Superconductivity and Spin Fluctuations

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The organizers of the Memorial Session for Herman Rietschel asked that I review some of the history of the interplay of superconductivity and spin fluctuations. Initially, Berk and Schrieffer showed how paramagnon spin fluctuations could suppress superconductivity in nearly-ferromagnetic materials. Following this, Rietschel and various co-workers wrote a number of papers in which they investigated the role of spin fluctuations in reducing the $T_c$ of various electron-phonon superconductors. Paramagnon spin fluctuations are also believed to provide the $p$-wave pairing mechanism responsible for the superfluid phases of $^3$He. More recently, antiferromagnetic spin fluctuations have been proposed as the mechanism for $d$-wave pairing in the heavy-fermion superconductors and in some organic materials as well as possibly the high-$T_c$ cuprates. Here I will review some of this early history and discuss some of the things we have learned more recently from numerical simulations.

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The interplay of magnetic spin fluctuations and superconductivity has an interesting history, beginning as a way to understand the suppression of $T_c$ in some of the traditional metals, then providing a mechanism for $p$-wave pairing in $^3$He, and finally as a suggested $d$-wave pairing mechanism for some organic superconductors, heavy-fermion systems, and possibly the high-$T_c$ cuprates. Here I will review some of the early history and discuss what has been learned in recent years from numerical studies.

In 1966 Berk and Schrieffer\cite{Berk} and Doniach and Engelson\cite{Doniach} discussed the behavior of nearly-ferromagnetic systems in terms of paramagnon spin...
fluctuations. Berk and Schrieffer showed how paramagnon fluctuations could lead to a strong suppression of the superconducting transition temperature in materials such as Pd. Figure 1 illustrates the Berk-Schrieffer paramagnon mediated interaction in the singlet pairing channel for a Hubbard model with an on-site renormalized interaction $\bar{U} n_{i\uparrow} n_{i\downarrow}$. The particle-hole graphs on the left contain the contribution from the transverse spin-fluctuations and the bubble graphs to the right contain the longitudinal spin fluctuations. For a nearly-ferromagnetic system, this singlet channel interaction has the form

$$V_s(q, \omega) \approx \frac{3}{2} \frac{\bar{U}^2 \chi_0(q, \omega)}{1 - \bar{U} \chi_0(q, \omega)}$$

with

$$\chi_0(q, \omega) = \int \frac{d^3 p}{(2\pi)^3} \frac{f(\varepsilon_{p+q}) - f(\varepsilon_p)}{\omega - (\varepsilon_{p+q} - \varepsilon_p) + i\delta}$$

the usual Lindhard function. A schematic plot of $V_s(q,0)$ is shown in Fig. 2. The peak at $q = 0$ is set by the Stoner enhancement factor $(1 - \bar{U} \chi_0(0))^{-1}$.

Now, just as the usual electron-phonon interaction is characterized by a dimensionless parameter $\lambda$, the paramagnon spin-fluctuation interaction has

$$\lambda_{SF} = -\int_0^\infty \frac{\langle \text{Im} V_s(q,w) \rangle}{w} dw = -\text{Re} \langle V_s(q,0) \rangle.$$ 

Here the bracket indicates an average of the momentum transfer over the fermi surface appropriate for a constant s-wave gap. From the sketch of $V_s(q,0)$ in Fig. 2, one clearly sees that $\lambda_{SF}$ is negative and the paramagnon spin-fluctuation exchange suppresses s-wave superconductivity.

Thus, as Berk and Schrieffer showed, one could understand why nearly-ferromagnetic metals such as Pd were not superconducting. In the late ’70’s and early ’80’s, Herman Rietschel and his co-workers used this approach...
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Fig. 2. Schematic plot of $V_s(q)$ versus $q$ for a spherical fermi surface.

to discuss the possibility that metals which had significantly smaller Stoner enhancement factors might nevertheless have their $T_c$ values limited by paramagnon exchange. For example, they noted that band structure and frozen phonon calculations of the electron-phonon coupling suggested that $Nb$ and $V$ might be expected to have transition temperatures as high as 18K. They then discussed the possibility that while paramagnon exchange did not suppress the $T_c$'s of $Nb$ and $V$ to zero, it could provide an explanation for why they were well below 18K. In particular, they concluded that since a “high electronic density of states $N(0)$ favors the occurrence of spin fluctuations, paramagnon effects are one, if not the limiting factor for high superconducting transition temperatures.” Rietschel et. al. extended these ideas to discuss a variety of materials including $VN$, $Nb_{1-x}V_xN$ and $V_2Zr$. To appreciate this work, one needs to realize that this occurred at a time when the success of the Eliashberg theory suggested that ab-initio calculations of $T_c$ were possible and furthermore that such calculations might provide an understanding of the maximum superconducting $T_c$ that could be reached. In particular, while increasing the electron density of states $N(0)$ might increase the effective electron-phonon coupling parameter, it could also increase the suppression arising from the Stoner-enhanced spin fluctuations and thus there could be some optimum situation and hence maximum $T_c$.

Now, previous to this, in 1971, Layzer and Fay had suggested that paramagnetic spin fluctuations could provide a $p$-wave pairing mechanism for $^3He$, explicitly implementing an earlier suggestion for odd-channel pairing by Emery. The paramagnon exchange interaction in the triplet channel,
illustrated for $S_z = 1$ in Fig. 3, gives an effective pairing interaction

$$V_t \approx -\frac{\bar{U}^2}{2} \frac{\chi_0(q, \omega)}{1 - U\chi_0(q, \omega)}.$$  

In this approximation, $V_t(q)$ is just minus one-third $V_s(q)$. Averaging this interaction over the fermi surface with a p-wave form factor for the gap gives a positive (attractive) effective pairing interaction strength because $V_s(q)$ is peaked at small momentum transfers. After the discovery of superfluid $^3$He in 1973, Anderson and Brinkman showed how the feedback of the superconducting state modified the paramagnetic spin fluctuations favoring the formation of the anisotropic p-wave Anderson-Morel state over the Balian-Werthamer state when the spin fluctuations are strong.

Finally, moving forward to 1986, a paper by Emery appeared in which he suggested that back-scattering from spin fluctuations could lead to the pairing of holes on neighboring organic stacks in the Beckgaard salts. In addition, three papers were submitted in June of '86 which argued that antiferromagnetic spin fluctuations might mediate $d$-wave pairing in the heavy-fermion materials. To see how this can happen, Fig. 4 shows the singlet Berk-Schrieffer interaction, eq. (1), versus $q$ for a two-dimensional system with antiferromagnetic fluctuations. In this case $V_s(q)$ peaks near $(\pi, \pi)$ rather than at $q = (0, 0)$. This may come about from band-structure nesting effects as it does in the weak-coupling treatment of the nearly half-filled Hubbard model or because of strong-coupling, short-range valence bond correlations such as in the 2-leg Hubbard or $t$-$J$ ladders. Basically, it is the short-range spin fluctuations that drive the pairing.
rise to pairing. First consider the usual BCS equation

$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}. \quad (5)$$

For the traditional electron-phonon superconductors, $V$ is negative and slowly varying over the fermi surface. This leads to a gap, $\Delta_p$, which has the same sign over the fermi surface and which is only weakly anisotropic. However, for an interaction which becomes more positive at large momentum transfer, and a large fermi surface, the gap must change sign on the fermi surface as schematically illustrated in Fig. 5 in order to satisfy the BCS gap, eq. (5). That is, suppose $\Delta_{p'}$ is positive for $p'$ near $(0, \pi)$. Then the strong scattering for $p - p' \simeq (\pi, \pi)$ produces a negative gap $\Delta_p$ at $p = (\pi, 0)$ according to eq. (5) so that a $d_{xy}$ gap of the form $\Delta_p = \Delta_0(\cos p_x + \cos p_y)$ provides a solution of the BCS gap equation.

Alternatively, a spatial Fourier transform of the interaction $V_s(q, \omega = 0)$

$$V_s(\ell) = \sum_q e^{i\vec{q}\cdot\vec{\ell}} V_s(q, \omega = 0) \quad (6)$$

gives the result sketched in Fig. 6. Here $\vec{\ell}$ is the separation of the electrons making up the pair. The pairing interaction $V_s(\ell)$ is clearly repulsive on site but becomes attractive on near-neighbor as well as some longer-range sites. The electrons making up the pair can bind when they spatially arrange themselves to take advantage of the attractive regions. Note that the electrons making up the pair come from states within the spin-fluctuation

Fig. 4. Sketch of $V_s(q)$ versus $q$ for a two-dimensional system with short-range antiferromagnetic spin fluctuations.
Fig. 5. Illustration showing how a $d$-wave gap can provide a solution of the BCS gap eq. (5) for a pairing interaction which increases at large momentum transfer like the type illustrated in Fig. 4.

energy of the fermi surface so that a $d_{x^2-y^2}$-wave is formed (for the 2D case) rather than an extended $s$-wave.

This was the kind of picture that was evolving in mid 1986 and the hope was that further measurements would tell whether superconductivity in the heavy-fermion materials and possibly some of the organic materials were indeed mediated by a magnetic spin-fluctuation mechanism. However, there was already at that time a publication, submitted in April 17 of that year by Bednorz and Muller,\(^1\) which would change the direction of research and lead to an intense questioning of the validity of the antiferromagnetic spin-fluctuation pairing mechanism. In fact, to this day, there is no widely agreed-upon pairing mechanism for the high-$T_c$ cuprate problem although there is renewed interest in the antiferromagnetic spin-fluctuation exchange as the mechanism for pairing in the heavy-fermion materials as well as the organics.

In addition, with the passage of time, we have, in fact, learned more about the structure of the pairing mechanism for various basic systems such as the Hubbard and $t$-$J$ models. There have been Gutzwiller variational calculations,\(^2\) auxiliary boson mean-field treatments,\(^2\) conserving fluctuation exchange diagramatic calculations,\(^3\) as well as various phenomenological spin-fluctuation mediated pairing calculations.\(^4\) Here I will focus on some of what we have learned about the pairing interaction from numerical calculations. Monte Carlo calculations\(^5\) for both the doped
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Fig. 6. Fourier transform of the singlet-pairing interaction $V_s(q)$ of Fig. 4 arising from the short-range antiferromagnetic spin fluctuations on a square lattice. Here one member of the singlet pair is located at the origin and the other at a surrounding site $\ell$. The potential is strongly repulsive for both electrons on the same site, as shown by the large positive bar at the origin. However, the potential is attractive on near-neighbor sites.

2D Hubbard model and the 2-leg Hubbard ladder\cite{27} find that the effective particle-particle interaction in the singlet channel peaks at large momentum transfer. Figure 7 shows Monte Carlo results for a doped $8 \times 8$ Hubbard lattice with $U = 8t$ and a site filling $\langle n \rangle = .875$. The peak in the interaction at large momentum transfers Fig. 7b evolves as the temperature $T$ is lowered in a similar manner to the evolution of the peak in the magnetic spin susceptibility $\chi(q)$, Fig. 7a. The structure of the pairing interaction in Fig. 7b, shown for momentum transfer along the $(1,1)$ direction, is similar to the increase at large momentum transfer found in weak-coupling calculations, Fig. 4.

A similar data set for the two-leg Hubbard ladder\cite{27} is shown in Fig. 8. In this case one is dealing with a spin-gapped system in which the antiferromagnetic correlations decay exponentially and the spin-fluctuations can be pictured as local fluctuations of the rung and leg singlet bonds. Nevertheless, as seen in Fig. 8 the temperature dependence of the large-momentum structure of the pairing interaction is similar to the spin susceptibility and the overall structure is similar to the results for the 2D Hubbard model.

Using these effective two-particle interactions along with the Monte Carlo calculation of the single-particle Green’s function, we have solved the particle-particle Bethe-Saltpeter equations\cite{28} and shown that the leading eigenvalue is associated with the $d_{x^2-y^2}$-wave (or in the case of the 2-leg
ladder, the $d_{x^2-y^2}$-wave-like pairing instability. However, the temperatures for which we can carry out these Monte Carlo calculations are limited by the fermion sign problem and at the lowest temperatures we have reached, approximately half the effective exchange energy, the $d$-wave eigenvalue is only of order 0.3. A pairing instability would occur if this eigenvalue reaches 1, where there would be a Kosterlitz-Thouless transition for the 2D system. Other types of Monte Carlo calculations\cite{29} suggested that the ground state of the basic 2D Hubbard model with only a near-neighbor hopping $t$ and an onsite Coulomb interaction $U$ has only short-range, $d$-wave correlations. Numerical density matrix renormalization group calculations do find power law $d_{x^2-y^2}$-like pairing correlations for the doped 2-leg Hubbard ladder, but in order for these correlations to be dominant over the charge-density correlations one needs to have a ratio of the rung-to-leg hopping larger than unity\cite{30} or consider other modifications of the basic model involving next-near-neighbor hopping or an additional contribution to the exchange interaction. Of course, both of these will be present in the actual system. In particular, in the $CuO$ system, an additional exchange coupling, beyond that which is present in a one-band Hubbard model arises from processes in which an intermediate state has two holes on an $O$. We have found, in fact, that the addition of such an exchange term to the Hubbard ladder gives rise to a significant enhancement of the pairing correlations.\cite{31}
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Fig. 8. a) Momentum dependence of the magnetic susceptibility $\chi(q)$ for a 2-leg ladder with $U = 4t$, $\langle n \rangle = 0.875$ and $t_\perp = 1.5t$. Here $q_y = \pi$ and $\chi(q)$ is plotted as a function of $q_x$. b) Momentum dependence of the effective interaction $V(q)$ for $U = 4t$, $\langle n \rangle = 0.875$ and $t_\perp = 1.5t$. Here $V(q)$ is measured in units of $t$, $q_y = \pi$ and $V(q)$ is plotted as a function of $q_x$. From ref. [27].

Thus, although there remain strong theoretical divisions regarding the role of magnetic spin fluctuations as a $d$-wave pairing mechanism, our numerical results support this possibility. Furthermore, recent experimental results on the heavy-fermion materials $CePd_2Si_2$, $CeIn_3$, and $UPd_2Al_3$ and the layered organic superconductors $\kappa$-$(BEDT-TTF)_2X$ provide experimental support for this type of pairing mechanism in these systems. The ultimate resolution of the high-$T_c$ cuprate problem remains to be sorted out. In this connection, it is encouraging that numerical calculations find evidence for both $d_{x^2-y^2}$ pair formation and domain wall formation which appear to arise from the interplay of short-range, spin-correlations and the kinetic energy of the doped holes in the $t$-$J$ model.

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