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Superconductivity of itinerant electrons coupled to spin chains

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A one-dimensional model of itinerant electrons interacting with an antiferromagnetic spin-$\frac{1}{2}$ chain is introduced and solved. The model is designed to create ferromagnetic spin polarons around each itinerant electron. The model is mapped onto a sine-Gordon Hamiltonian of three massless Bose fields. A renormalization-group analysis of the bosonic theory shows that the original model possesses quasi-long-range odd-parity superconductivity and spin-density-wave order. The relevance to high-temperature and heavy-fermion superconductors is discussed.

The recent discovery of high-temperature superconductivity in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ (Ref. 1) has rekindled interest in nonphonon mechanisms of superconductivity. In addition, there is little doubt that superconductivity of the heavy-fermion compounds is strongly influenced by their magnetic properties.[2] In both cases, neutron scattering[3] has revealed the presence of antiferromagnetic spin fluctuations. These experiments have stimulated studies of superconductivity mediated by antiferromagnetic spin fluctuations.[4-8] Weak coupling analyses have considered exchange of antiferromagnetic fluctuations in a Migdal-type approximation and obtain anisotropic singlet superconductivity.[4] The sensitivity of the anisotropic superconductivity to disorder and inelastic scattering makes this an unlikely mechanism of high-temperature superconductivity.[6,7] Strong coupling methods[8] consider a polaronic picture in which controlled analytic calculations are difficult to perform. In the light of this situation, it is clearly of interest to explore whether simplified soluble models are available which can clarify the interaction between itinerant electrons and localized spin fluctuations.

We introduce a one-dimensional model, soluble in the continuum limit, described by the Hamiltonian H:

$$\begin{aligned} H = & -t\sum_{i,\sigma}(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i,\sigma}) \\ & +J\sum_{i}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z) \\ & +(M/2)\sum_{i}S_i^z(c_{i,\uparrow}^{\dagger}c_{i,\uparrow}-c_{i,\downarrow}^{\dagger}c_{i,\downarrow})\,, \end{aligned} \tag{1}$$

where $c_{i,\sigma}^{\dagger}$ creates an electron with spin σ in a Wannier orbital at the unit cell i and $\mathbf{S}_i$ is a localized spin-$\frac{1}{2}$ operator for a different Wannier orbital in unit cell i. The electrons move along the chain via the hopping matrix element t and interact with the localized spins via the spin-diagonal coupling M. The localized spins interact antiferromagnetically with each other with the exchange constant J and the anisotropy constant Δ $(0\leq\Delta\leq 1)$. H is a simplified one-dimensional version of the two-dimensional models of high-temperature superconductors considered by Emery[5] and Hirsch:[8] $\mathbf{S}_i$ is the analog of the spin of the holes in copper $3d_{x^2-y^2}$ orbitals while $c_{i,\sigma}^{\dagger}$ represents the dopant holes in the oxygen $2p$ orbitals. Unlike these authors, however, we allow for direct hopping between the oxygen sites. A similar crude mapping can also be made to heavy fermion superconductors where $\mathbf{S}_i$ represents localized f electrons and $c_{i,\sigma}$ the itinerant electrons.

The physics of H can be understood in terms of a competition between the antiferromagnetic order on the spin chain preferred by the terms proportional to J, and the ferromagnetic polaron which each itinerant electron likes to form around itself as a consequence of the coupling M. Two parallel spin itinerant electrons will prefer to share the cost of the localized spin exchange energy by occupying the same polaron. This pairing of parallel spin electrons can therefore be a possible source of odd-parity superconductivity (OS) with the total spin of the Cooper pairs equal to ± 1.

Using bosonization,[9] we will solve the continuum limit of H. The electrons will be shown to possess quasi-long-range OS order with total Cooper pair spin ± 1 coexisting with spin-density-wave order polarized in the x-y plane. This order occurs for all Δ between 0 and 1, and all positive values of t, J, and $|M|$. If $|M|$ becomes too large, however, certain electron correlation functions decay on the scale of the lattice cutoff and it is not possible to use the techniques of this paper to define a sensible continuum limit. These are the central conclusions of this paper. Direct interactions among the itinerant electrons can also be introduced without affecting the solubility of the problem or the OS order as discussed briefly at the end of the paper. However, introducing an off-diagonal spin coupling like $S_i^+c_{i,\downarrow}^\dagger c_{i,\uparrow}+S_i^-c_{i,\uparrow}^\dagger c_{i,\downarrow}$ introduces complications which are not examined in this paper.

We begin with a review of the solution of the exactly solvable[10] Hamiltonian

$$H_0=J\sum_i(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z)$$

using continuum methods introduced by Luther and Peschel.[11] Introduction of the Jordan-Wigner fermion representation of the spin operators

$$S_i^z=a_i^\dagger a_i-\tfrac{1}{2}\,,\; S_i^+=(-1)^ia_i^\dagger\exp\left[i\pi\sum_{j=1}^{i-1}a_i^\dagger a_i\right]$$

transforms H_0 to the half-filled band sector of

$$H_0'=-(J/2)\sum_i(a_i^\dagger a_{i+1}+a_{i+1}^\dagger a_i)+J\Delta\sum_i{:}a_i^\dagger a_i{:}{:}a_{i+1}^\dagger a_{i+1}{:}\,.$$

We now take the continuum limit of H_0' by linearizing the fermion spectrum about the Fermi level: This introduces the left and right moving fermion fields Ψ_{1s} and Ψ_{2s} which move with the Fermi velocity $v_s=Jd$, where d is the lattice spacing. The fermion interaction terms can be taken to the continuum limit by using the following representation of the normal ordered lattice fermion density operator

$$:a_i^\dagger a_i:=d:[\Psi_{1s}^\dagger(r_i)\Psi_{1s}(r_i)+\Psi_{2s}^\dagger(r_i)\Psi_{2s}(r_i)+\Psi_{1s}^\dagger(r_i)\Psi_{2s}(r_i)e^{-i2k_Fr_i}+\Psi_{2s}^\dagger(r_i)\Psi_{1s}(r_i)e^{i2k_Fr_i}]:. \tag{2}$$

Finally, we bosonize the continuum fermion fields using the representation

$$\Psi_{1s,2s}(x)=\frac{1}{\sqrt{2\pi\alpha}}\exp\left[\pm i\sqrt{\pi}\Phi_s(x)-i\sqrt{\pi}\int_{-\infty}^x dx'\Pi_s(x')\right], \tag{3}$$

where Φ_s and Π_s are canonically conjugate boson fields and all momentum integrals are cut off by the factor $e^{-\alpha p}$. This transforms H_0 to its final form:

$$H_{\rm ob}=\tfrac{1}{2}\int dx v_s\left[K_s\Pi_s^2+\frac{1}{K_s}(\nabla\Phi_s)^2\right]-\int dx y_s\cos(\sqrt{16\pi}\Phi_s)\,. \tag{4}$$

Our prescription for the continuum limit yields the values $v_s=Jd(1+4\Delta/\pi)^{1/2}$, $K_s=(1+4\Delta/\pi)^{-1/2}$, and $y_s=J\Delta d/(2\pi^2a^2)$. The cosine term arises as a consequence of the umklapp scattering condition $4k_Fd=2\pi$.[12] Standard methods yield the renormalization-group (RG) equations

$$\frac{dy_s}{dl}=(2-4K_s)y_s,\quad \frac{dK_s}{dl}=-fK_s^3y_s^2\,, \tag{5}$$

where f is a numerical factor of order unity which is dependent upon the RG prescription and e^l is the scale factor of the RG. The flows described by Eqs. (5) represent a Kosterlitz-Thouless-type transition.[13] The coupling y_s renormalizes to zero provided the renormalized coupling K_s^* is greater than $\frac{1}{2}$. Spin-correlation functions can now be calculated using the renormalized Hamiltonian which describes a free massless Bose field. Undoing the chain of transformations outlined above we obtain

$$\langle S^z(0)S^z(x)\rangle\sim(-1)^x(x)^{-2K_s^*}$$

and

$$\langle S^+(0)S^-(x)\rangle\sim(-1)^x(x)^{-1/(2K_s^*)}\,.$$

Thus, the correlation functions can only be isotropic when $K_s^*=0.5$ which must therefore coincide with the point $\Delta=1$. A direct field theoretical analysis has also shown that $H_{\rm ob}$ has a hidden SU(2) symmetry at the point $K_s^*=0.5$.[14] For $\Delta<1$, we must have $K_s^*>0.5$, until K_s^* reaches 1 at the pure XY limit $\Delta=0$. In the range $\Delta>1$, the coupling y_s becomes relevant and the theory is no longer massless. To summarize, the infrared properties of H_0 for Δ between 0 and 1 can be calculated using a free massless Bose theory with the coupling K_s^* between 1 and 0.5.

We now address the solution of H. In the continuum limit, the lattice fermion fields $c_{i,\uparrow}$ and $c_{i,\downarrow}$ give rise to left- and right-moving fermion fields for the two spin species: $\Psi_{1\uparrow}$, $\Psi_{2\uparrow}$ and $\Psi_{1\downarrow}$, $\Psi_{2\downarrow}$. We bosonize these fermion fields by introducing the Bose fields $\Phi_\uparrow$ and $\Phi_\downarrow$ and their conjugate momenta $\Pi_\uparrow$ and $\Pi_\downarrow$. The bosonic representation of the term proportional to M is particularly simple: this a consequence of the fact that in general $2k_F\pm 2k_F'\neq 2n\pi$ where k_F' is the Fermi momentum of the itinerant electrons and n is any integer. All the large momentum transfer terms in Eq. (2) make no contribution. We may then directly bosonize the term $:\Psi_{1s}^\dagger\Psi_{1s}+\Psi_{2s}^\dagger\Psi_{2s}:$ which is known to be equivalent to the operator $(1/\sqrt{\pi})\nabla\Phi_s$. The itinerant electron fermion fields have a similar representation. This procedure yields the bosonized version of H,

$$H_b=\tfrac{1}{2}\int dx\left[v_sK_s\Pi_s^2\frac{v_s}{K_s}(\nabla\Phi_s)^2+v_\sigma K_\sigma\Pi_\sigma^2+\frac{v_\sigma}{K_\sigma}(\nabla\Phi_\sigma)^2+v_\rho K_\rho\Pi_\rho^2+\frac{v_\rho}{K_\rho}(\nabla\Phi_\rho)^2\right]+\int dx[m\nabla\Phi_s\nabla\Phi_\sigma-y_s\cos(\sqrt{16\pi}\Phi_s)]\,, \tag{6}$$

where $\Phi_\sigma=(\Phi_\uparrow-\Phi_\downarrow)/\sqrt{2}$ and $\Phi_\rho=(\Phi_\uparrow+\Phi_\downarrow)/\sqrt{2}$. The parameters v_s, K_s, and y_s have the same values as in Eq. (4). The Fermi velocities $v_\rho,v_\sigma\approx td\delta$ where δ is the concentration of the itinerant electrons. The coupling constants K_ρ and K_σ are both equal to unity but have been introduced here to facilitate the introduction of direct interactions among the itinerant electrons later in this paper. The coupling m is given by $m=Md/(\sqrt{2}\pi)$.

The RG analysis of H_b can be performed in a manner similar to the ordinary sine-Gordon theory.[15] The RG equation for y_s can be derived from the equation

$$\langle\cos[\sqrt{16\pi}\Phi_s(0)]\cos[\sqrt{16\pi}\Phi_s(x)]\rangle\sim x^{-\gamma};$$

we find

$$\frac{dy_s}{dl} = \left[2 - 4v_s K_s \left(\frac{\cos^2(\theta/2)}{\sqrt{\lambda_1}} + \frac{\sin^2(\theta/2)}{\sqrt{\lambda_2}}\right)\right] y_s\,, \qquad (7)$$

where $\tan\theta = (2m\sqrt{v_s v_\sigma K_s K_\sigma})/(v_\sigma^2 - v_s^2)$ and

$$\lambda_{1,2} = (v_\sigma^2 + v_s^2)/2 \pm [(v_\sigma^2 - v_s^2)^2/4 + m^2 v_s v_\sigma K_s K_\sigma]^{1/2}\,.$$

The renormalizations of v_s and K_s begin at order y_s^2 and are dependent upon the RG scheme. The remaining couplings m, v_σ, K_σ, v_ρ, and K_ρ remain invariant under RG to all orders in y_s. The Eq. (7) has some notable features. Recall that for $m=0$ [when Eq. (7) reduces to Eq. (5)], the coupling y_s was irrelevant provided $K_s^* > K_{Ls}$ with $K_{Ls} = 0.5$. We can now show that turning on the coupling m *reduces* the value of K_{Ls}. Figure 1 plots the boundary between the regions of relevant and irrelevant y_s, as a function of $(K_s^*)^{-1}$ and m. With y_s irrelevant, the spin excitations are gapless and the system can be described by a quadratic Hamiltonian of three Bose fields. When y_s is relevant, the localized spins become Ising-like and the continuum methods of this paper can no longer be used reliably. We conclude from Fig. 1 that for all Δ between 0 and 1, the coupling y_s is irrelevant;[16] this conclusion holds for all values of the parameters m, v_s^*, v_σ, v_ρ, K_σ, and K_ρ, for which the quadratic part of H_b is positive definite.

In the regime where y_s is irrelevant, correlation functions of the fermion operators can be calculated. Of particular interest are the singlet even-parity superconductivity (SS), odd-parity superconductivity (OS), charge-density-wave (CDW), and spin-density-wave (SDW) response functions. Without stating it explicitly, we will henceforth only consider OS and SDW order parameters with total spin equal to ± 1. The spin-zero components are equal in leading order to the SS and CDW response functions, respectively. We represent the response functions in the form $\chi_l(q,\omega_n)$ where l is any one of the order parameters SS, OS, CDW, or SDW, q is the momentum, and ω_n the Matsubara frequency. We find in general that $\chi_l \sim [\max(q,\omega_n)]^{-\alpha_l}$. A positive value of α_l, therefore, indicates the presence of a diverging susceptibility and

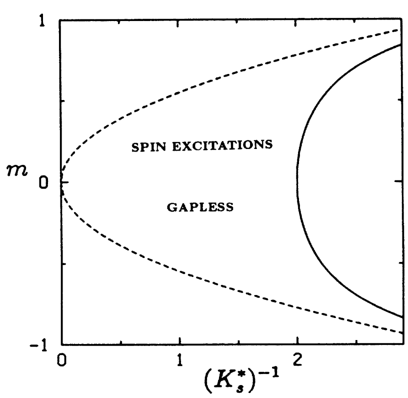

FIG. 1. Plot of the regions in which y_s is relevant or irrelevant for the Hamiltonian H_b as a function of m and K_s^*. The dashed line indicates the limit on the values of $|m|$ above which H_b is not positive definite.

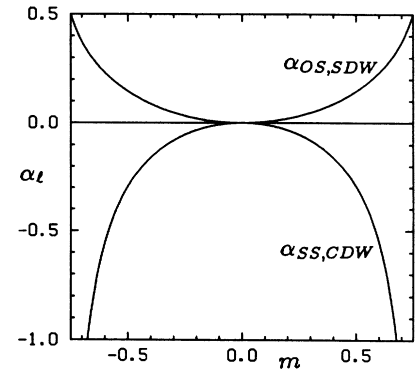

FIG. 2. Exponents α_l as a function of the coupling m for the case K_σ and $K_\rho = 1$, $K_s^* = 0.5$, $v_s^* = 1$, $v_\sigma = 0.3$. Positive values of α_l correspond to quasi-long-range order in the corresponding order parameter.

quasi-long-range order in the corresponding order parameter. The representation of these correlation functions in terms of the continuum Fermi fields is standard.[9] Using the analogs of Eq. (3) we obtain

$$\alpha_{\rm OS} = 2 - \frac{1}{K_\rho} - \frac{1}{v_\sigma K_\sigma}[\sqrt{\lambda_2}\cos^2(\theta/2) + \sqrt{\lambda_1}\sin^2(\theta/2)]\,,$$

$$\alpha_{\rm SDW} = 2 - K_\rho - \frac{1}{v_\sigma K_\sigma}[\sqrt{\lambda_2}\cos^2(\theta/2) + \sqrt{\lambda_1}\sin^2(\theta/2)]\,,$$

$$\alpha_{\rm SS} = 2 - \frac{1}{K_\rho} - v_\sigma K_\sigma\left(\frac{\cos^2(\theta/2)}{\sqrt{\lambda_2}} + \frac{\sin^2(\theta/2)}{\sqrt{\lambda_1}}\right), \qquad (8)$$

$$\alpha_{\rm CDW} = 2 - K_\rho - v_\sigma K_\sigma\left(\frac{\cos^2(\theta/2)}{\sqrt{\lambda_1}}\right),$$

where the parameters θ, λ_1, and λ_2 were defined below Eq. (7), although they must now be expressed in terms of the *renormalized* parameters v_s^* and K_s^*. In the absence of direct interactions among the electrons we have $K_\rho, K_\sigma = 1$. As a consequence, the SS,CDW and OS,SDW exponents are mutually equal. Figure 2 plots the exponents α_l as a function of the coupling m. We find that $\alpha_{\rm OS}$ and $\alpha_{\rm SDW}$ are positive while $\alpha_{\rm SS}$ and $\alpha_{\rm CDW}$ are negative for all values of the parameters m, K_s^*, v_s^*, v_σ, and v_ρ. The system therefore has quasi-long-range OS and SDW order. The result mentioned in the Introduction has therefore been established.

Finally, we address the effect of direct interactions among the itinerant electrons by adding the interactions of the extended Hubbard model:

$$H' = H + U\sum_i n_{i,\uparrow}n_{i,\downarrow} + V\sum_i (n_{i,\uparrow} + n_{i,\downarrow})(n_{i+1,\uparrow} + n_{i+1,\downarrow})\,,$$

where $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$. The concentration of the itinerant electrons δ is taken to be much smaller than 1. Under these circumstances H' can be solved using the methods of this paper. The bosonized form of H' differs from H_b only in that $K_\rho^*, K_\sigma^* \neq 1$ and by the presence of a $y_\sigma \cos(\sqrt{8\pi}\Phi_\sigma)$ term. The results of such an analysis are shown schemati-

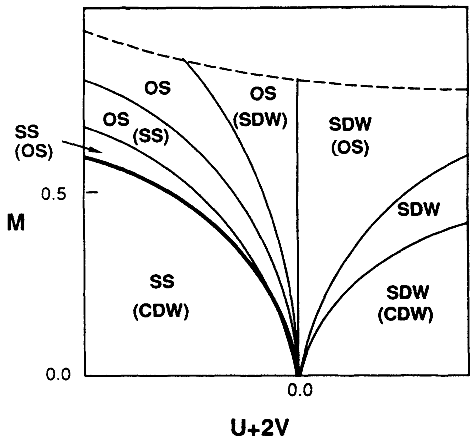

FIG. 3. Schematic phase diagram of H' as a function of M and $U+2V$. The Hamiltonian H corresponds to the vertical line $U+2V=0$. If a given phase has two types of divergent fluctuations, the less divergent one is indicated in brackets. The dark line is a Kosterlitz-Thouless-type transition, while all other phase boundaries correspond to the order parameter exponents α_l continuously passing through zero. The dashed line is the limit of stability of H_b'.

cally in Fig. 3. The thick line represents a Kosterlitz-Thouless transition where y_σ becomes irrelevant and there is a discontinuity in the value of K_σ^*; all other transitions correspond to the exponents α_l going continuously through zero. For $M=0$, H' exhibits SS and CDW order for attractive interactions and SDW and CDW order for repulsive interactions. Turning on the coupling M introduces OS order in a finite band around $U+2V=0$. In particular, the OS order is stable to the introduction of a finite amount of repulsive interactions.

To conclude, we have introduced in this paper a one-dimensional Hamiltonian H which is solvable by bosonization techniques. The Hamiltonian describes itinerant electrons interacting with an antiferromagnetic spin chain. The electrons exhibit odd-parity superconductivity, mediated by the tendency of parallel spin electrons to occupy the same spin polaron. The solution was obtained from a complete RG analysis of the bosonized equivalent of H: three coupled massless Bose fields with cosine self-interactions.

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[16]For this to be true, we need, in addition, that $1 \geq K_s^* \geq 0.5$ for $0 \leq \Delta \leq 1$ even in the presence of the coupling m. A convenient renormalization scheme which shows this is obtained by expanding correlation functions in powers of m and evaluating each term in the renormalized theory of the uncoupled fields.