Quantal Phases, Disorder Effects, and Superconductivity in Spin-Peierls Systems

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In view of recent developments in the investigation on cuprate high-T_c superconductors and the spin-Peierls compound $CuGeO_3$, we study the effect of dilute impurity doping on the spin-Peierls state in quasi-one-dimensional systems. We identify a common origin for the emergence of antiferromagnetic order upon the introduction of static vacancies and superconductivity for mobile holes.

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The evolution of a disordered spin-gapped state [hereafter referred to as a spin liquid (SL)] into a superconductor as observed in the underdoped regime of the cuprate oxide compounds continues to pose a major mystery. Here we address this problem from a new perspective: the comparison of the effect of static and mobile vacancies.

Doping the CuO_2 planes with static nonmagnetic impurities provides valuable information on the SLs. While monovalent Li can lead to additional complications [1], Cu → Zn substitution which introduces vacancies without excess holes serves as an ideal probe: enhancement of antiferromagnetic fluctuatuation accompanying the nucleation of local $s = 1/2$ moments is observed [2,3], apparently indicating that the state is a spin singlet with *confined* spinon excitations. Disorder-induced antiferromagnetism (AF) is a property also shared among several quasi-1D spin-singlet systems, most notably in the spin-Peierls compound $CuGeO_3$ [4], intensively studied in the past several years [5]. Such an analogy has attracted much attention; the effect of disorder on the density of states of the staggered flux state has been discussed [6] in this light, as well as a possible explanation [7] of the extreme sensitivity of the 40 meV magnetic resonance peak to Zn impurities. However, the precise relation, if any, between such responses of SL against *static* impurities and the superconducting instability observed in the cuprates (or spin ladders) in the presence of *mobile* holes remains unclear. This is the issue we discuss.

In this Letter we have chosen to reexamine the simplest confining SL, the quasi-1D spin-Peierls (SP) system within the above scope. The primary aim is to invoke nonperturbative methods, which takes advantage of the one dimensionality, and to extract a physical picture which may well be generic to a wider family of confining SLs. Additional motivations come from experiments, however; while carrier dopings of ar has not been realized in $CuGeO_3$, a possible proximity/coexistence of d-wave superconductivity with a SP-like (or bond-centered density wave) state in underdoped cuprates [8] has been inferred by very recent neutron scattering data of longitudinal optical phonon dispersions in $La_{1.85}Sr_{0.15}CuO_4$ and $YBa_2Cu_3O_{6.95}$ [9].

Let us summarize in physical terms what follows. Theories on impurity effects in spin chains have often focused on either the formation of local spin moments [using Abelian bosonization (AB)] or quantum interferences among a preassigned array of antiferromagnetically aligned spins in the presence of a few vacant sites (employing semiclassical methods). The former cannot account for directional fluctuations of the spins, while the latter may overemphasize the role of local spin moments by assuming them even in a spin-singlet state. Our remedy is to devise a version of non-Abelian bosonization (NAB) which simultaneously resolves both aspects. We derive an effective action reproducing the known AB theory for SP systems [10], *with* two additional terms, each related to the directional fluctuations of the AF order parameter and the Berry phases. The contribution of these new terms is appreciable only near an impurity-induced spin moment. This local weight transfer together with the Berry phase effect (which keeps the spin moments in registry with the underlying AF pattern) is what gives rise to AF order in the *static* impurity case. An important aspect here is the length (or energy) scales involved. Adiabatic adjustment of the spins to the charge deficiency requires the healing length of the charge to be sufficiently shorter than that for the spins. Meanwhile when *mobile* holes are doped, the same basic conditions are seen to enhance superconducting instability, enabling us to make contact with a pairing picture proposed in several earlier works. In this case, the local AF enviroment provided by the spectral weight transfer enhances intrasublattice hopping as well as mediates intersublattice attraction. The adiabaticity condition ensures slow fluctuation of the AF enviroment, necessary for coherent motion of the holes.

To model a SP system, we incorporate the one-band Peierls-Hubbard model at half filling,

$$H = \sum_{i\sigma}[t - (-1)^i \delta t](c^\dagger_{i\sigma}c_{i\sigma} + \text{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

with $U > 0$. Interchain coupling (which fixes the preference of the dimer pattern and hence confines disorder-induced spinons) will be assumed. We start by a semiclassical description of the bulk state; treating the U term as a commensurate spin density wave (cSDW) saddle point solution $\vec{\varphi} = \langle c^\dagger \frac{\vec{\sigma}}{2} c\rangle$, with $\vec{\varphi}_i = (-1)^i m\vec{n}_i$ ($|\vec{n}_i| = 1$, $m \sim \frac{t}{U}e^{-6\pi t/U}$ [11]), we get a 4-component Dirac-fermion-type Hamiltonian density [12]

$$\mathcal{H}_F = [R^\dagger, L^\dagger]\begin{bmatrix} -iv_F\partial_x, -\Delta_0 Q e^{-iQ(\phi_0/2)} \\ -\Delta_0 Q e^{iQ(\phi_0/2)}, iv_F\partial_x \end{bmatrix}\begin{bmatrix} R \\ L \end{bmatrix}, \tag{2}$$

where the right (R) and left (L) movers each carry a spin index, $Q \equiv \vec{n}\cdot\vec{\sigma}$, $\Delta_0 \equiv \sqrt{(4Um/3)^2 + (2\delta t)^2}$, and $\tan(\frac{\phi_0}{2}) \equiv \frac{3\delta t}{2Um}$. To see the physics embodied in the mass term (off-diagonal elements) assume temporarily that $\vec{n} \equiv \hat{z}$. The effective spin-dependent potential energy $V_\sigma(x) \equiv e^{i2k_Fx}V_\sigma(2k_F) + e^{-i2k_Fx}V_\sigma(-2k_F)$ experienced by each spin component $\sigma = \pm 1$ can be read off using $\mathcal{H}_{\text{off-diag}} = \sum_\sigma R_\sigma^\dagger L_\sigma V_\sigma(2k_F) + L_\sigma^\dagger R_\sigma V_\sigma(-2k_F)$:

$$V_\sigma(x) = \begin{cases} 2\Delta_0 \sin[2k_F x + (\frac{\pi}{2} + \frac{\phi_0}{2})] & (\sigma = +1). \\ 2\Delta_0 \sin[2k_F x - (\frac{\pi}{2} + \frac{\phi_0}{2})] & (\sigma = -1). \end{cases} \tag{3}$$

The minima of the potential are located at $x_{\min} = Xa$ (a: lattice constant), where $X = (2n-1) - \frac{\phi_0}{2\pi}, n \in \mathbf{Z}$ for $\sigma = +1$ and $X = 2n + \frac{\phi_0}{2\pi}, n \in \mathbf{Z}$ for $\sigma = -1$, which invites the following interpretation. When $\phi_0 = 0$, odd sites (even sites) are occupied by down spins (up spins) (the cSDW theory). Turning on electron-lattice coupling ($\phi_0 \neq 0$) shifts the position of these down spins (up spins) to the right (the left) resulting in a regular array of strong (odd-even) and weak (even-odd) bonds. The antiparallel spin pairs on the strong bonds form bond-centered density waves. Returning to the general case, this picture remains locally valid with the replacement $\hat{z} \to \vec{n}$ provided $\vec{n}$ fluctuates on a scale longer than a.

A low energy theory is obtained by treating the corresponding Lagrangian $\mathcal{L}_F = \bar{\Psi}[\mathbf{1}\otimes\not{\partial} - \Delta_0 Q e^{iQ(\phi_0/2)\gamma^5}]\,\Psi$ (where $\bar{\Psi} \equiv \Psi^\dagger\gamma_0$, $\gamma^5 \equiv i\gamma_0\gamma_1$, and $e^{iQ(\phi_0/2)\gamma^5} \equiv \cos\frac{\phi_0}{2}\mathbf{1}\otimes\mathbf{1} + i\sin\frac{\phi_0}{2}Q\otimes\gamma^5$) in a derivative expansion of $\vec{n}$. Perturbative terms enter only beyond quadratic order [13], and the resulting action—coming from the anomaly of the SU(2) current $\mathbf{j}_\mu^5 \equiv \bar{\Psi}\gamma_\mu\gamma^5\frac{\vec{\sigma}}{2}\Psi$—is the O(3) nonlinear sigma (NLσ) model with vacuum angle $\theta = \pi - \phi_0 - \sin\phi_0$ [12,14], which signals a spin gap for $\phi_0 \neq 0$.

Having discussed the bulk system at half filling, we now introduce a dilute density of nonmagnetic impurities (vacancies). To this end, keeping ϕ_0 constant (justified in the presence of interchain coupling), we bosonize. In doing so we must go beyond the usual AB with a fixed spin quantization axis in order to retain the spin directional degree of freedom $\vec{n}$. We describe in some detail how this can be done. The AB scheme derives from the fermion-boson correspondence

$$R_\sigma \propto e^{(i/2)[\theta_+ + \theta_- + \sigma(\phi_+ + \phi_-)]}, \qquad L_\sigma \propto e^{(i/2)[-\theta_+ + \theta_- + \sigma(-\phi_+ + \phi_-)]} \tag{4}$$

(in conventions of Ref. [15]) and translates fermionic operators into the language of a set of conjugate charge ($\theta_\pm$) and spin ($\phi_\pm$) phase fields. We attempt a modification by the simple replacement $\sigma \to Q = \vec{n}\cdot\vec{\sigma}$. Constructing Fermi bilinears according to this rule, one readily sees that it corresponds to parametrizing the $k = 1$ Wess-Zumino-Witten (WZW) field $g \in$ SU(2) appearing in the NAB rules [13] as $g = e^{-i\phi_+ Q}$. (The dual fields ϕ_- and θ_- are gauge degrees of freedom which do not arise unless considering chiral currents or Cooper channels.) Note that we differ from the usual way [11] of relating Abelian phase fields to the WZW model. To give firmer grounds to this identification observe that Eq. (4) and its non-Abelian generalization may be viewed as a family of chiral transformations acting on a bosonic vacuum free of charge or spin solitons. The spin part of the free fermion theory therefore has an induced SU(2) connection and is consistently evaluated as

$$Z_{\text{spin}} = \int \mathcal{D}\vec{n}\,\mathcal{D}\phi_+ \int \mathcal{D}\bar{\Psi}\,\mathcal{D}\Psi e^{-\int d\tau\,dx \bar{\Psi}[\mathbf{1}\otimes\not{\partial} + U_5\not{\partial}U_5]\Psi} = \int \mathcal{D}\vec{n}\,\mathcal{D}\phi_+ e^{-S_{\text{wzw}}[g]}|_{g=e^{-i\phi_+ Q}} = Z_{\text{wzw}}, \tag{5}$$

where $U_5 \equiv e^{-(i/2)\phi_+ Q\gamma^5}$. The bosonization dictionary remains unaltered for the charge sector, while the spin part receives corrections related to the fluctuations of $\vec{n}$. For instance, the $k = 2k_F$ component of the spin operator reads $\vec{S}_{k=2k_F} \propto \sin(2k_F x + \theta_+)\sin\phi_+\vec{n}$, whereas the uniform component is

$$\vec{S}_{k=0} = \mathbf{J}_R + \mathbf{J}_L = \frac{1}{2\pi}\partial_x\phi_+\vec{n} + \vec{S}_{\text{additional}} \tag{6}$$

in which $\vec{S}_{\text{additional}} = \frac{1}{2\pi}\cos\phi_+\sin\phi_+\partial_x\vec{n} - \frac{1}{2\pi}\times \sin^2\phi_+\vec{n}\times\partial_x\vec{n}$. Canonical quantization of $\vec{n}$ and ϕ_+ yields the correct (Kac-Moody) algebra for the currents $\mathbf{J}_R$ and $\mathbf{J}_L$. The bosonized Lagrangian for $\mathcal{L}_F$ is $\mathcal{L} = \mathcal{L}_{\theta_+} + \mathcal{L}_{\text{wzw}}(g)|_{g=\exp(-i\phi_+Q)} + \mathcal{L}_{\text{mass}}(\theta_+, \phi_+, \vec{n})$, where the free fermion parts for the charge and spin are, respectively, $\mathcal{L}_{\theta_+} = \frac{1}{4\pi}(\partial_\mu\theta_+)^2$ and

$$\mathcal{L}_{\text{wzw}}(g)|_{g=\exp(-i\phi_+Q)} = \frac{1}{4\pi}(\partial_\mu\phi_+)^2 + \frac{1}{8\pi}\sin^2\phi_+(\partial_\mu\vec{n})^2 + i[2\phi_+ - \sin(2\phi_+)]q_{\tau x}, \tag{7}$$

with $q_{\tau x} = \frac{1}{4\pi}\vec{n}\cdot\partial_\tau\vec{n}\times\partial_x\vec{n}$, the topological charge density of instantons. The last two terms in Eq. (7) are new; they are terms that disappear on taking $\vec{n} =$ const, reproducing the AB expression for a free Tomonaga-Luttinger liquid. On the other hand, a bulk spin gap will fix ϕ_+, and (for $\phi_+ \neq 0$) these terms will yield an O(3) NLσ model with a θ term. The mean value of ϕ_+ is determined from the interaction $\mathcal{L}_{\text{mass}}$, but the latter needs to be handled with some care. Straightforward bosonization gives

$$\mathcal{L}_{\text{mass}} = \frac{2}{\pi\alpha}\sin\theta_+\cos\left(\phi_+ - \frac{\pi}{2} + \frac{\phi_0}{2}\right), \tag{8}$$

where α is a short distance cutoff. Being a relevant term, this locks ϕ_+ in the bulk problem to the value $\phi_+ = \frac{\pi}{2} - \frac{\phi_0}{2}$. (We assume that $\sin\theta_+$ attains a mean value; i.e., the Umklapp term present at half filling opens up the charge gap.) Plugging this into $\mathcal{L}_{\text{wzw}}$, we recover the NLσ

model with the θ angle previously mentioned. But to see the full correspondence with the AB result, we should go beyond this semiclassical approximation; noting that the portion of the mass term $\Delta_0 \cos\frac{\phi}{2}(R^\dagger_\alpha Q_{\alpha\beta} L_\beta + \text{H.c.})$ had originated (prior to the decoupling) from a backscattering process, we should correct Eq. (8) into the form

$$\mathcal{L}_{\text{mass}} = \frac{2\Delta_0}{\pi\alpha} \sin\theta_+ \sin\!\left(\frac{\phi_0}{2}\right)\cos\phi_+ + D\cos 2\phi_+ , \tag{9}$$

where we now have complete agreement with the well-known AB result for the spin-Peierls system [10], supplemented with the second and third terms of Eq. (7). The D term is marginally irrelevant, and the effective value of θ is now governed by the first term of Eq. (9). For $\phi_0 \neq 0$ this gives $\phi_+ = 0$ and hence $\theta = 0$, in which case the magnitude of the staggered spin $m\vec{n}$ is quenched, making the second term in Eq. (7) ineffective. (The formula for $\vec{S}_{k=2k_F}$ infers that $\theta = 0$ and π each correspond to a spin-singlet and a Néel state.) The case $\phi_0 = 0$ (no dimerization) is special; only the D term is present and the effective θ angle is undetermined, indicating a dynamically induced axial U(1) symmetry. This suggests a physical picture of fluctuating dimers reminiscent of a long-ranged resonating-valence-bond state [10]. The above arguments expose an intimite and rather unexpected relation between the θ angle and the spin phase fields of AB, which only becomes evident in the present "rotating frame." In the remaining part we seek its consequences, concentrating on the case $\phi_0 \neq 0$.

We are now ready to discuss vacancies. From the formula for the charge density $\rho = \frac{1}{\pi}\partial_x\theta_+$, this is represented by a π kink of θ_+. From either Eq. (8) or Eq. (9), this is seen to invert the sign of the potential energy, which must be compensated by a π kink of ϕ_+. The latter corresponds to, according to Eq. (6), the liberation of a spin 1/2 degree of freedom in the background of the singlet state. (*Note that this argument does not apply in the absence of the spin gap, i.e., for* $\phi_0 = 0$.) It is possible to show that along the lines of Ref. [16] the spectral weight $\text{Im}\chi(k,\omega)$ for fixed ϕ_+ can be estimated as $\sim \cos^2\phi_+/\sqrt{(k-\pi)^2 + m^2}$ for the gapped part, while another contribution $\sim |\sin\phi_+/(k-\pi)|$ represents a spin wavelike part. Hence the π kink of ϕ_+ should indeed cause a transfer of spectral weight into subgap states, which is a characteristic feature of the present system. Physically, a vacancy at site $x = X_i$ should release a spin of $\vec{S} \sim \frac{1}{2}(-1)^{X_i/a}\vec{n}(X_i)$, which fixes the sign of the kink of the ϕ_+ field to be $\delta\phi_+ = \pi\sum_{X_i}(-1)^{X_i/a}\Theta(x - X_i) = (-1)^{X_i/a}\theta_+$. ($\Theta$ is the step function.) This should be true under the adiabaticity condition $\xi_c \ll \xi_s$, where ξ_c (ξ_s) is the charge (spin) correlation length. The continuum limit, however, does not distinguish to which of the two sublattices a given point $x = X_i$ belongs. Such lattice effects can be particularly important when dealing with Berry phases [17]. To continue working in the continuum, we are thus led to introduce *two* charge phase fields θ_+^A and θ_+^B, one for each sublattice. This leads to a simple expression for the deviation $\delta\phi_+$ of ϕ_+ from the bulk value $\bar{\phi}_+$,

$$\delta\phi_+ = \theta_+^A - \theta_+^B, \tag{10}$$

which is the principal equation of this Letter. Now let us see how this affects the topological term, $\mathcal{L}_{\text{top}} = i[2\phi_+ - \sin(2\phi_+)]q_{\tau x}$. Again using $\xi_c \ll \xi_s$, the effect of $\delta\phi_+$ on the term $-i\sin(2\phi_+)q_{\tau x}$ cancels out on average, and

$$\mathcal{L}_{\text{top}} = i[2\bar{\phi}_+ - \sin 2\bar{\phi}_+]q_{\tau x} + 2i[\theta_+^A - \theta_+^B]q_{\tau x} , \tag{11}$$

provided the average separation of vacancies $l > \xi_s$. Next, we note [18] that formally $q_{\tau x} = \frac{1}{4\pi}\partial_x A_0$, where $A_0(\tau,x) \equiv \partial_\tau\vec{n}\cdot\vec{a}[\vec{n}(\tau,x)]$, and the monopole vector potential $\vec{a}$ satisfies $\nabla_{\vec{n}} \times \vec{a} = \vec{n}$. Integrating by parts, the second term in Eq. (11) becomes $\mathcal{L}'_{\text{top}} = -\frac{i}{2\pi}\partial_x(\theta_+^A - \theta_+^B)\vec{a}\cdot\partial_\tau\vec{n}$. For static vacancies, this yields the action $S'_{\text{top}} = \frac{i}{2}\sum_{X_i}(-1)^{X_i/a}\omega[\vec{n}(\tau,X_i)]$, where $\omega[\vec{n}(\tau)] = \int d\tau\, A_0$ is the solid angle subtended by $\vec{n}(\tau)$ in the course of its evolution. These terms are the Berry phases of spin 1/2 objects induced by vacancies. Together with the bulk contributions consisting of the NLσ model and the first term of Eq. (11) [we use for the potential Eq. (8)], this is essentially the action derived in Ref. [19] for the doping of a spin ladder. Following similar arguments, we arrive at the final action for the induced spins $\{\vec{n}(X_i)\}$,

$$S_{\text{eff}}[\{\mathbf{n}_j\}] = \sum_j \frac{i}{2}(-1)^{X_j/a}\omega[\mathbf{n}_j(\tau)] - \int d\tau\, J_{\text{eff}}\, e^{-|X_j - X_{j+1}|/\xi}\mathbf{n}_j(\tau)\cdot\mathbf{n}_{j+1}(\tau) , \tag{12}$$

where $\mathbf{n}_j \equiv \vec{n}(X_j)$ and $J_{\text{eff}} = 1/\xi \cdot \sin^2\frac{\phi_0}{2}$. Absorbing the signs into the spins $\mathbf{N}_j \equiv (-1)^{X_j/a}\mathbf{n}_j$, this becomes a random exchange Heisenberg model, with diverging spin correlation and staggered susceptibility at $T = 0$ [19]. We expect, in agreement with, e.g., Ref. [20], that the essential physics of the disorder-induced AF observed in $CuGeO_3$ is captured within this model.

Turning to the case of mobile vacancies (holes), the part of the action involving θ_+^A and θ_+^B reads

$$\mathcal{L}(\theta_+^A, \theta_+^B) = \frac{1}{8\pi}[\partial_\mu(\theta_+^A + \theta_+^B)]^2 + \frac{1}{8\pi}[\partial_\mu(\theta_+^A - \theta_+^B)]^2 + 2i[\theta_+^A - \theta_+^B]q_{\tau x} . \tag{13}$$

This coincides with the action proposed by Shankar [21] on semiphenomenological grounds for hole motions in an antiferromagnetic background. We have arrived at this form from an electron system containing both spin and charge sectors. Hereon we may basically adapt the arguments of Ref. [21]. Refermionizing $\mathcal{L}(\theta_+^A, \theta_+^B)$ we see that it is equivalent to two massless fermions

$$\mathcal{L}_{\rm hole} = \bar{\psi}_A(\partial\!\!\!/ + iA\!\!\!/)\psi_A + \bar{\psi}_B(\partial\!\!\!/ - iA\!\!\!/)\psi_B \qquad (14)$$

coupled to the gauge fields $A_\mu = \partial_\mu \vec{n} \cdot \vec{a}$ each describing intrasublattice (next nearest neighbor) hopping of the holes [21,22]. Because the fermions ψ_A and ψ_B have opposite gauge charges, there is an attractive interaction. The spin-singlet superconducting susceptibility is the correlation fuction of (in terms of the original electrons) $\psi^A_{R\sigma}(x)\psi^B_{L-\sigma}(x) \sim e^{(i/2)(\theta^A_+ - \theta^B_+)} e^{(i/2)(\theta^A_- + \theta^B_-)} e^{i\phi_+}$. The nontrivial combination here is $\theta^A_+ - \theta^B_+$, but Gauss law constraints can be incorporated [21] to show it is massive. Then the susceptibility obeys a power law with exponent -1 and should become an Emery-Luther superconductor when including interactions among neighboring sites, which seems to be consistent with available numerical results on dimerized *t-J* models [23]. This would suggest the possibility of the coexistence of the spin-gapped state (i.e., spin-Peierls state) with superconductivity. Superconductivity in quasi-1D spin-gapped systems may become relevant in view of the recent advances in hole injection via field-effect transistors [24]. Finally we note certain differences from Ref. [21]; first the picture relies on a confining SL, therefore breaking down at the Heisenberg point $\phi_0 = 0$; i.e., a spin gap is required. A second feature is the difference in the vacua structure; we had effectively $\theta = 0$ irrespective of the value of $\phi_0 \neq 0$ and hence zero weight for the NLσ model part, so the collapse of a θ-vacua structure with hole doping [21] is not seen, which marks a departure from semiclassical methods.

In conclusion, we have seen the enhancement of superconducting susceptibility—closely related to pairing scenarios based on t'-J-type interactions [22]—emerge from the same origin as the disorder-induced AF. The origin is the coupling of the charge density fluctuation to the spin gauge fluctuation, represented compactly in Eq. (10). This suggests that validity of such pairing pictures in a particular spin-gapped system can be inferred from testing its response to static nonmagnetic impurities. In this respect we mention recent hole-doping experiments in the Haldane-gap material Y_2BaNiO_5 [25], a system where static impurities do not induce AF. The authors find no enhancement of conductivity and ascribe it to the comparable magnitude of the charge and spin gaps.

Since our framework can be readily applied to charge stripes modeled as arrays of 1D electron gases coupled to spin-gapped chains [26], similar treatments should provide useful insight. Such work is now in progress.

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