Effect of inter-band nesting on superconductivity in stacked honeycomb lattices

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Abstract

In order to exemplify our idea that inter-band nesting can favor superconductivity arising electron repulsion in layered, non-Bravais lattices, we have looked into the two-band Hubbard model on a stack of honeycomb lattices with the fluctuation exchange approximation. By systematically varying the band filling and transfers, the inter-band nesting is indeed found to give rise to gap functions that change sign across the bands, with a time-reversal-broken $d_1 + id_2$ intra-band pairing symmetry.

Key words: superconductivity;electron correlation;Hubbard model

Superconductivity from electron-electron repulsion is fascinating in many ways. Althoght there is a growing consensus that high-T_c cuprates may be related to the electron correlation, we are only beginning to understand the link between the underlying band structure and the way in which the electron-mechanism superconductivity appears. Usually the repulsion-originated (i.e., spin-fluctuation mediated) superconductivity should have, as in the cuprates, strongly anisotropic gap functions having nodes, which greatly suppress T_C. However, if the system has multi-bands in such a way that a strong inter-band nesting accommodates the pair scattering (the Coulombic matrix elements that scatter pairs of electrons across the Fermi surface) between different pieces of the Fermi surface, the gap function changes sign across the bands, which greatly enhances T_C[1].

In this paper, we study whether such an inter-band nesting mechanism can be realized in a three-dimensional system, by taking the repulsive Hubbard model on a stack of honeycomb lattices as a prototype. There, the honeycomb, a typical non-Bravais lattice, provides two pieces of the Fermi surface arising from the two bands, while the stacking can provide a natural nesting direction.

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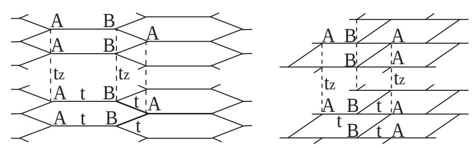

Fig. 1. 3D layered honeycomb lattice (left panel: A and B indicate sublattices), which is topologically equivalent to the lattice in the right.

We study the spin-fluctuation-mediated superconductivity with the fluctuation exchange approximation (FLEX)[2,3]. The model is a two-band Hubbard model with repulsion U. Here we take a non-staggered stacking of honeycomb layers as realized in MgB2 and GIC (Fig.1), where t and t_z denote intralayer and interlayer hopping, respectively. Hereafter we take $t = -1$.

In the two-band FLEX[4,5], Green's function, self-energy, spin susceptibility, and the gap function all become 2×2 matrices. We have obtained these self-consistently with FLEX to plug in Eliashberg's equation. The transition temperature (T_c) is determined as the temperature at which maximum eigenvalue λ of this equation becomes unity.

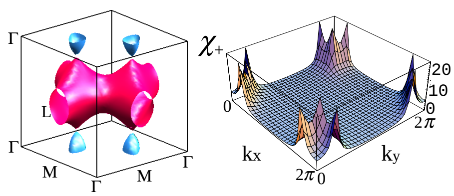

Fig. 2. Fermi surface (left) and $\chi_+(k_z = \pi)$ (right) for the optimized parameter set of $U = 8, n = 1.15, t_z = 0.7$ at $T = 0.01$, where the gap function has opposite signs across the two bands while the intra-band pairing symmetry is d (nodes not shown here).

We search superconductivity from electron repulsion. In general, pairing instability mediated spin fluctuations in 3D systems has been shown to be much weaker than that in 2D systems as shown by Arita et al[6]. Furthermore, 3D systems have strong tendencies toward magnetic orders, so that to identify 3D systems that favor superconductivity from electron repulsion becomes a challenging problem. Here we have optimized the occurrence of the pairing instability in the layered honeycomb lattice by varying t_z and the band filling n. Namely, we have searched for sets of parameter values that give large λ without encountering antiferromagnetic instability at low temperature[7]. The resulting best parameter set is found to be $U = 8$, $n = 1.15$, $t_z = 0.7$. The Fermi surface and the spin susceptibility χ_+ are shown in Fig.2, where peaks of χ_+ around $(0, 0, \pi)$ reflect strong inter-band nesting. To prevent the antiferromagnetic instability for such a large U (see Fig.3(b)), we have selected a slightly bad nesting, so that the peaks of χ_+ deviate from $(0, 0, \pi)$.

In Fig.3(a) we can see that $T_c \sim 0.001$. The pairing symmetry with largest λ is "d wave" where the gap function changes sign as $+-+-$ azimuthally (i.e., within each band) and has opposite signs across the two bands. This solution is doubly degenerate, d_1, d_2, which can be understood by a group theoretical Γ_6^+ representation for the honeycomb system. The true gap function below T_c to minimize the free energy should be a complex linear combination, $d_1 + id_2$, which breaks the time-reversal symmetry. This gap function has *point nodes* on the Fermi surface as shown in Fig.4.

Acknowledgements

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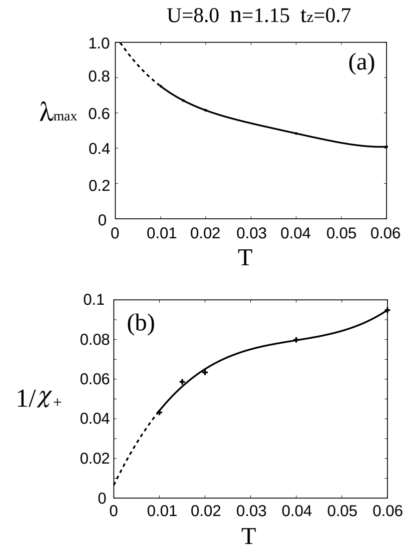

Fig. 3. Eigenvalue of Eliashberg's equationλ (a) and $1/\chi_+$ (b) versus temperature for the optimized parameter set employed in the previous figure. Dotted line is a spline extrapolation to lower temperatures.

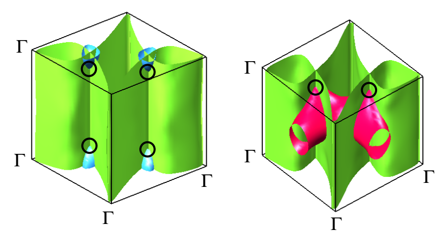

Fig. 4. Nodal planes as well as the Fermi surface are shown, where the results for the doubly-degenerate d waves, d_1 and d_2 are superposed. Left (right) panel represents bonding (anti-bonding) band, and the circles in each panel indicate the intersections of the crossing lines of the two sets of nodal planes with the Fermi surface.

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