Thermoelectric power in half-filled bands

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(Received 11 September 1978)

We extend the argument of Beni and Coll for the Hubbard model to show that the thermoelectric power of the lattice gas vanishes at concentration 1/2 because of particle-hole symmetry. This result is valid in the presence of phonon coupling, and, unlike the fermion case, is valid on close-packed as well as alternate lattices.

I. INTRODUCTION

In a recent paper,[1] Beni and Coll have shown that an electron system consisting of a half-filled band described by the Hubbard model exhibits a vanishing thermoelectric power as a result of particle-hole symmetry. The purpose of the present comment is to show that an analogous result can be obtained for the lattice-gas model. This model has received considerable attention recently in connection with superionic conductors.[2-9] The thermoelectric power contains important information about the microscopic transport mechanism in these materials[7] and the significance of the particle-hole symmetry for a lattice-gas concentration of $\frac{1}{2}$ has not been widely appreciated.

II. LATTICE-GAS MODEL

The Hamiltonian for the lattice-gas model is[4,7]

$$H=\sum_j h_j \tag{1}$$

$$h_j \equiv \frac{U}{2}\sum_\delta n_j n_{j+\delta}+\frac{t}{2}\sum_\delta (c^\dagger_{j+\delta}c_j+c^\dagger_j c_{j+\delta}) + \hbar\omega b^\dagger_j b_j+\lambda n_j(b^\dagger_j+b_j)\,, \tag{2}$$

where δ is summed over nearest neighbors, $c^\dagger_j$ and n_j are the usual particle operators, and $b^\dagger_j$ are phonon operators. It is important to note that the lattice-gas particle operators obey spin commutation relations,[4] i.e., they commute off site but anticommute on site. The parameter t controls the particle hopping between neighboring sites, ω is the phonon frequency, and λ is the polaron coupling constant. For simplicity we have assumed local coupling to dispersionless phonons, although this is not essential to the argument.

The thermopower S is related to the heat of transport Q by[7]

$$S=-Q/qT, \tag{3}$$

where q is the particle charge and T is the temperature. The heat of transport is in turn given by the Kubo formula[7]

$$Q=\frac{q\langle \vec{J}_U\cdot\vec{J}\rangle_0}{\langle \vec{J}\cdot\vec{J}\rangle_0}-\mu\,, \tag{4}$$

where $\vec{J}$ is the charge current, $\vec{J}_U$ is the energy current, and μ is the chemical potential. The subscript on the brackets indicates that the zero-frequency part of the retarded version of the correlation function is to be used.

The current operators required in (4) may be obtained for the Hamiltonian by standard procedures[1,7]:

$$\vec{J}=(iqt/\hbar)\sum_{j\delta}\vec{\delta}c^\dagger_{j+\delta}c_j\,, \tag{5}$$

$$\vec{J}_U=(i/\hbar)\sum_j \vec{R}_j[H,h_j]\,, \tag{6}$$

where $\vec{R}_j$ is the position of the jth site.

III. PARTICLE-HOLE SYMMETRY

We now investigate the transformation properties of Q under particle-hole exchange. To simplify the discussion we will temporarily neglect the phonon coupling. Consider a canonical transformation which obeys

$$\Phi c^\dagger_k \Phi^{-1}=c_k\,. \tag{7}$$

This has the properties

$$\Phi n_k \Phi^{-1}=1-n_k\,, \tag{8}$$

$$\Phi(H-\mu N)\Phi^{-1}=H-\tilde{\mu}N+\text{constant}\,, \tag{9}$$

where

$$\tilde{\mu}=Uz-\mu \tag{10}$$

and z is the coordination number of the lattice. In the calculation of Beni and Coll the canonical transformation involved special site-dependent phase factors. These were necessitated by an extra minus sign appearing in the transformation of the hopping term in the Hamiltonian due to the an-

ticommutation of the fermion operators. This restricted their result to alternate lattices.[1] In the present case the lattice-gas operators commute off-site and no special phase factors are required. The symmetry argument that will be presented here is thus valid on both close-packed and alternate lattices.

A straightforward application of the transformation shows that the current operators transform as

$$\Phi \vec{J} \Phi^{-1} = -\vec{J}\,, \tag{11}$$

$$\Phi \vec{J}_U \Phi^{-1} = \vec{J}_U - (zU/q)\vec{J}\,. \tag{12}$$

Applying these results to Eq. (4) yields

$$Q(\mu) = -Q(\tilde{\mu}) \tag{13}$$

or, in terms of the concentration c

$$Q(c) = -Q(1-c)\,. \tag{14}$$

At concentration $\frac{1}{2}$ $\mu = \tilde{\mu} = Uz/2$ and $c = 1 - c$. This clearly shows that the lattice-gas contribution to the heat of transport and hence the thermopower vanishes at concentration $\frac{1}{2}$. This result has not been widely appreciated. For example, a recent paper by Kobayashi and Yamada[9] incorrectly predicts a nonvanishing lattice-gas thermopower for concentration $\frac{1}{2}$. A factor of 2 error in their expression for the energy current [their Eq. (4)] leads to this conclusion in violation of the present theorem.

As pointed out by Beni and Coll, the inclusion of phonon coupling of the form in Eq. (2) does not destroy the particle-hole symmetry. It turns out that phonon coupling decreases the first term in (4) by an amount equal to the polaron energy $E_B = \lambda^2/\hbar\omega$, but the chemical potential μ is also decreased by E_B so that the heat of transport is independent of the phonon coupling constant.[7,10] This fact is important because phonon coupling does modify the activation energy for hopping.[3,4] The difference between the heat of transport and the activation energy is a direct measure of the phonon coupling in superionic conductors.[7]

ACKNOWLEDGMENTS

Research was supported by AFOSR 76-3106.

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