Unconventional Pairing in Doped Band Insulators on a Honeycomb Lattice: Application to Superconducting $\beta$-MNC1 (M=Hf, Zr)

Kazuhiko Kuroki

1 Department of applied Physics and Chemistry, The University of Electro-Communications, Chofu, Tokyo 182-8585, Japan
E-mail: kuroki@vivace.e-one.uec.ac.jp

Abstract. We investigate the possibility of realizing unconventional superconductivity in doped band insulators on the square lattice and the honeycomb lattice, where the latter is found to be a good candidate. We discuss the possibility of applying the theory to the superconductivity in doped layered nitride $\beta$-MNC1 (M=Hf, Zr).

1. Introduction
Layered nitride $\beta$-MNC1\(^1\) (M=Hf, Zr) is one of the most interesting group of superconductors in that they exhibit relatively high $T_c$ (up to 25.5K for M=Hf) despite the extremely low density of states at the Fermi level \(^2\) as well as the weak electron phonon coupling.\(^4\) $\beta$-MNC1 is composed of alternate stacking of honeycomb MnN bilayer and Cl bilayer. The bilayer honeycomb lattice structure consisting of M and N is considered to be playing the main role in the occurrence of superconductivity. The mother compound is a band insulator and becomes a superconductor upon doping electrons by Na or Li intercalation.

In the present study, we first generally study the possibility of unconventional superconductivity by doping band insulators on a square or honeycomb lattice. We find that the honeycomb lattice is a good candidate for realizing such a possibility. Then we discuss the possibility of applying the theory to $\beta$-MNC1.
of unconventional superconductivity by doping carriers in band insulators (Fig.1(a)). As shown in Fig.2, we find that the introduction of $\Delta$ rapidly suppresses superconductivity. Thus, in the case of the square lattice, chances for realizing unconventional superconductivity in the above sense are small.

3. Honeycomb lattice

Now let us compare the above result for the square lattice with those for another bipartite lattice, namely, the honeycomb lattice. The honeycomb lattice is a system with two sites in a unit cell, in which the two bands make point contact at $K$ and $K'$ points of the BZ, resulting in a zero gap density of states (Fig.1(b)). We show in Fig.3(a) the maximum value of the spin susceptibility as a function of temperature for the band filling of $n = 1.08$ (band filling $n =$ number of electrons/number of sites), which corresponds to a small amount of electron doping. Surprisingly, we find that the spin susceptibility is nearly independent of $T$, which is in sharp contrast with the case of square lattice. For example, for the square lattice with $n = 0.7$, which is already substantially away from half-filling, we still have a strong enhancement of the spin susceptibility upon lowering the temperature. With further hole doping to $n = 0.65$, the spin susceptibility is suppressed, but even in that case, there is a moderate increase of the spin susceptibility upon lowering the temperature. In Fig.3(b), we show the eigenvalue $\lambda$ of the linearized Eliashberg equation as functions of temperature. $T_c$ is the temperature where $\lambda$ reaches unity. The density of states at $E_F$ is nearly the same for the square lattice with $n = 0.65$ and the honeycomb lattice with $n = 1.08$, and also the spin susceptibility has similar values at low temperature, but still, the honeycomb lattice has larger $\lambda$ and higher $T_c$. Thus, the Hubbard model on the honeycomb lattice has relatively high $T_c$ despite the low density of states and the weak and temperature independent spin fluctuations.

Fig.4 shows the contour plot of the Green’s function squared, whose ridge corresponds to the Fermi surface. We see here two disconnected pieces of the Fermi surface. The spin susceptibility is maximized at wave vectors that bridge the opposite sides of each pieces of the Fermi surface. The gap has a $d$-wave form, where one of the nodes of the gap do not intersect the Fermi surface because of its disconnectivity, which may be one reason why superconductivity is favored despite the low density of states and the weak spin fluctuations. By symmetry, there are two degenerate $d$-wave gaps, and the most probable form of the gap below $T_c$ is the form $d + id$, where the gap is fully open on the Fermi surface, and the time reversal symmetry is broken.

Now we introduce the level offset between A and B sites as we did for the square lattice. In this case also, a band gap opens in the center (Fig.1(b)), so we once again investigate the possibility of superconductivity by doping band insulators. In this case, we find that superconductivity is relatively robust against the introduction of $\Delta$. This may be because the density of states is already low in the original honeycomb lattice, so that the introduction of $\Delta$ does not affect superconductivity so much.

4. Application to $\beta$-MNCl

We now consider applying the above theory to $\beta$-MNCl. Although $\beta$-MNCl has a bilayer honeycomb lattice structure, we find[9] that the two bands closest to $E_F$ obtained in the first principles calculation[5, 6] can roughly be reproduced by a single layer honeycomb lattice model consisting of alternating $d$ and $p$ orbitals with a level offset between $d$ and $p$. If we consider on-site repulsive interaction on both $d$ and $p$ orbitals, the model is similar to the one studied in section 2, except that some distant hopping integrals have to be considered so as to reproduce the first principles band structure accurately. Consequently, within the FLEX+Eliashberg equation approach, we obtain relatively high $T_c$ of around 30K. The relatively high $T_c$ despite the low density of states is consistent with the experimental observation. As for the pairing symmetry, a fully open gap is observed in the experiments,[8] and this is consistent with the present theory.
Figure 1. (a) The density of states for the square lattice with $\Delta = 0$ (black) and $\Delta = t$ (red). (b) The density of states (upper) and the band dispersion (lower) for the honeycomb lattice with $\Delta = 0$ (black) and $\Delta = 1.5t$.

Figure 2. $T_c$ as functions of the level offset $\Delta$ obtained by FLEX+Eliashberg equation for the square lattice with $U = 6t$, $n = 0.7$ (black) or for the honeycomb lattice with $U = 6t$ and $n = 1.08$ (red).

provided that the $d+id$ state is realized. It is hence interesting to investigate experimentally the possibility of time reversal symmetry breaking in the superconducting state of this material.

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Figure 3. (a) The maximum value of the spin susceptibility as functions of temperature obtained by FLEX for the square lattice with $n = 0.7$ or $n = 0.65$ and for the honeycomb lattice for $n = 1.08$. $U = 6t$ in all cases. (b) The eigenvalue of the linearized Eliashberg equation with the same parameter values as in (a). The temperature at which $\lambda = 1$ is the $T_c$.

Figure 4. The contour plots of the FLEX result at the lowest Matsubara frequency for the honeycomb lattice with $U = 6t$, $n = 1.08$, and $T = 0.01t$ (a) The Green's function of the upper band squared, (b) the spin susceptibility, (c) the superconducting gap function.

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