Statistics of holons in the quantum hard-core dimer gas

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The nature of holons, and in particular, their statistics, are studied in the context of a two-dimensional quantum hard-core dimer gas. This model has been shown to embody the low-energy physics of the short-ranged resonating-valence-bond state. We find that, depending on detailed energetic considerations, the holons either bind a half flux quantum of "statistical flux," in which case they are fermions, or they are free, in which case they are bosons. The exchange energy is shown to favor a fermionic hole while the hole kinetic energy (which generally exceeds the exchange energy) favors bosonic holes. Finally, it is shown that even in the bosonic case, flux quantization is in units of $hc/2e$.

I. INTRODUCTION

The notion[1–3] that quasiparticles with unusual quantum numbers (e.g., fractional charge) and unusual statistics (e.g., fractional statistics) can describe the low-energy excitations of two-dimensional quantum systems has played an important role in understanding the fractional quantum Hall effect,[2] and more recently has been invoked in the context of high-temperature superconductivity.[3–11] In particular, in Ref. 3 it was suggested that in a system with a short-ranged resonating-valence-bond (RVB) ground state, the quasiparticles created on doping are charge e, spin-0 holons satisfying Bose statistics. While the reverse charge spin relation of the quasiparticle is unambiguous, and indeed is a rather general consequence of singlet pairing,[12] the statistics of the quasiparticles is a subtle issue. The subtlety arises because in two dimensions, statistics are a matter of convenience; the statistics of a particle can be changed at will by attaching a partial flux quantum of "statistical flux" to each particle.[1] At best, one particular choice of statistics is natural if it eliminates all long-range pieces of the particle kinetic energy. Partly for this reason, the assignment of statistics has proven to be highly controversial; in Refs. 4–8 the holons were identified as bosons, in Ref. 9 as half-fermions, and in Refs. 10 and 11 as fermions. The important point here is that even when there exists an unambiguous natural choice for the statistics of the low-energy quasiparticles, that choice can change depending on detailed energetic considerations which determine whether a particle will or will not bind a flux. Indeed, Read and Chakraborty[11] have pointed out that exactly this issue arises in the context of the spinons and holons in a short-ranged RVB state.

In this paper we will analyze a simple model of a short-ranged RVB superconductor, the quantum hard-core dimer gas,[5] in which the statistics of the holon can be understood completely. (By inference, the statistics of the spinon can be understood in the same way, although there are a variety of technical issues which make the case of the spinon more complicated.) We find that the two-dimensional dimer model has vortex excitations which carry one half flux quantum of statistical flux; the purely magnetic interactions in the model cause a bare holon to bind a vortex, thereby turning it into a fermion. These conclusions are in agreement with the results of Chakraborty and Read[11] based on an analysis of the nearest-neighbor RVB state with phases chosen to satisfy the Marshall[13] sign rule. However, we find that the holon kinetic energy causes the holon to unbind from the vortex leaving a bare (i.e., bosonic) holon as the low-energy quasiparticle. Moreover, we argue that in three dimensions and higher, where statistics are robust, the holon is always a boson. Finally, we show that the presence of vortex excitations leads to electromagnetic flux quantization in units of $hc/2e$, even when the ground state is a Bose condensate of charge e bosons.

II. THE MODEL

Recently, it has been shown that there is a class of models[14] whose ground state and low-lying excited states lie in the subspace spanned by the nearest-neighbor valence-bond states. These models are described by a Hamiltonian which is the sum of the so-called Klein Hamiltonian,[15] H_K, plus any of a broad class of perturbing Hamiltonians, H'. The ground-state manifold of H_K is the subspace $\Omega_{\rm NNVB}$ spanned by the nearest-neighbor valence-bond states. We treat H' using degenerate perturbation which amounts to projecting H' into $\Omega_{\rm NNVB}$. In another paper[5] we do this for a representative H' which is the sum of a nearest-neighbor antiferromagnetic Heisenberg interaction plus a holon kinetic energy; however, none of our main results depend sensitively on the exact nature of the perturbation. Since the states in $\Omega_{\rm NNVB}$ are clearly in one-to-one correspondence with the states of a hard-core dimer gas, by simply orthogonalizing the valence-bond states the system can be mapped onto a hard-core quantum dimer gas on a lattice. Roughly, a dimer represents a valence bond. The nonorthogonality of the valence-bond states is represented *exactly* by the presence of longer-range interactions in the dimer Hamiltonian; the fact that the valence-bond states are, in a sense, nearly orthogonal is reflected in the fact that the dimer Hamiltonian $H_{\rm dim}$ is short ranged (in the sense of exponentially falling).

The details of the derivation of the hard-core dimer model from the perturbed Klein model are discussed in Ref. 5; we sketch the procedure here. First, we must define a phase convention for valence-bond states. We have adopted the convention that a valence-bond between sites i and j is created by

$$b_{ij}^{\dagger} = \frac{1}{\sqrt{2}} (c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} + c_{j\uparrow}^{\dagger} c_{i\downarrow}^{\dagger}) , \tag{1}$$

where $c_{is}^{\dagger}$ creates an electron of spin s on site i. A valence-bond state is created by the set of $b_{ij}^{\dagger}$ corresponding to a dimer configuration c. The valence-bond states can be orthogonalized by the method of Lowdin,[16] and we define a "dimer" state to be the member of the resulting orthonormal set corresponding to dimer configuration c. The matrix elements of the H_{dim} are then the matrix elements of H' between dimer states. We have shown that for short-ranged perturbations, only short-ranged terms in H_{dim} are important; so for simplicity, we will consider a model consisting of only the shortest-range term of each type. We do not expect other terms in the dimer Hamiltonian to affect our conclusions. Therefore, we consider the model represented below:

$$H_{\text{dim}} = H_J + H_{J'} + H_T , \tag{2}$$

$$H_J = J \sum \left[\, |\, = \,\rangle \langle \, \| \, | + \text{H.c.} \right] + V \sum \left[\, |\, = \,\rangle \langle \, = \, | + | \, \| \, \rangle \langle \, \| \, | \right] , \tag{3}$$

$$H_{J'} = J' \sum \left[\, | \, \text{⌐·⌐} \, \rangle \langle \, \text{⌐·⌐} \, | + \text{H.c.} \right] , \tag{4}$$

$$H_T = -t \sum \left[\, | \cdot \, | \, \rangle \langle \, \_\, \cdot \, | + \text{H.c.} \right] + V_h \sum \left[\, | \cdot \;\; \cdot \rangle \langle \cdot \;\; \cdot | \, \right] , \tag{5}$$

where the sums in Eq. (3) run over all plaquettes, the sum in Eq. (4) over the neighborhood of each hole, and the first sum in Eq. (5) runs over all triplets of nearest-neighbor sites, while the second sum is over nearest-neighbor pairs of sites. The matrix elements of a bra containing a particular local dimer configuration with an arbitrary dimer state ket is zero unless the two dimer configurations match, in which case it is one. In Eqs. (3)–(5), a bar represents a dimer and a dot represents an empty site or bare holon. The first two terms, H_J and $H_{J'}$, are purely magnetic in origin and so are proportional to the exchange coupling; the final term H_T arises from electron hopping between sites. For a nearest-neighbor antiferromagnetic exchange interaction, we expect J and J' both to be positive; we shall see that this favors a ground-state superposition of dimer states with the relative phases that are expected on the basis of the Marshall rule.[11,13] For a sufficiently frustrated magnetic system it is possible for the ground state to violate the Marshall rule, i.e., it is also reasonable to consider the model with J and J' negative. In contrast, the pure hopping Hamiltonian always favors a $\mathbf{k}=\mathbf{0}$ state, so t is always expected to be positive. Thus the hole kinetic energy favors a totally symmetric superposition of dimer states and for positive J and J', the doped system is somewhat frustrated. It is useful to include the longer-range interaction J' in the Hamiltonian even though we except it to be small compared to J, since without it the purely magnetic part of the Hamiltonian has a conserved winding number [defined in Ref. 4(b)] about each hole and thus H_J is block diagonal. The "pinwheel operator" in Eq. (4) removes this unphysical aspect of the static-hole model. The various terms in the dimer Hamiltonian can be interpreted as a pure dimer kinetic energy (J), a dimer potential energy (V), a holon kinetic energy (t), and a holon-holon repulsion (V_h).

III. STATISTICS OF THE HOLONS IN THE 2D MODEL

An arbitrary state $|\psi\rangle$ in the dimer Hilbert space can be represented as a liner combination of dimer states $|c\rangle$ with specified amplitude A_c and phase θ_c,

$$|\psi\rangle = \sum_c A_c e^{i\theta_c} |c\rangle , \tag{6}$$

where c specifies a dimer configuration (including, implicitly, the locations of the holes). For a finite-size system, if there is a choice of phases which makes the expectation value of all off-diagonal matrix elements of the Hamiltonian negative (i.e., if the system is unfrustrated), then the ground-state wave function has those phases. In many cases, it is convenient to define a phase field $a(l)$ which lives on the links l of the lattice such that

$$\theta_c = \sum_{l \in c} a(l) . \tag{7}$$

Notice that in the absence of the hole kinetic energy there is a gauge invariance, analogous to the U(1) gauge symmetry discussed by Baskaran and Anderson[17] for the Heisenberg model, such that all energies are invariant under

$$a(l) \to a(l) + \chi(\mathbf{R}) + \chi(\mathbf{R}') , \tag{8}$$

where $\mathbf{R}$ and $\mathbf{R}'$ are the lattice sites on either end of link l, and $\chi(\mathbf{R})$ is an arbitrary function of $\mathbf{R}$. Indeed, we[18] have recently shown that the dimer model defined above is equivalent to compact lattice quantum electrodynamics (QED), and even in the presence of dynamical holes the model can be made gauge invariant by defining a new field $\phi(\mathbf{R}) = |\phi(\mathbf{R})| e^{i\alpha(\mathbf{R})}$ associated with the holons such that

$$\theta_c = \sum_{l \in c} a(l) + \sum_{\mathbf{R} \in c} \alpha(\mathbf{R}) , \tag{9}$$

where the second sum is over all unoccupied sites (occupied by holons); under a gauge transformation, a still transforms as in Eq. (8), and

$$\phi(\mathbf{R}) \to \phi(\mathbf{R}) e^{i\chi(\mathbf{R})} . \tag{10}$$

Because of the gauge invariance of the model, the relevant information about θ_c can be summarized by specifying the distribution of a flux in the system; we refer to this as "statistical flux." For J positive, the off-diagonal matrix elements of H_J are all negative if there is a half-integer flux quantum through each plaquette. If in addition J' is positive, and if we introduce an additional half flux-quantum distributed in an arbitrary fashion through the four plaquettes which surround each holon, then all the matrix elements of $H_{J'}$ are negative as well. As discussed by Lederer and Takahashi[19] in the context of the Hubbard model, this choice of phase corresponds to the so-called "$s+id$" state.[20] Thus, in the absence of the holon kinetic energy, the effect of $H_{J'}$ is to cause each holon to bind a half flux quantum of statistical flux.

The holon number (topological charge[4(a)]) couples to the statistical gauge-field in the same way as electromagnetic charge couples to the electromagnetic gauge field, which follows from Eq. (10). To see this explicitly, imagine that there is a half integer flux quantum through the plaquette at the origin. We work in a singular gauge in which there is a Dirac sting running along the positive y axis, which is to say $a(l)=\pi$ for the column of links which cross the string, and $a(l)=0$ for all other links as shown in Fig. 1(a). Thus, the phase can be expressed as $e^{i\theta_c}=(-1)^{n_c}$ where n_c is the number of dimers which cross the y axis at positive y. As shown in Fig. 1(b), when a holon moves past the string, the number of dimers crossing the string changes by ± 1. In other words, if a holon makes a closed orbit around the flux quantum, the wave function changes sign; this is just the Aharonov-Bohm phase corresponding to a half flux quantum.

Since all the bare particles in the theory are bosons, i.e., dimers which consist of a tightly bound electron pair, it is clear that the bare holon is a boson,[4] and this can be checked directly. Thus, in the usual way[1(a)] of two-dimensional systems, a holon-fluxoid bound state can be treated either as a boson, in which case the bosons interact via a long-ranged gauge force, or, more simply, as a weakly interacting fermion. This conclusion reproduces, in the context of the hard-core dimer model, the earlier conclusions of Read and Chakraborty.[11] However, we see at once that the statistics of the low-energy state (quasiparticle) of the holon is determined by energetic considerations. If J' were negative, then the bare holon would have lower energy by order of $|J'|$ than the holon-fluxoid pair; as a result the holon would be a boson. More to the point, in the presence of a nonzero holon kinetic energy, the holon will be a boson, even for positive J', so long as $t \gg J'$. This follows from the fact that repeated holon hopping generates an effective coupling between the dimer states connected by the pinwheel operator as shown in Fig. 2; the holon kinetic energy is minimized if all dimer states which differ by the rearrangements of dimers in the vicinity of the holon enter with equal phases. (In the Appendix we estimate the critical value of the ratio of t to J' at which the unbinding transition occurs.) Again, this is consistent with the results of Lederer and Takahashi[19] who found in the context of the short-ranged RVB state in the Hubbard model that the holon kinetic energy is minimized if the superposition is locally "s-like" in the neighborhood of each holon. Since we expect physically that

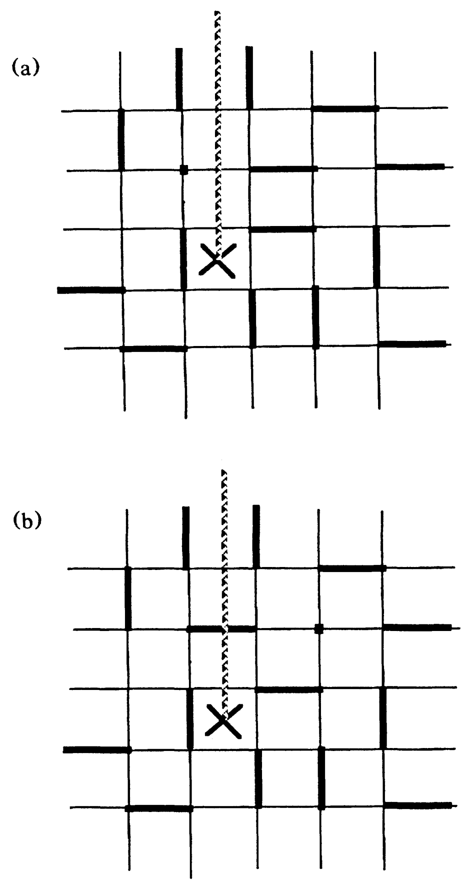

FIG. 1. A vortex excitation at the origin (marked by an ×) with a Dirac sting lying along the positive y axis. Shown are representative dimer configurations (dimers are represented by bars and a holon by a dot) and information about the phases with which they enter the sum in Eq. (6). There is one half-quantum of statistical flux through each plaquette and an additional half flux quantum through the marked plaquette. Thus, $a(l)=\pi$ for all the links that are cut by the string. In (a) there are no dimers crossing the Dirac string, while after the holon crosses the string [in (b)] there is one.

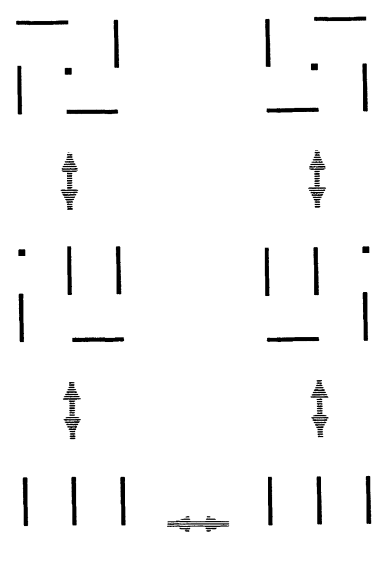

FIG. 2. An effective pinwheel operation can be generated by repeated action of the holon kinetic energy.

$t \gg J'$, the holons will generally be bosonic.

It is worth commenting briefly on the statistics of the spinons. Spinons are not present in the hard-core dimer model per se, since the model presupposes a gap in the spin excitation spectrum, and deals only with excitations at energies less than the spin gap.[5] Moreover, if we allow a finite density of spinon excitations, we are no longer guaranteed that the different valence-bond states are linearly independent; indeed the set of states consisting of nearest-neighbor valence-bonds plus unpaired spins is clearly overcomplete. However, at dilute spinon density, we can treat a spinon as a holon with an electron bound to it. Clearly, such a particle has electromagnetic charge 0 and spin $\frac{1}{2}$. It also carries the same topological charge as the holon, so it couples in an identical fashion to the statistical gauge field. Thus, a bare spinon is a fermion while a spinon-fluxoid pair is a boson. Unlike the holon, however, the spinon kinetic energy is neither large compared with J and J', nor is it clear whether it favors local s-like or $s+id$-like symmetry. It seems natural, as suggested in Refs. 10 and 11, that the spinon will bind a fluxoid and hence will be bosonic, but this presumably depends on the degree of frustration in the model. At any rate, since whenever the short-ranged RVB analysis is applicable there must be a gap to the spinon states, we are never interested in the low-temperature properties of a dense spinon gas, and so the statistics of the spinons is not of primary importance.

IV. SPIN, QUASISTATISTICS RELATION

In three dimensions, statistics are more robust than in two; we cannot simply change the statistics of the particles by adding a pure gauge field to the system as was the case in two dimensions. This suggests that the statistics can be determined on more fundamental ground. The spin-statistics theorem of relativistic quantum mechanics is such a connection. Unfortunately, its proof relies on Lorentz invariance. In the class of problems we are interested in, the spin is an internal quantum number of the bare particles of the problem, the electrons; it is not necessarily connected to any of the space-time symmetries of the system. The question we are interested in answering is; if the low-energy excitations of a collection of electrons have a quasiparticle description, are these quasiparticles required to have a particular spin (quasiparticle) statistics relation? In general, the answer must necessarily be that they do not. However, in three dimensions in particular, it *is* often the case that there is a connection between the spin and spatial rotational symmetries of the wave function. It is easy to see that if a two-quasiparticle wave function has any axis of symmetry such that it is invariant under a 180° rotation of both spin and space, then the quasiparticles must be bosons if they have integer spin and fermions if they have half-integer spin. This follows immediately from the fact that such a transformation interchanges the two quasiparticles. A rotation by 180° of two half integer spins produces a minus sign which, for an invariant wave function, must be canceled by a factor of -1 per exchange. Similarly, for integer spin, the exchange factor must be $+1$. Based on this argument, we feel that it is likely (though not proven) that in higher dimensions, the holons will be bosons and the spinons will be fermions.

V. FLUX QUANTIZATION

An issue of general importance is the issue of flux quantization in systems with quasiparticles with fractional charge and/or statistics. It was argued in Ref. 21 that, quite generally, charge fractionalization will not produce any effect on the Aharonov-Bohm periodicity of observable quantities in a non-simply-connected system, since the quasiparticle wave functions will be multivalued in just such a way as to leave the flux quantum unchanged. The issues of flux quantization and the effects of statistical transmutation are somewhat more subtle since they address issues of macroscopic phase coherence. Arguments similar in spirit to those in Ref. 21 were presented in Refs. 4(b) and 22 to demonstrate that in the present model, the reverse charge-statistics relations of the holons will not alter the fact that flux quantization will occur in units of $hc/2e$. Indeed, it can *almost* be argued on general grounds[23] that if the only bare charged particles are fermions with charge e, then flux quantization will always occur in units of $hc/2ne$ where n is an integer.

On the other hand, Wilzcek[1(a)] has shown that in two dimensions there is no way to distinguish a charge e boson from a charge e fermion bound to a half flux quantum. Yet there is no doubt that at zero temperature, a system of charge e bosons can condense into a superfluid state with flux quantum hc/e.

The resolution of this seeming paradox can be understood along lines first suggested by Wen.[7] It derives from the existence of vortex excitations which carry charge zero and half a flux quantum. Consider the purely magnetic model in which t is set equal to zero. We define the one vortex state to be the state in which an additional half flux quantum of statistical flux is threaded through an arbitray plaquette, e.g., the plaquette at the origin as is Fig. 1(a). This state is orthogonal to the ground state,[11] and has an excitation energy of order J. Note that there is no magnetic energy associated with the Dirac string since so long as the holon positions are held fixed, any process which rearranges the dimers will change the number of dimers crossing the string by an integer multiple of 2, except only those which involve a net circulation of dimers about the vortex. It is the existence of these vortices which is responsible for the fact that flux quantization is in units of $hc/2e$.

To see this, consider the cylindrical geometry shown in Fig. 3. We consider the periodicity of the ground-state energy $E(\Phi)$ of a condensate of change-e bosons which live on the surface of the cylinder as function of the electromagnetic flux Φ through the cylinder. Clearly, $E(\Phi)$ is periodic with period hc/e. However, there are two possible branches of $E(\Phi)$ as shown respectively in Figs. 3(a) and 3(b). If there is no statistical flux through the cylinder, then the energy is minimized when there is an integer number of electromagnetic flux quanta through the cylinder; if there is a half quantum of statistical flux

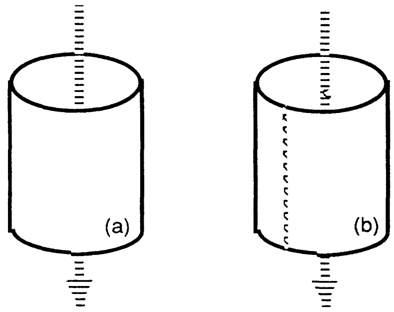

FIG. 3. Geometry for the discussion of flux quantization. Here, the electromagnetic flux through the center of the cylinder (indicated by the arrow) is varied. In (a) there is no net statistical flux through the cylinder, while in (b) there is half a flux quantum of statistical flux as indicted by the presence of a Dirac string.

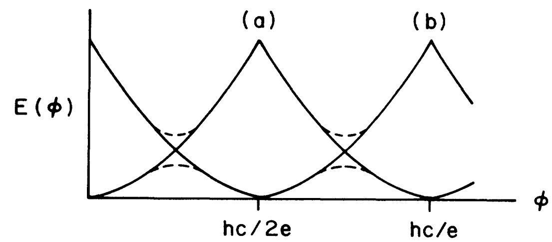

FIG. 4. Ground-state energy as a function of the electromagnetic flux through the cylinder in Fig. 3. Curve a is the branch corresponding to no statistical flux through the cylinder, curve b to half a flux quantum. The dashed curve includes the effect of mixing between the first two curves.

through the cylinder (i.e., if there is a Dirac string that bisects the cylinder) then the energy is minimized when there is a half odd-integer number of electromagnetic flux quanta through the cylinder, as shown in Fig. 4. This follows immediately from the fact that electromagnetic and statistical flux couple to the holon current in identical fashion. The two branches of $E(\Phi)$ are identical other than the offset of their zeros, since there is no energy associated with a Dirac string which has no ends. Were there no vortices, the system with half a statistical flux quantum through the cylinder could never mix with the fluxless system, and the only observable periodicity would be in units of hc/e. However, the presence of vortices with finite energy allows the system to tunnel from one sector to the other by creating a vortex-antivortex pair and pulling them off either edge of the cylinder. Thus, there is level mixing, and the true grounds-state energy has periodicity $hc/2e$, as shown in the dashed line in Fig. 4.

In the model Wilzcek considered, there are no independent dynamical degrees of freedom corresponding to the vortices, which is equivalent in our model to setting the creation energy of a vortex to infinity. In that limit, but only in that limit, the superconducting flux quantum would be hc/e. This resolves the apparent paradox. However, if the vortex creation energy is large but not infinite, the mixing caused by the vortices could be small, and it might be possible to do a "fast" experiment on small superconducting rings and observe flux quantization in units of hc/e.

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APPENDIX: HOLON-FLUXOID INTERACTION

Here we wish to estimate X, the critical ratio of J'/t such that for $J'/t > X$ the holon will bind a half flux quantum while for $J'/t < X$, the holon will be free. To do this, we compute the eigenstates and eigenvalues of the dimer Hamiltonian on the nine-site system pictured in Fig. 2, and we assume free boundary conditions. (Only a subset of the possible dimer configurations are pictured in the figure; in total there are 18 dimer states for free boundary conditions.) Of the 18 eigenstates of this Hamiltonian, only four have nonvanishing amplitude for the two dimer configurations with the holon on the central site. (For example, the configuration in the upper left-hand corner of the figure.) We will consider only these four states.

Of these four states, one of them is antisymmetric under rotation by $\pi/2$. This state is the lowest-energy state of the four for the pure magnetic Hamiltonian; its energy is $E_{\rm anti} = -J'$, independent of the other interactions. The other three states are symmetric under rotation. Their energies are obtained from the solution of the following cubic equation:

$$(J'-E)(2V+J-E)(V-E) - J'J^2 - 4t^2(2V+J-E) = 0 \, .$$

The lowest-energy solution of this equation is the symmetric ground state energy, $E_{\rm sym}$.

The antisymmetric state is the state in which there is an extra half flux quantum associated with the holon, so the unbinding transition occurs when $E_{\rm sym} = E_{\rm anti}$. Since the solution of a cubic equation is awkward, and our estimate is crude at best, we choose to evaluate $E_{\rm sym}$ for $V = J = 0$, so

$$E_{\rm sym} \approx \frac{J'}{2} - \left[\left(\frac{J'}{2} \right)^2 + (2t)^2 \right]^{1/2} .$$

In this approximation the critical value of $J'/t = \sqrt{2}/2$.

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