. B **41**, 4017 (1990).
[4] M. Ichioka *et al.*, Phys. Rev. B **53**, 15 316 (1996).
[5] Y. Wang and A. H. MacDonald, Phys. Rev. B **52**, R3876 (1995).
[6] See, e.g., M. I. Salkola, A. V. Balatsky, and D. J. Scalapino, Phys. Rev. Lett. **77**, 1841 (1996), and references therein.
[7] C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).

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