# Holes in a Quantum Antiferromagnet: New Approach and Exact Results

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(Received 20 March 1989)

It is shown that holes on the $A$ and $B$ sublattices of a spin-$s$ antiferromagnet behave as charges $\pm s$ coupled to a gauge field $a_\mu(\mathbf{n})$, $\mathbf{n}$ being the local order parameter. This general formalism can be pursued very far in $d=1$ where the finite-hole-concentration problem is described by massless fermions coupled to the $\sigma$ model. Many exact results follow: Holes superconduct, destroy the quasi-long-range order, and wipe out the $\Theta$ term which distinguishes between integer and half-integer models or describes bond-strength alternation.

PACS numbers: 75.10.Jm, 11.10.Ef, 71.30.+h, 74.65.+n

Superconductivity in the Cu-O layers[1] gives us a good motivation for studying antiferromagnets with holes. Prior to doping, the layers are Mott insulators with one spin-$\frac{1}{2}$ per site and Néel order. Upon doping the order is reduced and eventually replaced by superconductivity. Several theorists[2] have attempted to describe the holes, analytically and numerically. Here I develop the theory of holes for a certain class of models using path integrals. While some general consequences can be deduced in all dimensions, in $d=1$, I can go much further: I present several exact results for the problem with a *finite* concentration of holes.

To begin with, consider a bipartite lattice of $N$ sites with a spin $s$ at each site. Let

$$H=J\sum_{\langle ij\rangle}\mathbf{s}_i\cdot\mathbf{s}_j \tag{1}$$

be the nearest-neighbor Hamiltonian. Following Haldane[3] let us write a path integral for $Z=\mathrm{Tr}\exp(-\beta H)$ using at each site $I=\int(4\pi)^{-1}d\mathbf{\Omega}\,|\mathbf{\Omega}\rangle\langle\mathbf{\Omega}|$, where $\mathbf{\Omega}=(\Theta,\phi)$ lies on a unit sphere and labels the coherent state $|\mathbf{\Omega}\rangle$ obeying

$$\langle\mathbf{\Omega}'|\mathbf{\Omega}\rangle=(\cos\tfrac{1}{2}\Theta\cos\tfrac{1}{2}\Theta'+e^{i(\phi'-\phi)}\sin\tfrac{1}{2}\Theta\sin\tfrac{1}{2}\Theta')^{2s}, \tag{2}$$

$$\langle\mathbf{\Omega}|\mathbf{s}|\mathbf{\Omega}\rangle=s\mathbf{\Omega}. \tag{3}$$

The usual logic gives

$$Z=\int[\mathcal{D}\Omega]\prod_{i=1}^{M}\langle\mathbf{\Omega}_{1\cdots N}(\tau_i+\epsilon)|1-\epsilon H|\mathbf{\Omega}_{1\cdots N}(\tau_i)\rangle, \tag{4}$$

where $\mathbf{\Omega}_{1\cdots N}$ is the collective label for all $\Omega$'s at a given time slice, $\epsilon=\beta/M$, and $\mathcal{D}\Omega$ is the normalized measure in this discrete Euclidean space-time, with time $\tau_i$: $0\le\tau_i\le\beta$.

Let us first ignore $H$. Assuming smooth paths in $\tau$, Eq. (2) gives at each site

$$\langle\mathbf{\Omega}(\tau+\epsilon)|\mathbf{\Omega}(\tau)\rangle=[1+i\Delta\phi\sin^2\Theta/2]^{2s}$$
$$\simeq e^{is(1-\cos\Theta)\Delta\phi}. \tag{5}$$

The assumption of smooth paths is justified only in the limit of large $S$, when the overlap of coherent states at neighboring time slices drops rapidly as the state vectors begin to differ. Thus the $\sigma$-model derivation and the present variant in the presence of holes are all valid only in this large-$S$ limit. It is, however, possible that qualitative features, such as gap or no gap may be valid down to spin-$\frac{1}{2}$.

Haldane pointed out that we can write (5) in a rotationally invariant way:

$$\langle\mathbf{\Omega}'|\mathbf{\Omega}\rangle=e^{is\mathbf{A}(\mathbf{\Omega})\cdot\Delta\mathbf{\Omega}}, \tag{6}$$

where $\Delta\mathbf{\Omega}=\mathbf{\Omega}'-\mathbf{\Omega}$ and $\mathbf{A}(\mathbf{\Omega})$ is the potential of a unit monopole at the center of the sphere $|\mathbf{\Omega}|=1$. Thus,

$$\nabla_\Omega\times\mathbf{A}(\mathbf{\Omega})=\mathbf{\Omega}. \tag{7}$$

We are free to gauge transform $\mathbf{A}$: $\mathbf{A}\to\mathbf{A}+\nabla_\Omega\lambda$. The particular choice $\mathbf{A}=[(1-\cos\Theta)/\sin\Theta]\mathbf{e}_\phi$ reproduces Eq. (5). The choice I will use is $\mathbf{A}=-\cot\Theta\mathbf{e}_\phi$ for which $\mathbf{A}(\mathbf{\Omega})=\mathbf{A}(-\mathbf{\Omega})$.

Returning to Eq. (4), with $H=0$ still, we get

$$Z=\int[\mathcal{D}\Omega]\exp\left[is\sum_r\int_0^\beta\left(\mathbf{A}(\mathbf{\Omega}_r)\frac{d\mathbf{\Omega}_r}{d\tau}\right)d\tau\right], \tag{8}$$

where $r$ is the site label, and I wrote $d\mathbf{\Omega}=d\mathbf{\Omega}/d\tau\cdot d\tau$.

Restoring $H$ adds spatial coupling between the $\Omega$'s, and eventually we get the $\sigma$ model as reviewed elsewhere.[3] It is sufficient to recall that since $H$ is antiferromagnetic, at least *locally*, we have

$$\mathbf{\Omega}(\mathbf{r})=(-1)^r\mathbf{n}(\mathbf{r})+O(a), \tag{9}$$

where $(-1)^r$ is the parity of site $\mathbf{r}$, $\mathbf{n}$ is the smooth $\sigma$-model (order parameter) field, and $a$ is the lattice spacing. Thus

$$Z=\int[\mathcal{D}\Omega]\exp\left(is\sum_r\int_0^\beta\mathbf{A}(\mathbf{n})\cdot\frac{d\mathbf{n}}{d\tau}(-1)^r+S(H)\right), \tag{10}$$

where $S(H)$ are terms due to $H$, and I have used $\mathbf{A}(\mathbf{\Omega})=\mathbf{A}(-\mathbf{\Omega})$.

Let us now imagine we pull out the spin at site $\mathbf{r}_0$ at time $\tau_1$, i.e., make a hole there, and reinstate it at time

$\tau_2$.

It is clear that between $\tau_1$ and $\tau_2$ we must use a different Hilbert space since we have one less spin. But in the space-time path integral there is a simple way to describe the hole: *We use the same action as before but subtract the contribution the spin would have made at* $\mathbf{r}_0$ *between* $\tau_1$ *and* $\tau_2$; i.e., *add* $\delta S = -(-1)^{r_0} is\int_{\tau_1}^{\tau_2} a_0(\mathbf{r}_0,\tau)d\tau$ to the old action, where $a_0 = \mathbf{A}\cdot\partial_0\mathbf{n} \equiv \mathbf{A}\cdot\partial\mathbf{n}/\partial\tau$. This is the same as introducing a Wilson line $\exp[-is(-1)^r \times\int_{\tau_1}^{\tau_2} a_0(\mathbf{r}_0,\tau)d\tau]$ in the path integral for the $\sigma$ model.

Other effects due to hole will be discussed shortly. But first let us try to cast the above effect in an operator formalism. At each site we introduce an operator $\psi^\dagger$ which creates a hole and $\psi$ which destroys it, demand $\psi^2 = \psi^{\dagger 2} = 0$, $\{\psi,\psi^\dagger\} = 1$, and that $\psi^\dagger\psi$ commutes at different sites. *The hole creation does not do anything to the spin there and proceeds independently of it.*

We describe the static holes by

$$H_h = \sum_r is(-1)^r \psi^\dagger\psi a_0\,, \tag{11}$$

which clearly reproduces the Wilson line if we take the trace in the occupation number representation of $\psi$. Having checked this, we can switch to any other representation, say a Grassmann integral over $\psi$.

To fully understand this $H_h$, and the present formalism in general, let us consider the analogy with QED. There, $Z$ is a functional integral over the photon ($A$) and electron ($\psi$) variables with Boltzmann weight $\exp[S(A)+S_A(\psi)]$, where $S(A)$ is the Maxwell action $(-\frac{1}{4}f_{\mu\nu}^2)$ and $S_A(\psi) = \bar\psi(\partial\!\!\!/ - ieA\!\!\!/)\psi = \bar\psi D\!\!\!\!/\,\psi$. To evaluate $Z$, we can fix $A$, do the $\psi$ integral, and finally do the $A$ integral. In the second step we have at each $A$ {generated with probability $\exp[S(A)]$} an external field problem in $\psi$ of evaluating $\det D\!\!\!\!/ = \mathrm{Tr}\exp[-\beta H_A(\psi)]$, where $H_A(\psi)$ is the Dirac Hamiltonian of the electron minimally coupled to the current value of $A$. A term in it, such as $e\psi^\dagger\psi A_0$, describes the coupling of the charge to the background scalar potential $A_0$ *preassigned to that point whether or not the electron is there.* In our problem $H_h(\psi,a_0)$ is the analog of $H_A(\psi)$ while $A\to\mathbf{n}$; $S(A)\to S(\mathbf{n})$, the $\sigma$-model action, and $\psi$(bare electron) $\to\psi$(bare hole). If we evaluate $\mathrm{Tr}\exp(-\beta H_h)$ in the occupation number representation, it will, by design, do its job: Whenever $\psi^\dagger\psi = 1$, $is\psi^\dagger\psi a_0$ will kick in and neutralize the on-site evolution $is\mathbf{A}\cdot\partial\mathbf{n}/\partial\tau \equiv isa_0$.

So far we have focused on the on-site phase factor. Other effects due to the hole are similarly obtained by multiplying the other terms in the $\sigma$-model action by the projection operator $1-\psi^\dagger\psi = 1 - :\psi^\dagger\psi: - c$, where $:\psi^\dagger\psi:$ is the normal order parameter and $c$ is its vacuum expectation value. Now $:\psi^\dagger\psi:$ has dimension $d$ in $d$ spatial dimensions, and makes irrelevant corrections in all but the $:\psi^\dagger\psi: a_0$ term (which we have already considered and which is always marginal). The $c$ term renormalizes various couplings, velocities, etc., and also leads to a nearest-neighbor attraction between holes, reflecting the fact that in this configuration one less bond is broken. I thank G. Murthy for pointing this out. We will not consider this interaction further; which amounts to assuming that a compensating $NN$ Coulomb repulsion exists. This point will be discussed elsewhere.[4]

Let us return to Eq. (11) and deal with the $(-1)^r$ term. We can, of course, say that there is one kind of hole and that the gauge potential it sees varies *very* rapidly in space, as $(-1)^r a_0$. But it makes more sense in the continuum to double the unit cell (as one does in the $\sigma$-model derivation) and say that there are two kinds of holes (on the $A$ and $B$ sublattices) coupling with charge $\pm s$ to the smooth scalar potential $a_0$. This picture makes sense if the hopping between sublattices is neglected and if there is a net intrasublattice term $t_{AA} = t_{BB} = t$. Thus we are not talking about the simplest one-band Hubbard model, but its generalization. We will work in the low-energy sector wherein the large $J$ will preserve the integrity of the $A$-$B$ species. In a moment we will see more justification for the assumption that the holes move within one or the other sublattice.

Consider first a hole hopping from site 1 to site 2 in the same sublattice. Let $\mathbf{n}_1$ and $\mathbf{n}_2$ be the background field values. (Recall $\mathbf{n}$ and $\mathbf{\Omega}$ are equivalent within a given sublattice.)

The correct addition to $H_h$ is not $-t\psi_2^\dagger\psi_1$, but rather

$$\delta H = -t\psi_2^\dagger\psi_1 e^{is\mathbf{A}\cdot(\mathbf{n}_1-\mathbf{n}_2)} \equiv -t\psi_2^\dagger\psi_1 e^{i\delta}\,. \tag{12}$$

This is because $\psi_2^\dagger\psi_1$ moves the hole, without touching $\mathbf{n}$, whereas at the microscopic level the electron is transported by some operator $d = \sum_\sigma c_{\sigma 1}^\dagger c_{\sigma 2}$ which moves the spin *coherently* from site 2 to 1. Its matrix element in that language would have been

$$\begin{aligned} -t\langle\mathbf{n}_1, \text{hole at } 2\,|\,d\,|\,\text{hole at } 1,\mathbf{n}_2\rangle &= -t\langle\mathbf{n}_1|\mathbf{n}_2\rangle\langle\text{hole at } 2\,|\,\text{hole at } 2\rangle \\ &= -te^{is\mathbf{A}\cdot(\mathbf{n}_1-\mathbf{n}_2)} = -te^{i\delta}\,. \end{aligned} \tag{13}$$

In our scheme, $H_h$ from Eq. (12) reproduces this result when applied to hole motion in the given background $\mathbf{n}$.

Had we tried to move the hole from $A$ to $B$, then in place of Eq. (13) we would have obtained the overlap $-t_{AB}\langle\mathbf{\Omega}_A|\mathbf{\Omega}_B\rangle$. In view of Eq. (9), this number would be nearly zero. (Remember that the overlap of two coherent states of oppositely pointing $\mathbf{\Omega}$'s is zero.) *In other words, the real overlap to go from A to B is the overlap of orbital wave functions times the overlap on spin wave functions.* Given strong short-range antiferromagnetic correlations, the second factor strongly damps $NN$ hopping. It is this *combined* hopping element that is considered as negligible here. All this is justifiable in the large-$S$ limit where the desired short-range order is assured.

Returning to the main theme, the full hole Hamiltonian, in terms of

$$a_\mu = \mathbf{A}\cdot\partial_\mu\mathbf{n},\quad \mu = 0,1,\ldots, \tag{14}$$

is

$$H_h = \left[\sum_{\mathbf{r}} \psi_A^\dagger \psi_A isa_0 - \sum_{\mathbf{r}\delta} \psi_{A+\delta}^\dagger \psi_A \exp\left[-is\sum_\mu \mathbf{a}_\mu \cdot \boldsymbol{\delta}_\mu + \text{H.c.}\right]\right] + (A \to B, s \to -s) \tag{15}$$

in obvious notation. Under the gauge transformation of $\mathbf{A}$, $a_\mu$ behaves as follows: $a_\mu \to a_\mu + \nabla_{\mathbf{n}}\lambda \cdot \partial_\mu \mathbf{n} = a_\mu + \partial_\mu \lambda$ by the chain rule. The equations of motion are gauge invariant if at the same time $\psi_{A,B} \to e^{\mp is\lambda}\psi_{A,B}$.

It is clear that $A$ and $B$ holes will like to be near each other. A hole at $A$ for all times $\tau$ adds an oscillating Wilson line to the path integral, which will average $e^{-E_0\beta}$, $E_0$ being the energy of the hole. The same goes for a hole at $B$. Now consider two holes. If we put an $A$ and $B$ hole close to each other (in the scale of the correlation length, $\psi$), the phase factors cancel and it costs no energy, whereas two $A$ holes or two $B$ holes will cost energy $2E_0$. The exact forces between holes depends on the dynamics of the $a_\mu$ field. However, all forces will become exponentially small at large distances, as is clear in the CP(1) language. We have the holes, the gauge field, and the $z$ quanta of mass $m_\psi \sim 1/\psi$. In the presence of the latter, we will never see a confining potential, $kR$, between holes: Pair production of $z$ quanta will eventually make neutral "mesons" out of these holes for $kR > 2m_\psi$. These mesons will have the spin index of the $z$ quanta and the fermionic nature of the holes: These are just ordinary electrons.

Another general remark we can make about this gauge theory is that the field strength due to $a_\mu$ is [upon employing Eqs. (7) and (14) and a lot of partial differentiation]

$$f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu = \mathbf{n} \cdot (\partial_\mu \mathbf{n} \times \partial_\nu \mathbf{n}) . \tag{16}$$

To see what this means, multiply $f_{\mu\nu}$ by an area element $dx_\mu dx_\nu$. The right-hand side then tells us that the flux enclosed is simply the area of its image on the $\mathbf{n}$ sphere under the map $x \to \mathbf{n}(x)$ defined by the background $\mathbf{n}$ field. [In differential geometric terms $a_\mu$ and $f_{\mu\nu}$ are pull-backs of the one and two forms $\mathbf{A}$ and $\nabla \times \mathbf{A}$ from $|\mathbf{n}| = 1$ to space-time, under the map $x \to \mathbf{n}(x)$.]

Let us now pass from these general considerations, valid in any $d$, to $d=1$, where we can do some serious quantitative computations.

The spin chain by itself is given by an action

$$S_\theta = \frac{-1}{2g^2}\int d^2x[(\partial_0 \mathbf{n})^2 + v^2(\partial_x \mathbf{n})^2] + \frac{i\theta}{4\pi}\int \mathbf{n} \cdot (\partial_\mu \mathbf{n} \times \partial_\nu \mathbf{n}) d^2x , \tag{17}$$

where $g \sim 1/s$, $v$ is a velocity, $\theta = 2\pi s$ for a uniform chain, and some real number if one includes bond strength alternation. The coefficient of $i\theta$ is the instanton or winding number, $W$, and is just the integral of $f_{\mu\nu}$ from Eq. (16). (Remember $f_{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu}f_{\mu\nu}$ is scalar in $1+1$ dimensions.)

Consider now the holes, ignoring for a moment the gauge coupling. We have for the two species

$$H_{\text{holes}} = -t\sum[\psi_{A+1}^\dagger \psi_A + \text{H.c.} - 2\mu\psi_A^\dagger \psi_A] + A \to B . \tag{18}$$

Here $\psi$, whose statistics were deliberately left vague in $d \geq 2$, is definitely chosen to be fermionic. (If one begins with hard-core bosons described by Pauli matrices $\sigma_\pm$, one can use the Jordan-Wigner transformation to go to $\psi$ and the above $H$. The question of bare statistics for $\psi$ in $d>1$ is under investigation.)

Now we can Fourier transform, obtaining $E = 2t(\mu = \cos k)$, and fill up some number of levels by varying $\mu$. As usual,[5] we will linearize near $k = \pm k_F$, obtaining two components $\psi_1$ and $\psi_2$ of a Dirac field from a single $\psi$:

$$\psi(n) = e^{ik_F n}\psi_1(n) + e^{ik_F n}\psi_2(n) , \tag{19}$$

in terms of which, in the continuum, we get

$$H_{\text{holes}} = 2t\sin k_F \int [\psi_A^\dagger(\alpha \cdot p)\psi_A + \psi_B^\dagger(\alpha \cdot p)\psi_B]dx , \tag{20}$$

where

$$\alpha = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad p = -i\,\partial/\partial x . \tag{21}$$

If we now work out the gauge coupling, we get, not surprisingly, just the minimal coupling. The corresponding path integral is, in Euclidean space,

$$Z = \int [\mathcal{D}\psi][\mathcal{D}\mathbf{n}]e^{[S_F + S_\theta(\mathbf{n})]} , \tag{22}$$

where, upon rescaling $x$ by $2t\sin k_F$,

$$S_F = \int [\bar{\psi}_A(-\not{\partial} - i\not{a}s)\psi_A + \bar{\psi}_B(-\not{\partial} + i\not{a}s)\psi_B]dx\,d\tau , \tag{23}$$

where $\not{a} = a_\mu \gamma_\mu$ and $\gamma_\mu$ are $2\times2$ Euclidean $\gamma$ matrices.

*We thus have the remarkable result that a finite hole density corresponds to the addition of massless fermions coupled to the $\sigma$ model via a gauge coupling.*

Many dramatic effects follow since massless fermions can drastically alter instanton physics.[6]

The first effect is that the $\theta$ term is ineffective. The reason is simple: It can affect only configurations with instanton number, call it $W \neq 0$. But whenever $W \neq 0$, the Atiyah-Singer Index theorem[7] assures us that $\det(\not{\partial} \pm is\not{a}) = 0$. This will be explained in detail elsewhere.[4] Luckily in $1+1$ dimensions we can see this another way. Let us bosonize the fields $\psi_{A,B}$ to $\phi_{A,B}$ by the usual rules:[8]

$$-\bar{\psi}\not{\partial}\psi = -\tfrac{1}{2}(\nabla\phi)^2, \quad \bar{\psi}\gamma^\mu\psi = \frac{\epsilon_{\mu\nu}}{\sqrt{\pi}}\partial_\nu\phi \tag{24}$$

to obtain the action

$$S=\int\left[\frac{-(\nabla\phi_+)^2}{2}+\frac{-(\nabla\phi_-)^2}{2}+is\left(\frac{2}{\pi}\right)^{1/2}\phi-\epsilon_{\mu\nu}\partial_\mu a_\nu\right]d^2x+S_\theta\,, \tag{25}$$

where $\phi_\pm=(\phi_A\pm\phi_B)/\sqrt{2}$ and I have integrated $\partial_\nu\phi_-$ by parts. Now it is clear that the $\theta$ term can be eliminated by a shift in $\phi_-$ [recall Eqs. (16) and (17)]. Continuing further, if we integrate out $\phi_-$ completely, it is clearly seen to produce a logarithmic potential between instanton density; i.e., we get a term in the **n** sector given by

$$\delta S=\frac{s^2}{\pi^2}\int f_{\mu\nu}(\mathbf{x})\ln|\mathbf{x}-\mathbf{x}'|f_{\mu\nu}(\mathbf{y})d^2x\,d^2y\,. \tag{26}$$

Thus the instanton configurations are globally neutral.

All $\theta$-dependent effects are now purged and the behavior with spin-$s$ is monotonic and effects of bond strength alternation washed out. We expect all cases to be translationally invariant and only exponentially correlated. (Consider even $s$: It is surely massive without holes, and adding holes can only make it worse. Alternately we can see the gauge field will be massive because of the longitudinal coupling $a_\mu\epsilon^{\mu\nu}\partial_\nu\phi$ of $a_\mu$ to the $\phi$ field. Indeed, both fields will become massive.) An important consequence is that in the $\sigma$-model sector we expect massive spin-$\frac{1}{2}$ particles. [In the $CP(1)$ language the $z$ quanta become deconfined when the gauge field becomes massive.] This result, which rests on Witten's earlier work as well as the exact $S$-matrix of the O(3) supersymmetric $\sigma$ model,[9] will be discussed elsewhere.[4]

Although genuine off-diagonal long-range order is impossible in $d=1$, the superconducting susceptibility is

$$\langle\psi_A^\dagger\psi_B^\dagger(r)\psi_A\psi_B(0)\rangle\sim 1/r\,, \tag{27}$$

which is more singular than in the free fermion case ($1/r^2$). Thus the gauge interaction has produced an attraction between holes. [Equation (27) was obtained by bosonizing the operators on the left-hand side. The result factorizes into two parts involving exponentials of the fields $\phi_\pm$. Clearly, $\phi_+$ is massless; it produces the $1/r$. The field $\phi_-$ becomes massive and gets stuck at some value. This gets rid of the other $1/r$ that arises in free fermion theory.]

To conclude, we see that even hole motion restricted to sublattices can destroy the quasi-long-range order in $d=1$ at any finite concentration. In $d=2$, where there is genuine long-range order, a minimal concentration may be needed. As we increase doping, superconductivity will eventually be lost since we will not have enough short-range antiferromagnetic order to bind $A$ and $B$ holes. These ideas in $d=2$ are under further investigation.

Since completing this work, I have received a paper from Lee,[10] who reaches many similar conclusions following up on some of Wiegmann's ideas from Ref. 2.

I thank O. Alvarez, S. Kivelson, A. Millis, G. Murthy, and S. Sachdev and especially Dung-Hai Lee for their help. Acknowledgement is made to the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for the partial support of this research. This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara.

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