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Fluxoid quantization in the resonating-valence-bond model

D. J. Thouless
Department of Physics, University of Washington, Seattle, Washington 98195
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Fluxoid quantization in the resonanting-valence-bond model is investigated. It is shown that the explicit solution of the one-dimensional model is periodic with period $h/2e$ in the fluxoid, but that in the zero-temperature limit there are two families of states corresponding to odd and even multiples of $h/2e$. It is shown that for a general lattice, not necessarily bipartite, a topological constraint leads to the conclusion that $h/2e$ is the unit of fluxoid.

INTRODUCTION

In the resonating-valence-bond model for high-temperature superconductors, as proposed by Anderson[1] and modified by Kivelson, Rokshar, and Sethna,[2] electrons are arranged on the square lattice of copper atoms in such a way that each atom is bonded to *one* of its neighbors by a singlet electron pair. The ground state is a linear superposition of all the states that can be formed by such a dimerization of the lattice. If all atoms are covered by this dimerization no charge transport is possible, but singly charged vacancies can be formed in pairs by removing electron pairs. These vacancies are mobile and can lead to superconductivity if Bose-Einstein condensation occurs.

Since the charge-carrying boson is singly charged it has been argued by various authors that the unit of magnetic-flux quantization should be h/e rather than $h/2e$, which is contrary to the results observed in polycrystalline high-temperature superconductors.[3] In Ref. 2 it was shown that this argument is incorrect in a bipartite lattice, and topological restrictions ensure that the charged boson must go around a current-carrying ring in pairs, so that the correct quantum of flux is indeed $h/2e$ in this model. In this note two aspects of this problem are looked at in more detail. It is shown that the one-dimensional version of this model, which is just the well-known model of polyacetylene due to Su, Schrieffer, and Heeger,[4] is indeed periodic in the fluxoid with period $h/2e$, but there are two families of low-lying states according to whether the number of flux quanta is odd or even. Secondly, it is shown that the topological argument can be extended to arbitrary lattices, and is not restricted to bipartite lattices.

ONE-DIMENSIONAL MODEL

In one dimension the model leads to a variant of a model whose solution has been known for fifty years (see Lieb and Mattis[5] for references). Vacancies occur alternately on odd and even site numbers, since there must be an even number of bonded atoms between each pair of successive vacancies. Any vacancy can hop to its next-nearest-neighbor site unless there is a vacancy on the intervening site. This can be described by a Hamiltonian of the form

$$H=\sum_{\nu=1}[\mu b_\nu^\dagger b_\nu - V(b_{\nu-1}^\dagger b_{\nu+1}+b_{\nu+1}^\dagger b_{\nu-1})(1-b_\nu^\dagger b_\nu)] \ , \tag{1}$$

where $b_\nu^\dagger$ is a boson creation operator for a vacancy on the site ν, provided it is understood that only states with not more than one vacancy per site are considered. We also assume periodic boundary conditions for the system whose length L is an even multiple of the lattice constant a. The possible wave functions for N vacancies are of the form

$$\det(e^{ik_j(x_n+na)}) \ , \tag{2}$$

in the region defined by $x_n<x_{n+1}+a$, $x_N<x_1+L+a$, where the coordinates x_n are even or odd multiples of a for n even or odd. The condition for this wave function to vanish on the boundaries of the region is

$$k_j=2\pi(r_j+\delta)/(L+Na) \ , \tag{3}$$

where r_j is an integer and δ is a constant determined by the condition that the wave function is unchanged by the cyclic permutation $x_n \rightarrow x_{n+2}$. This condition gives

$$-\sum_j 2ak_j+2k_i(L+Na)=2\pi n \ , \tag{4}$$

where n is an integer. Solution of Eqs. (3) and (4) gives

$$\sum_j k_j=(2\pi/L)\sum_j(r_j+\tfrac{1}{2}) \tag{5a}$$

or

$$\sum_j k_j=(2\pi/L)\sum_j r_j. \tag{5b}$$

Girardeau[6] has pointed out that such a solution displays some sort of generalized Bose condensation. It does not show essential features of superconductivity or superfluidity such as persistent currents, fluxoid quantization, or quantization of circulation, because its excitation spectrum is essentially that of a noninteracting Fermi gas. Equation (5) shows that there are two inequivalent sets of states that cannot readily transform into one another. If we take the r_j to be the integers from $-N/2$ to $N/2-1$ then Eq. (5a) gives the ground state if the magnetic flux is zero, but Eq. (5b) gives the ground state if the flux is $h/2e$. Which of these two families of states lies lowest is an oscillatory function of the enclosed flux with period h/e.

Thermal excitations mix these families of states. The center-of-mass momentum $\sum k_j$ for the noninteracting Fermi gas is in free motion, so it has a mean-square value $8NVa^2/k_BT$. This results in a variance of δ equal to $Nk_BT/32\pi^2V$, so thermal motion mixes these states when the temperature T is of the order of V/Nk_B. Thus the metastability disappears at nonzero temperatures in the macroscopic limit. It is, of course, to be expected that a one-dimensional model should have its superconductivity destroyed by thermal fluctuations at any nonzero temperature.

FLUXOID QUANTIZATION FOR A GENERAL LATTICE

In Ref. 2 it was shown that for a bipartite lattice there is a topological constraint on the charge transport by singly charged vacancies that makes the quantum of fluxoid $h/2e$. In fact, there is a more general argument of this sort that can be applied to any lattice. For simplicity I consider a uniform strip of triangular lattice, for which each row transverse to the length of the strip has an even number of $2K$ atoms, as shown in Fig. 1; the argument is readily generalized to strips which contain many connected layers, or which have an odd number of atoms in each cross section. The strip is connected to itself in the form of a ring of length L. In the absence of vacancies each atom is bonded to one other atom, so that each atom has one bond ending at it. Each gap between two of the rows of $2K$ atoms is crossed by a number of bonds which is either even for each gap or odd, since an even number of bonds ends on the row of atoms. If a row of atoms contains a single vacancy, then this number changes from odd on one side of the row to even on the other. The bonds can rearrange locally by electrons tunneling through doubly charged states of the atoms, but the parity of the number of bonds in a gap cannot change.

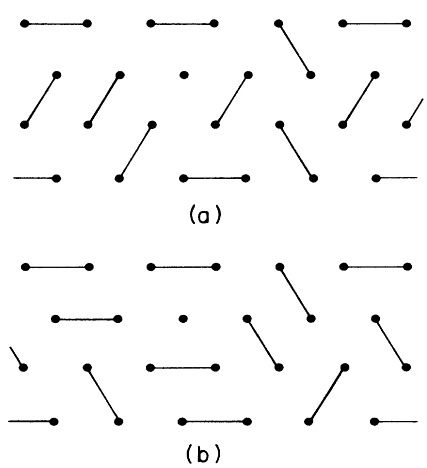

FIG. 1. A section of a ring showing valence bonds between pairs of atoms, with one positively charged vacancy. In (a) an odd number of bonds crosses vertical gaps between atoms to the left of the vacancy, while an even number crosses the gaps to the right of the vacancy. The configuration shown in (b) can be obtained from (a) by transporting the vacancy once around the ring, and that configuration has an even number of bonds crossing gaps to the left, and an odd number crossing gaps to the right.

Transport of a single vacancy right around the ring changes the parity in every gap, as is shown in Figs. 1(a) and 1(b). Therefore the Bose statistics of the vacancies cannot lead to any superposition of states obtained from one another by any transport of the vacancies an odd number of times around the ring. The original configuration can be reached by transport of a pair of vacancies once around the ring, or by a single vacancy twice around the ring. Therefore the effective charge that determines the quantum of fluxoid quantization is $2e$ and not e.

General, plausible, but not compelling arguments were put forward by Yang[7] to show that for fermions the denominator of the quantum of flux should be an even multiple of e. There are exceptions to this rule, and a superfluid plasma of $^3He^+$ ions should have flux quanta h/e according to Yang's arguments.

CONCLUSIONS

Vacancies in a one-dimensional resonating-valence-bond model behave very much like hard-core bosons, with no persistent currents, and no flux quantization except in the zero-temperature limit; this is just what should be expected for a one-dimensional model. In the low-temperature limit energy is periodic in flux with period $h/2e$. Low-lying states for odd and even multiples of flux $h/2e$ are separated from one another. These two families of states are mixed by nonzero temperatures of order V/Nk_B.

For the general lattice it can be shown that transport of a single vacancy around a ring does not restore the configuration to its original state, but it must be transported twice around the ring, so that the quantum of fluxoid is $h/2e$.

The same conclusion could be drawn by considering the wave function of the bonds rather than the wave function of the vacancies. The one-dimensional model can be solved by writing down a similar wave function for the nonoverlapping valence-bond pairs, and transport of two vacancies once or one vacancy twice around the ring is equivalent to the transport of a single electron pair around the ring.

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