Fictitious flux confinement: Magnetic pairing in coupled spin chains or planes

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The spinon and holon excitations of two-leg Heisenberg or lightly doped t-J ladders are shown to be bound in pairs by string confinement forces given approximately by the antiferromagnetic exchange energy across the rungs, $F=J_\perp\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp/b$. These forces originate from fictitious flux tubes associated with the half-Fermi statistics of the excitations. It is conjectured that similar confinement forces, determined by the antiferromagnetic exchange energy across the layers, are partially responsible for the spin gap and the pairing of charge carriers in multilayer CuO superconductors.

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Two-leg Heisenberg or lightly doped t-J ladders[1] can, according to a recent proposal,[2] be described approximately by an RVB-type spin liquid. Specifically, one assumes a magnetic tight-binding model on the ladder, with flux π per plaquet and hopping magnitudes $\tilde{t}$ along the chains and $\tilde{t}_\perp$ across the rungs. One then fills the lower band twice, once with up-spin electrons and once with down-spin electrons. Upon elimination of doubly occupied sites via a Gutzwiller projection, one obtains a reasonable approximation[2] of the ground state of the Heisenberg ladder with $J_\perp/J=\tilde{t}_\perp/\tilde{t}$.

Spinon and holon excitations for this liquid may be created either via Anderson's projection technique[3] or via midgap states.[4] As the topology of the ladder dictates that midgap states can only be created in pairs, the second method automatically yields spinon-spinon bound states (magnons) rather then isolated spinons, which reflects the fact that the spinons or holons are confined in pairs.

In the first part of this paper, I will explain the form and origin of the confinement forces between the spinons and holons of the ladder, and calculate the spinon mass and the bound-state resonances based on a heuristic identification of the spin gap of the Heisenberg ladder as the zero-point energy of the string oscillator. In the second part, I will postulate similar confinement forces in systems of (weakly) coupled magnetic planes, make some assumptions regarding both the nature of the spin liquid in the planes and the confinement forces due to the interplane coupling, and obtain an estimate for the spin and charge gaps in bilayer CuO superconductors (25 and 30 meV, respectively, for $YBa_2Cu_3O_{6+x}$).

In order to determine the functional form and strength of the confining potential between the spinon or holon excitations of the two-leg Heisenberg ladder, we create two holons at sites i and j via Anderson's projection technique,[3]

$$|\psi_{i,j}\rangle = c_{i\uparrow}c_{j\downarrow}\mathcal{P}_{\mathrm{G}}c_{i\uparrow}^{\dagger}c_{j\uparrow}|\psi_{\mathrm{SD}}\rangle, \tag{1}$$

where $|\psi_{\mathrm{SD}}\rangle$ is the Slater determinant ground state obtained by filling the lower magnetic tight-binding band twice, and numerically compare the energy expectation value of this configuration to the energy of the exact ground state for a Heisenberg ladder with two stationary holes at these sites.[5] The results are shown in Figs. 1 and 2; we find a linear potential

$$V(x)=F|x|, \quad F\approx J_\perp|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|/b, \tag{2}$$

where x is the distance between the spinons or holons in the direction of the chains, $\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp$ the spin correlation across the rungs, and b the bond length along the chains. The confinement energy is hence approximately equal to the antiferromagnetic exchange energy across the rungs between the spinons; the reason for this emerges from a comparison of the individual spin correlations on each link, as reproduced in Fig. 3 for two typical configurations: an invisible string between the holons destroys the antiferromagnetic correlations on all the rungs between them.

The origin of this string is explained in Fig. 4: the fictitious flux tube associated with the half-fermi statistics[8] of the spinons or holons,[7,9] which manifests itself in an adjustment by π (Refs. 4 and 2) of the fictitious flux through the adjacent plaquets in the magnetic tight-binding model before Gutzwiller projection, effectively annihilates the hopping terms on the rungs between them.

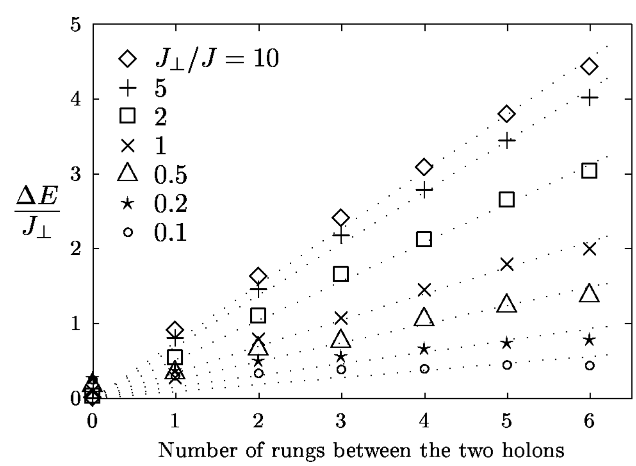

FIG. 1. The confinement energy, defined here as the energy of a pair of holons measured relative to the exact ground-state energy of a pair of holes, as a function of the number of rungs between the holons or holes for a 2×8 ladder with open boundary conditions and $\tilde{t}_\perp/\tilde{t}$ vs $J_\perp/J$ as in Table I. The data were obtained with one holon localized at the end of the ladder and the other localized at various positions on the same chain, as illustrated in Fig. 3(a); a finite-size correction has been taken into account for $J_\perp/J=0.2$ and 0.1.

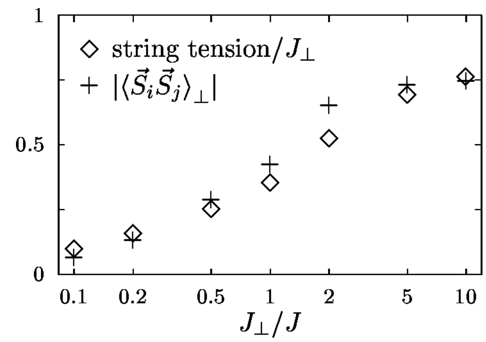

FIG. 2. The string tension in units of $J_\perp$ given by the slope of the dotted lines fitted though the data points in Fig. 1 in comparison with the spin correlations $|\langle \vec{S}_i \vec{S}_j \rangle_\perp|$ across the rungs in the ground state as taken from Table I for different ratios $J_\perp/J$. The discrepancy around $J_\perp/J=2$ arises from the enhanced correlations $|\langle \vec{S}_i \vec{S}_j \rangle_\parallel|$ along the chains in the presence of the holons, which were neglected in Eq. (2).

If we were to know the effective mass of the spinon, we could calculate the resonances of the string oscillator

$$\left(-\frac{1}{2m_{\rm red}} \nabla^2 + F|\mathbf{r}| \right) \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}), \qquad (3)$$

where $m_{\rm red} = \frac{1}{2} m_{\rm sp}$ is the reduced mass of a spinon pair. We then could compare the oscillator ground-state energy to the spin gap in the Heisenberg ladder, which is just the energy required to create a spinon-spinon bound state; apart from a possible correction due to a chemical potential for spinons which we neglect, these should be equal. In the present case,

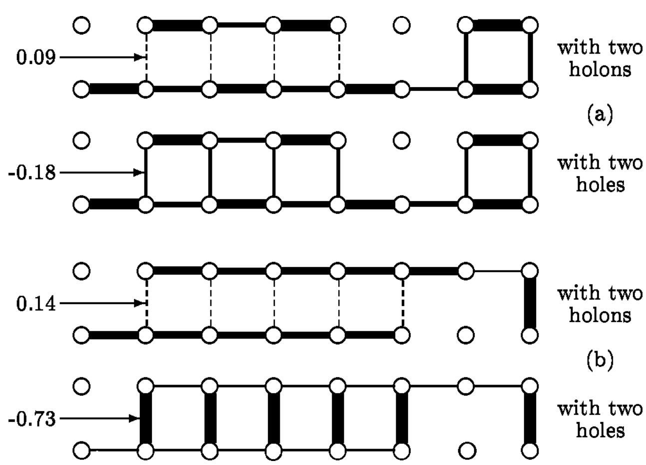

FIG. 3. Spin correlations $\langle \vec{S}_i \vec{S}_j \rangle$ between nearest neighbors in the presence of two holons compared with two holes for two representative configurations of a 2×8 ladder with open boundary conditions and (a) $J_\perp/J=0.5$ or (b) $J_\perp/J=5$. The conventions are adopted from White and Scalapino (Ref. 6); the thickness of the lines is proportional to $|\langle \vec{S}_i \vec{S}_j \rangle|$; solid lines indicate antiferromagnetic, and dotted lines ferromagnetic correlations. The state containing two holons was obtained from Gutzwiller projected magnetic bands using Anderson's method for constructing spinons; the state containing two holes is just the exact ground state of the Heisenberg ladder with two static vacancies at the positions indicated.

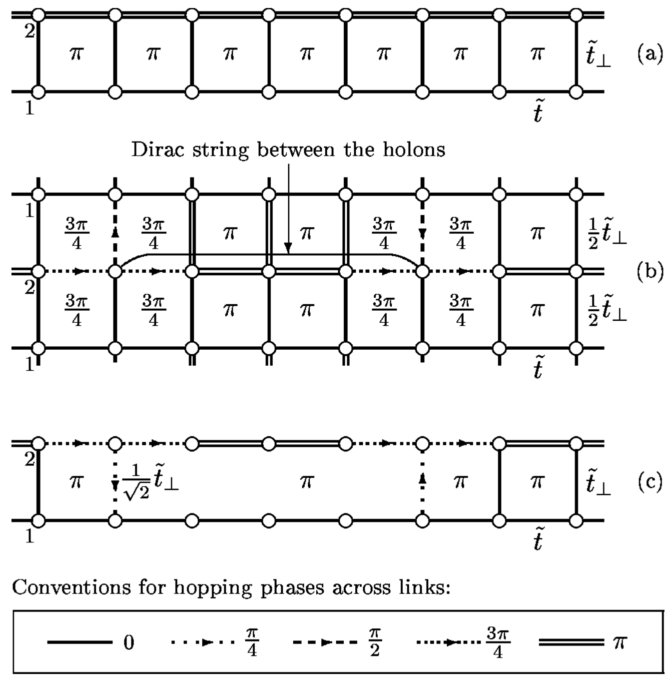

FIG. 4. Magnetic tight-binding configurations before Gutzwiller projection for (a) the ground state of the t-J ladder at half-filling and [(b) and (c)] in the presence of two holons at a distance of 4 lattice spacings. The holons in (b) were created following the procedure for the Kalmeyer-Laughlin chiral spin liquid (Ref. 7), suggested in Ref. 2 after mapping the flux ladder into a flux lattice subject to a periodic boundary condition with a periodicity of only two lattice spacings in the y direction. The lattice is subsequently reconverted into a ladder (c). Note that the Dirac string annihilates all the hopping terms across the rungs between the holons, while the hopping magnitudes along the chains remain unaffected.

we use the known value $\Delta \approx J_\perp/2$ for the spin gap[10,12] to calculate the spinon mass and the spinon-spinon resonances in the weak coupling regime $J_\perp < J$. In one dimension, the solutions of Eq. (3) are given in terms of the Airy function $\mathrm{Ai}(x)$,[13]

$$\psi_n(x) = \left(\frac{x}{|x|} \right)^n \mathrm{Ai}\left(\frac{|x|}{x_0} - \lambda_n \right), \quad E_n = F x_0 \lambda_n, \qquad (4)$$

where $x_0 = 1/(2m_{\rm red}F)^{1/3}$ is the characteristic lengthscale of the oscillator, and λ_n are the extrema or zeros of $\mathrm{Ai}(-x)$ for n even or n odd, respectively, which are listed in Table II. Even values for n correspond to spinons in a spin-triplet configurations, and odd values to a spin-singlet configuration. Equating $E_0 = \Delta$, we obtain

$$m_{\rm sp} = \frac{F^2 \lambda_0^3}{E_0^3} = \frac{8|\langle \mathbf{S}_i \mathbf{S}_j \rangle_\perp|^2 \lambda_0^3}{J_\perp b^2} = 3.25 \frac{J_\perp}{J^2 b^2}, \qquad (5)$$

where we have approximated $|\langle \mathbf{S}_i \mathbf{S}_j \rangle_\perp| \approx 0.62 J_\perp/J$ according to Table I for weakly coupled ladders. The spacing of the eigenvalues λ_n implies that the internal resonance frequencies of the spinon-spinon bound states or magnons are higher than the energies required to create a second or third magnon. At first glance, one might hence expect that these reso-

TABLE I. Energy expectation values in units of $\max(J_\perp, J)$ and nearest-neighbor spin correlations for the spin liquid trial wave functions in comparison with the exact ground states of a 2×10 Heisenberg ladder with periodic boundary conditions. The ratios of the hopping magnitudes before projection have been $\tilde{t}_\perp/\tilde{t} = 0.75(J_\perp/J)^{0.5}$ for $J_\perp/J \leqslant 1$ and $\tilde{t}_\perp/\tilde{t} = (J_\perp/J)^{0.6}$ for $J_\perp/J \geqslant 2$.

$J_\perp/J$	$E_{\rm tot}$ exact	$E_{\rm tot}$ trial	% off	overlap	$\langle\vec{S}_i\vec{S}_j\rangle_\parallel$ exact	$\langle\vec{S}_i\vec{S}_j\rangle_\parallel$ trial	$\langle\vec{S}_i\vec{S}_j\rangle_\perp$ exact	$\langle\vec{S}_i\vec{S}_j\rangle_\perp$ trial
0	−9.031	−9.015	0.2	0.997	−0.452	−0.451	0.000	0.000
0.01	−9.031	−9.015	0.2	0.997	−0.452	−0.451	−0.006	−0.006
0.02	−9.032	−9.015	0.2	0.997	−0.451	−0.451	−0.012	−0.012
0.05	−9.039	−9.015	0.3	0.995	−0.451	−0.450	−0.031	−0.031
0.1	−9.062	−9.018	0.5	0.990	−0.450	−0.448	−0.062	−0.064
0.2	−9.155	−9.055	1.1	0.974	−0.445	−0.440	−0.123	−0.130
0.5	−9.755	−9.559	2.0	0.947	−0.420	−0.406	−0.269	−0.286
1	−11.577	−11.395	1.6	0.968	−0.354	−0.358	−0.450	−0.424
2	−8.594	−8.566	0.3	0.992	−0.222	−0.205	−0.638	−0.651
5	−7.664	−7.661	0.0	0.999	−0.085	−0.093	−0.732	−0.729
10	−7.539	−7.539	0.0	1.000	−0.040	−0.044	−0.746	−0.745
∞	−7.500	−7.500	0.0	1.000	0.000	0.000	−0.750	−0.750

nances decay rapidly into several magnons, and are difficult if not impossible to observe. The pronounced momentum dependence of the magnon dispersion [see, for example, Fig. 4(b) of (Ref. 2)], on the other hand, shows that the two-magnon continuum near $(k_x,k_y)=(\pi,0)$ only begins at energies $\approx 4\Delta$, so that the lowest singlet spinon-spinon bound state at $\Delta_{\rm singlet}\approx 2.3\Delta$ could well correspond to a sharp resonance below this continuum. This state might even be responsible for a large part of the low-energy spectral weight observed in the optical conductivity measurements by Windt *et al.*[11] in $(\mathrm{Ca,La})_{14}\mathrm{Cu}_{24}\mathrm{O}_{41}$.

It is now easy to estimate the size of the magnon. Using $\mathrm{Ai}(|x|-\lambda_0)\approx \mathrm{Ai}(-\lambda_0)\exp(-\frac{1}{3}x^2)$, we write the ground state

$$\psi_0(x)=\exp\left(-\frac{x^2}{2\xi^2}\right) \qquad \text{with} \quad \xi=\sqrt{\frac{3}{2}}x_0=0.97\frac{J}{J_\perp}b. \tag{6}$$

This result illustrates why the spin gap in the weak-coupling regime can be $\frac{1}{2}J_\perp$ while the antiferromagnetic exchange energy across each rung is only of order $\frac{1}{2}J_\perp^2/J$: the number of decorrelated rungs is of order $J/J_\perp$. The oscillator spectrum predicts a ratio of singlet to triplet gap $\lambda_1/\lambda_0=2.3$, which agrees roughly with the result $m_s/m_t=3$ found by bosonization for the limit of weakly coupled chains.[12]

This calculation can also be applied to spinon-holon bound states (holes) in the ladder. The only difference is that the reduced mass in Eqs. (3) and (4) is replaced by

$$\frac{1}{m_{\rm red}}=\frac{1}{m_{\rm sp}}+\frac{1}{m_h} \quad \text{where} \quad m_h=\frac{1}{2t_{\rm eff}b^2} \tag{7}$$

is the effective mass of the holon; according to Table II of Ref. 2, $t_{\rm eff}=\frac{1}{2}E_{t_\parallel}=0.77t$ for $J_\perp=J$ and $t_{\rm eff}=0.95t$ in the weak-coupling limit $J_\perp \ll J$. The values for the energies E_n and the size ξ of the bound state are those given in Eqs. (4) and (6) above, multiplied by $\mu^{1/3}$ with

$$\mu=\frac{1}{2}\left(1+\frac{m_{\rm sp}}{m_h}\right)=\frac{1}{2}\left(1+6.50\frac{t_{\rm eff}J_\perp}{J^2}\right). \tag{8}$$

I will now turn to the speculative part of this article, and explain part of my thinking on CuO superconductivity. To begin with, I make the following assumptions: First, the ground state of the two-dimensional t-J model at the relevant hole dopings is a spin liquid, which supports spinons and holons as elementary excitations.[3] (My understanding[14] of this liquid is that it is a liquid in both the spin degrees of freedom and in the nonrelativistic plaquet chiralities;[15] this *chirality liquid* may be seen as a significant generalization of Laughlin's chiral spin liquid,[7] which is a liquid in the spins but effectively aligns the chiralities and thereby violates the discrete symmetries P and T. These symmetries are preserved in my construction. The spinon and holon excitations supported by the chirality liquid carry a chirality quantum number, which can be $+$ or $-$; this number determines the sign of the winding phases associated with their half-Fermi statistics.) Second, the spinon and holon masses in a system of coupled t-J planes are comparable to their values in a system of coupled chains estimated above.

The main difference between fictitious flux confinement in a system of coupled planes as compared to coupled chains is that the one-dimensional array of decorrelated rungs is replaced by a puddle of decorrelated interplane links. To see this, imagine several ladders (which are not necessarily straight) embedded in a system of coupled planes such that the rungs align with interplane links, and connect two spinon sites i and j along various paths in the planes with these ladders. The fictitious flux connecting the spinons will then destroy the correlations across all the rungs on each ladder.

The simplest estimate for the strength of the confining force is to assume a circular droplet of decorrelated links between the spinons, with a diameter given by the spinon-spinon distance r. (This is presumably not a valid approxi-

TABLE II. The lowest (dimensionless) energy eigenvalues for the linear oscillator in one and two dimensions.

	1D string		2D string oscillator		
n	λ_{2n}	λ_{2n+1}	λ_{n0}	λ_{n1}	λ_{n2}
0	1.0188	2.3381	1.7372	2.8721	3.8175
1	3.2482	4.0879	3.6702	4.4930	5.2629
2	4.8201	5.5206	5.1697	5.8671	6.5415

mation for large spinon separations, but may be reasonable for the ground state of the oscillator.) It yields a harmonic potential

$$V(r)=\frac{\pi r^2}{4b^2}J_\perp|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|\equiv\frac{1}{2}Dr^2. \tag{9}$$

The ground state energy of the spinon-spinon bound state is hence given by

$$E_0=\sqrt{\frac{D}{m_{\mathrm{red}}}}=\sqrt{\frac{\pi}{3.25}|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|J^2}=0.77\sqrt{J_\perp J}, \tag{10}$$

where we have used Eq. (5) and $|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|\approx 0.62J_\perp/J$. This estimate for the spin gap[16] in $YBa_2Cu_3O_{6+x}$ is directly related to the optical magnon gap in the ordered antiferromagnet $YBa_2Cu_3O_{6.2}$, which has been measured by inelastic neutron scattering:[17] $E_{\mathrm{opt.}}=2\sqrt{J_\perp J}\approx 70$ meV. This yields a spin gap of 27 meV. The charge gap is just the gap to create a spinon-holon bound state: substituting $J=120$ meV, $J_\perp=10$ meV $t=500$ meV, and $t_{\mathrm{eff}}=0.9t$ for $YBa_2Cu_3O_{6+x}$ into Eq. (8), we obtain 33 meV.

I wish to remark at this point that the microscopic details of the chirality liquid[14] mentioned above yield a linear potential as an estimate for the confining force,

$$F_{2\mathrm{d}}=\frac{1}{b}\sqrt{\frac{E_{00}J_\perp|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|}{2}}, \tag{11}$$

where E_{00} is the spin gap given by the ground-state energy of the string oscillator [Eq. (3)] with string tension $F_{2\mathrm{D}}$ in two dimensions. This oscillator has to be solved numerically; the solutions are

$$\psi_{nl}(r,\varphi)=e^{\pm il\varphi}\phi_{nl}\left(\frac{r}{r_0}\right), \quad E_{nl}=F_{2\mathrm{D}}r_0\lambda_{nl}, \tag{12}$$

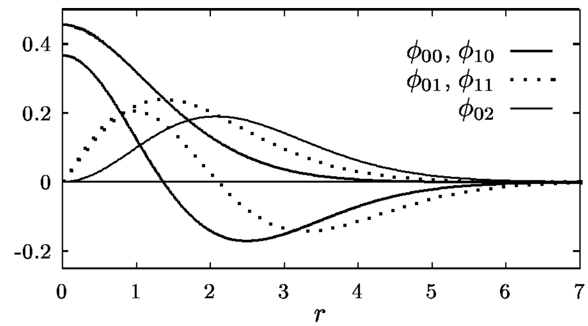

FIG. 5. Radial wave functions for the lowest-energy eigenstates of the linear oscillator in two dimensions.

with $r_0=1/(2m_{\mathrm{red}}F_{2\mathrm{D}})^{1/3}$, λ_{nl} as listed in Table II, and $\phi_{nl}(r)$ as plotted in Fig. 5.

Solving Eqs. (11) and (12) for E_{00} yields

$$E_{00}=\sqrt{\frac{J_\perp|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|\lambda_{00}^3}{4m_{\mathrm{red}}}}=\sqrt{\frac{1}{2}J_\perp J}, \tag{13}$$

where we have used Eq. (5) and $|\langle \mathbf{S}_i\mathbf{S}_j\rangle_\perp|\approx 0.62J_\perp/J$ once more. This yields spin and charge gaps of 25 and 30 meV for $YBa_2Cu_3O_{6+x}$. It should of course be borne in mind that these numbers are only rough estimates; many important details, including the *d*-wave symmetry of the superconducting order parameter, have not been taken into account here.

In conclusion, I have elucidated the mechanism responsible for the confinement of spinons and holons in *t*-*J* ladders. By equating the spin gap in undoped ladders with the zero-point energy of the spinon-spinon bound state, I obtained an estimate for the energies of the internal resonances of spinon-spinon or spinon-holon bound states. I further explained how similar confinement forces in systems of weakly coupled planes give rise to spin and charge gaps which are by magnitudes larger than the antiferromagnetic exchange energy stored in the links connecting the planes.

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