Pseudogap enhancement due to magnetic impurities in d-density waves

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We study the effect of quantum magnetic impurities on d-wave spin density waves (d-SDW). The impurity spins are aligned coherently according to the spin space anisotropy of the condensate. Both the order parameter and transition temperature increases due to the coherent interplay between magnetic scatterers and d-SDW. This can explain the recent experimental data on the pseudogap enhancement of Ni substituted NbBa2(Cu1−yNi)yO6.8 from Pimenov et al. (Phys. Rev. Lett. 94, 227003 (2005)).

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The nature of the pseudogap phase of high $T_c$ superconductors is highly controversial. Among many others, Chakravarty et al.1 proposed that it results from d-density wave order. This phase is a charge density wave (CDW) with a gap of d-wave symmetry. This causes the lack of periodic charge modulation, and evokes the notion "hidden-order". However, there are many other unconventional density wave phases, with similar properties to d-density waves.4,5,6 For example, d-wave spin density waves (d-SDW) are almost identical to d-CDW except the hidden spin space anisotropy, and can account for several experimental results in the pseudogap phase of high $T_c$ superconductors equally well as d-CDW does.

Last year, Pimenov et al.7 reported that the pseudogap energy in underdoped NbBa2CuO6.8 is enhanced by substituting Cu in the CuO2 plane with Ni by measuring the c-axis optical conductivity. We have established recently1 that the pseudogap phase should be d-wave density wave through the analysis of both the giant Nernst effect and the angle dependent magnetoresistance.8 However, we cannot decide whether it is d-wave charge or spin density wave. The earlier Pauli limiting behaviour of d-density waves suggested d-CDW.9,10,11,12 However, it is easily seen that d-SDW also exhibits Pauli limiting when the spin anisotropy axis in d-SDW lies in the a − b plane. Further a recent analysis of impurity scattering under general conditions suggests that such an enhancement of d-density wave order is impossible, if the condensate is d-CDW and/or the impurity is nonmagnetic.13,14,15 This leaves us the unique possibility that d-density waves need to be d-SDW and the impurity scattering is of Kondo type.

Therefore we consider in the followings d-SDW in the presence of magnetic impurities with the Kondo coupling. The study of magnetic impurities has a long history.16,17 In order to couple the impurity spins to the underlying d-SDW, the Kondo coupling has to be non-local and has to have a d-wave component as in Ref. 18. The interaction between quantum magnetic impurities and d-SDW is similar in essence to the RKKY interaction, but the electrons mediating the coupling between the spins are not free but participate in collective phenomenon, and belong to the density wave condensate. This leads to the enhancement of the pseudogap energy, similarly to ferromagnetic superconductors.19,20 There, the Pauli term due to an external magnetic field can compensate the exchange term due to ferromagnetism, and superconductivity will be revived. It is worth mentioning that d-density waves have unusual magnetic properties with the inclusion of spin-orbit coupling as well.21

In general, nonmagnetic impurities such as Zn, lead to the destruction of the underlying phase,21,22 regardless to its symmetry, and are thought to belong to the unitary scattering limit. Ni impurities have also similar impact on superconductors due to the lack of spin space anisotropy, and act as simple potential scatterers in the Born limit. In the situation considered below, their magnetism can couple directly to the order parameter of d-SDW, completely modifying the simple scattering picture. No such mechanism is expected to exist in superconductors, hence magnetic Ni impurities suppress superconductivity similarly to Zn.

As a model, we consider an effective low-energy Hamiltonian describing d-wave spin density waves (d-SDW),23,24 interacting with randomly distributed quantum magnetic impurities:

$$H = \sum_{\mathbf{k},\sigma} \left[ \varepsilon(\mathbf{k}) a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + i\Delta \sigma f(\mathbf{k}) a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k}-\mathbf{Q},\sigma} \right] + \sum_{\mathbf{r},\mathbf{R}_j} J(\mathbf{r} - \mathbf{R}_j) \mathbf{S}_j \mathbf{s}(\mathbf{r}).$$  \hspace{1cm} (1)

Here $\varepsilon(\mathbf{k})$ is the kinetic energy spectrum, $\Delta$ is the d-SDW order parameter, $f(\mathbf{k}) = (\cos(k_x a) - \cos(k_y a))/2$ is the gap function with d-wave symmetry. For simplicity, and to make connection with earlier analysis, we study a commensurate situation with best nesting vector $\mathbf{Q} = (\pi/a, \pi/a)$. A magnetic impurity ($\mathbf{S}_j$) at $\mathbf{R}_j$ interacts with the electron spin density ($\mathbf{s}(\mathbf{r})$) through the non-local Heisenberg exchange coupling. Its matrix element describing scattering with $\mathbf{Q}$ is expanded in terms of Fermi surface harmonics, and we retain the term possessing d-wave symmetry, namely $J(\mathbf{k}, \mathbf{Q}) \propto f(\mathbf{k})$, where $f(\mathbf{k})$ is the d-wave component of the electron density.
the others are unable to couple to the wavevector dependence of the gap. To investigate the effect of magnetic interaction on d-SDW, we study its change on the grand canonical potential perturbatively. To lowest order, one finds

$$\Delta \Omega = - \frac{2J \Delta}{\rho} \sum \frac{S_j^z \cos(Q R_j)}{n_j}, \quad (2)$$

which suggests that each impurity feels a local aligning "magnetic" field manifested through $\Delta/P \cos(Q R_j)$. $S^z$ is the component of the impurity spin parallel to the spin of underlying d-SDW which lies in the $a-b$ plane. Depending on the sign of $\Delta$, the impurity will order locally in ferro- or antiferromagnetic fashion with respect to the local field, but the overall arrangement of impurities will follow an antiferromagnetic pattern due to the $\cos(Q R_j)$ factor, as is visualized schematically in Fig. 1.

![FIG. 1: (Color online) The impurity spin configuration is sketched in the ordered phase. The solid line denotes the alternating field dictated by the impurity-density wave interaction, the colored objects represent the impurity spins.](image)

To make this picture more quantitative, we perform a two order parameter mean field theory, one for the d-SDW and another for the impurities by assuming that the impurity spins are aligned as $S_j^z = m \cos(Q R_j)$. The mean field decoupled magnetic interaction reads as

$$H_{s-d} = J N \sum \frac{i m e^{i q R_j} f(k) \sigma a_{k+q, \sigma} a_{k-Q, \sigma}}{N \rho} = - \frac{J}{\rho} \sum \frac{2S_j^z + m J 2 \Delta}{n_j} \quad (3)$$

Here $N$ is the number of unit cells, $P$ is the d-SDW interaction and $N_i$ is the number of impurity atoms. To average over impurities, we use the standard approach to consider only non-crossing ladder type diagrams. Usually, in the first order Born approximation, nonmagnetic impurities simply shift the chemical potential $\mu$. In our case, however, magnetic impurities couple to the order parameter, $\Delta$, and in the first order Born approximation, the new energy spectrum is given by

$$E_{\pm}(k) = \frac{\varepsilon(k) + \varepsilon(k - Q) \pm}{2}$$

$$\pm \sqrt{\left(\frac{\varepsilon(k) - \varepsilon(k - Q)}{2}\right)^2 + f^2(k) (\Delta + n_i J m)^2}. \quad (4)$$

The use of the Born approximation is justified from the fact that Ni impurities in unconventional superconductor can convincingly be described with it, while Zn substituted samples call for the unitary limit. The stability conditions of the order parameters can be obtained from the grand canonical potential, which takes the form

$$\Omega = N \frac{\Delta^2}{\rho} - T \sum_{\mathbf{k} \in \text{RBZ}} \ln \left(1 + e^{\beta \epsilon_{\mathbf{k}}(\mathbf{k}) - \mu}\right)$$

$$+ \frac{J m}{\rho} N_i 2 \Delta - T N_i \ln \left(\frac{\sinh(\beta J \Delta(2S + 1)/P)}{\sinh(\beta J \Delta/P)}\right). \quad (5)$$

Here $S$ is the impurity spin quantum number, RBZ stands for the reduced (antiferromagnetic) Brillouin zone. The first two terms are characteristic to density waves, the third one stands for the electron-impurity interaction, while the latter describes to certain extent the quantum nature of the magnetic impurity, as opposed to classical spins. After minimization with respect to $\Delta$ and $m$, the coupled gap equations are obtained as

$$\Delta = \frac{2P}{N} \sum_{\mathbf{k} \in \text{RBZ}} \left(f(E_-(\mathbf{k})) - f(E_+(\mathbf{k}))\right) \frac{\Delta + n_i J m f^2(\mathbf{k})}{E_+(\mathbf{k}) - E_-(\mathbf{k})}.$$  

$$2m = (2S + 1) \coth(\beta J \Delta(2S + 1)/P) - \coth(\beta J \Delta/P), \quad (6)$$

$$n_i = N_i/N, f(x)$$ is the Fermi distribution function. The first one is the usual BCS type gap equation, while the second one with Brillouin function on the right hand side accounts for the quantum nature of the magnetic impurity. Regardless to the detailed form of the kinetic energy spectrum, Eq. 6 can be solved at $T = 0$ to give $m = S$, the impurity spin is aligned completely. The above gap equations can further be simplified in the continuum limit and assuming perfect nesting ($\varepsilon(k) + \varepsilon(k - Q) = 0$), but we would like to emphasize that our result are robust with respect to variation of the kinetic energy spectrum, commensurability and imperfect nesting. With this, the zero temperature d-SDW order parameter is determined from

$$\frac{2n_i J S}{\rho_0 \Delta_0} = \frac{(\Delta + n_i J S)}{\Delta_0} \quad (7)$$

with $\rho_0$ the normal state density of states, $\Delta_0$ is the order parameter of the pure system at $T = 0$. In spite of its relative simplicity, this formula constitutes the main result of this paper and is shown in Fig. 2 for various interactions. For any finite $n_i J$, $\Delta$ is enhanced with respect to its pure value $\Delta_0$. The steady increase stems from Eq. 6, since impurities act like a source term. These findings are in accordance with Ref. 6, where a steady increase of the pseudogap has been reported with respect to Ni impurity concentration, by focusing on the suppression of the electric conductivity. Our result indicates that this can arise from the coherent interplay of

$$\varepsilon(k) + \varepsilon(k - Q) \pm$$

$$\sqrt{\left(\frac{\varepsilon(k) - \varepsilon(k - Q)}{2}\right)^2 + f^2(k) (\Delta + n_i J m)^2}. \quad (4)$$
magnetic impurities and d-SDW. Moreover, the experimentally measured pseudogap energy scale is not simply $\Delta$, but $\Delta + n_i JS$ as seen from Eq. [4], causing further enhancement of the pseudogap. As opposed to this, Zn impurities act like potential scatterers, and provide us with pair-breaking effect, leading to the destruction of the superconducting or density wave condensate.

\begin{figure}
\centering
\includegraphics[width=0.45\textwidth]{Fig2}
\caption{(Color online) The concentration and magnetic coupling dependence of the order parameters is shown ($\Delta$ with blue solid, $m$ with red dashed line) at $T = 0$ in the weak-coupling limit for $P \rho_0 = 0.7$, 0.5 and 0.3 from bottom to top. Note the strong increase in $\Delta$ even for low impurity concentrations.}
\end{figure}

The change in the transition temperature ($T_c$) is different from the Abrikosov-Gor’kov formula deduced for non-magnetic impurities, and reads as

$$\ln \left( \frac{T_c}{T_{c0}} \right) = \frac{1}{P \rho_0} \frac{2n_i J^2 S(S + 1)}{3PT_c + 2n_i J^2 S(S + 1)}. \quad (9)$$

The right hand side of this equation is always positive, hence similarly to $\Delta$, $T_c$ also enhances in the presence of magnetic impurities. For arbitrary temperatures, the gap-equations have been solved numerically, and are shown in Fig. [3] for $S = 1$, characteristic to Ni. When the Heisenberg coupling ($J$) is large, the spins retain their maximum value ($S$) up until the close vicinity of $T_c$, and a small amount of impurities increase significantly $\Delta$. On the other hand, for weaker $J$, the d-SDW order parameter follows the usual BCS like temperature dependence, and $m$ reaches its maximum value only at low temperatures.

We mention here, that the finite value of $m$ results in small amplitude antiferromagnetic modulation of the localized spins. Recently such weak low temperature staggered magnetization lying in the $a-b$ plane has been observed in YBa$_2$Cu$_3$O$_6$ with an amplitude $m_0 = 0.05\mu_B$ well above the superconducting transition temperature (55 K) at 310 K. We believe that this antiferromagnetism is related to the interaction between the pseudogap phase and localized moments. Indeed, the measured magnetic intensity closely resembles to that in YBa$_2$Cu$_3$O$_6$. Albeit orbital antiferromagnetism does not exist in our d-SDW model as opposed to its d-CDW counterpart, the sensitivity of its order parameter to local magnetic fields provides us with weak antiferromagnetism, similarly to URu$_2$Si$_2$.

\begin{figure}
\centering
\includegraphics[width=0.45\textwidth]{Fig3}
\caption{(Color online) The temperature dependence of the order parameters is shown ($\Delta$ with blue solid, $m$ with red dashed line) in the weak-coupling limit for $P \rho_0 = 0.5$ and $S = 1$. The top panel shows weak impurity-electron coupling $\Delta_0/J = 4.5$ with $n_i = 0$, 0.03, 0.1 and 0.2 with increasing $T_c$. In the bottom panel, strong impurity-electron coupling is used with $\Delta_0/J = 0.45$, $n_i = 0$, 0.01, 0.03 and 0.06 with increasing transition temperature. For stronger coupling, small concentration causes dramatic increase in both $\Delta$ and $T_c$.}
\end{figure}
magnetic impurities. The impurities will align following the spin density oscillations of electrons, leading to an enhancement of the ordering amplitude. We predict the realization of the aforementioned coherent interplay between magnetic impurities and condensate in the SDW phase of Bechgaard salts (TMTSF)$_2$X with X=PF$_6$, ClO$_4$, AsF$_6$ etc. polluted with magnetic scatterers.

In conclusion, we have demonstrated that magnetic impurities are coherently aligned in a d-wave spin density wave, causing the increase of the order parameter of the condensate. This can be identified with the pseudogap energy scale, whose enhancement is in agreement with a recent experiment in Ni substituted NdBa$_2$\{Cu$_{1-y}$Ni$_y$\}O$_{6.8}$. As was pointed out, magnetic correlations play an important role in the explanation. We predict, that beyond the pseudogap enhancement in NdBa$_2$\{Cu$_{1-y}$Ni$_y$\}O$_{6.8}$, small amplitude antiferromagnetic ordering should be observable due to the Ni impurities, similarly to YBa$_2$Cu$_3$O$_{6.5}$.

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