Thermal Evolution of Spin-Polarons

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We study the thermodynamics of a single hole in the $U = \infty$ Hubbard model using a Monte Carlo method which samples graphs that contribute to the partition function; there are no finite-size effects. The heat capacity and magnetic susceptibility indicate a sharp transition between a high temperature spin-polaron and a compact ferromagnetic droplet at low temperature. When applied to trapped vacancies in solid ^{3}He, this transition would occur near 5 mK.

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A single hole in an otherwise half-filled band with infinite on-site repulsion ($U = \infty$ Hubbard model) is one of the simplest models of highly correlated fermions. In nature, this model is realized by solid ^{3}He with a trapped vacancy, provided the temperature is well above the nuclear-spin ordering temperature T_J. The single energy in the model is the hopping matrix element t for the hole; for solid ^{3}He, $t \approx 50T_J$ [1]. At temperatures below the energy scale t, the hole is quantum mechanically delocalized and as a result stirs up the surrounding configuration of spins. As first noticed by Nagaoka [2] and Thouless [3], for the case of near-neighbor hopping on a *bipartite* structure this situation is not as hopeless (theoretically) as one might expect. There, the fermionic nature of the spins plays no role so that all configurations of the surrounding spins, accessed by the hole traversing a closed path, have the same sign. Moreover, if all configurations also appear with the same weight, as one would expect for high delocalization in a confined region, then the net spin wave function is the maximally symmetric, or *ferromagnetic,* state. Consequently, in bcc ^{3}He, a bipartite lattice, a vacancy would be surrounded by a ferromagnetic "droplet." This droplet description of the polaron was originally worked out by Andréev [4] and Héritier and Lederer [5].

A very different picture of hole motion in the strongly interacting limit was introduced by Brinkman and Rice [6]. They argued that hole motion that does not restore the spin configuration contributes with less statistical weight than a more restricted motion involving self-retracing paths. While neglecting all but the self-retracing paths gives a good approximation to the density of states, polaron formation is missed completely. The latter, in the Brinkman-Rice treatment, is understood as a phenomenon occurring in the *tails* of the hole band.

In this Letter we study the thermodynamics of a hole on the square and bcc lattices in a range of temperatures that extends from high temperatures, where the Brinkman-Rice approximation is valid, down to temperatures low enough for the droplet description to be appropriate. We find that the crossover between these regimes is quite abrupt and is marked by large oscillations in the heat capacity.

Our simulation method samples graphs contributing to the high-temperature expansion of the partition function Z; this approach has also been used by Handscomb [7]. Each graph may uniquely be identified with a closed path taken by the hole. For a system of N sites and $N - 1$ spin-S fermions, the partition function can be written as a sum over paths p:

$$\frac{Z}{\Omega} = \sum_p \frac{(-\beta)^{n_p}}{n_p!} s_p , \tag{1}$$

where $\beta = t/T$, $\Omega = N2^{N-1}$, and n_p (taking the values $0, 2, 4, 6, \ldots$) is the length of path p. The "spin factor" s_p is given by $(2S + 1)^{-(v_p - 1 - c_p)}$, where c_p is the number of cycles in the permutation of fermions induced by moving the hole around path p, visiting v_p sites; s_p takes into account the fact that not all configurations of the spins visited by path p contribute to the trace. We restrict ourselves to the spin-$\frac{1}{2}$ case in this Letter. For the self-retracing paths in the Brinkman-Rice approximation, $c_p = v_p - 1$, and the spin factor is unity. On bipartite networks, where only even n_p appear, all the terms in (1) are positive and can be sampled by Monte Carlo techniques.

A refinement of this approach [8] resums (1) to give

$$\frac{Z}{\Omega} = \sum_{p'} W(n_{p'}, \beta) s_{p'} , \tag{2}$$

where the prime on p denotes that only paths having no consecutive direction reversals, or "hair," are considered; $n_{p'}$ takes the values $0, 4, 6, 8, \ldots$. The functions $W(n_{p'}, \beta)$ take into account all possible ways of adding hair to a hairless path p' by inserting self-retracing paths of arbitrary length at all points of the hairless path; they depend only on the length of the path, $n_{p'}$. This resummation takes advantage of the fact that the spin factor depends only on the hairless part of the path. The Brinkman-Rice approximation corresponds to the "hairless part" being a single point ($n_{p'} = 0$). The functions $W(n_{p'}, \beta)$ are easily computed and tabulated using generating functions [9].

To illustrate the Monte Carlo method, we show how the energy is computed; the manner in which the heat capacity

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and the susceptibility are computed is analogous, though a little more complicated. The energy is given by

$$E = -t \frac{\partial \ln Z}{\partial \beta} \tag{3}$$

$$= -t \frac{\sum_{p'} [W'(n_{p'}, \beta)/W(n_{p'}, \beta)] W(n_{p'}, \beta) s_{p'}}{\sum_{p'} W(n_{p'}, \beta) s_{p'}}, \tag{4}$$

where $W' = \partial W/\partial \beta$, all the temperature dependence being in the W functions. As suggested by expression (4), a Monte Carlo approach involves sampling hairless paths p' with $W(n_{p'}, \beta) s_{p'}$ as their statistical weight, while averaging the quantity $W'(n_{p'}, \beta)/W(n_{p'}, \beta)$. The ensemble of hairless paths can be sampled in the usual way, by performing elementary moves that modify the path, and then accepting or rejecting the new path as detailed balance dictates.

We have adopted elementary moves that change $n_{p'}$ by ± 2, ± 4, or switch the order of two consecutive, noncollinear hops of the hole (leaving $n_{p'}$ unchanged). As the paths get quite long at low temperatures, it becomes costly to recompute the spin factor after each move. We have therefore implemented an algorithm that is able to calculate the *change* in the spin factor at a constant cost in time as the temperature is lowered [9].

In contrast to the usual high temperature series expansion technique, where a finite number of terms are calculated exactly, the present method samples contributions from potentially any term while identifying the statistically dominant paths. Equilibrium in the simulation is established when the averaged properties of paths (length, diameter, etc.) reach a steady state and may be considered "typical" of the given temperature. A typical path for spin-$\frac{1}{2}$ fermions on the square lattice at $\beta = 111.11$ is shown in Fig. 1 (bottom). The compact droplet shape is in sharp contrast to a typical path for spin-0 fermions at the same β, Fig. 1 (top). For $S = 0$, of course, the hole is simply a free fermion (in a filled band) and typical paths are expected to appear diffuse.

In the droplet model, valid at low temperatures, the free energy per hole is given by

$$F(r) = -\gamma t + \frac{k^2(r)}{2m^*} + TN(r) \ln(2S + 1), \tag{5}$$

where γ is the coordination number of the network, $k(r)$ is the wave vector of the hole when it is confined in a circular (spherical) well of radius r, m^* is the effective mass of a free fermion at the top (or bottom) of the band, and $N(r)$ is the number of spins contained in a disk (sphere) of radius r. Minimizing with respect to r and substituting this r into the first two terms gives the energy as a function of T. Differentiating with respect to T, we then obtain the heat capacities: $C_{\text{square}} = (1.774\ldots)\beta^{1/2}$ and $C_{\text{bcc}} = (3.755\ldots)\beta^{3/5}$.

The excess susceptibility of a hole relative to infinite temperature is defined by

$$\Delta\chi = \beta[\langle S_z^2 \rangle - \langle S_z^2 \rangle_{T=\infty}], \tag{6}$$

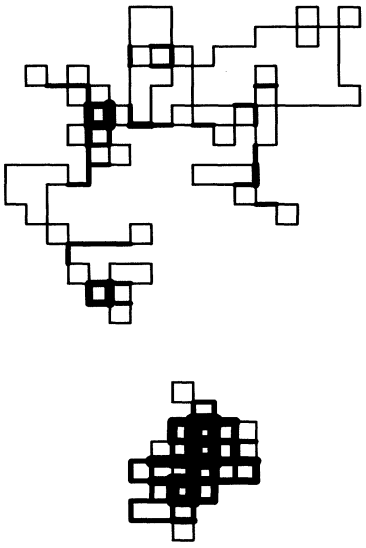

FIG. 1. Effect of spin: Typical paths at $\beta = 111.11$ for (top) spinless case and (bottom) spin-$\frac{1}{2}$ case. The thickness of a line is proportional to the number of times the hole has traveled along it.

where S_z is the total z component of spin. Within the droplet model, the spins inside the droplet are treated as a single spin of magnitude $N(r)S$. Using the results for $N(r)$ given by the free energy minimization above, we obtain $\Delta\chi_{\text{square}} = (2.184\ldots)\beta^2$ and $\Delta\chi_{\text{bcc}} = (6.794\ldots)\beta^{11/5}$. We note that $\Delta\chi = 0$ in the Brinkman-Rice approximation.

Plots of $\Delta\chi$ (Figs. 2 and 3) show two distinct regimes with a clearly defined crossover temperature T_0. At T_0, the steady increase in $\Delta\chi$ upon lowering the temperature appears to get arrested, forming a plateau. By inspecting the hairless paths generated in the simulation, one ar-

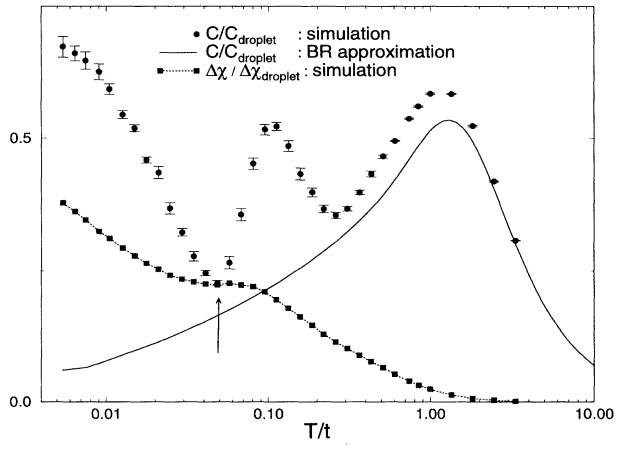

FIG. 2. Rescaled heat capacity C and excess susceptibility $\Delta\chi$ for one polaron on the square lattice. The transition to a ferromagnetic droplet occurs at T_0, shown by the arrow. The error bars for $\Delta\chi$ are smaller than the symbols.

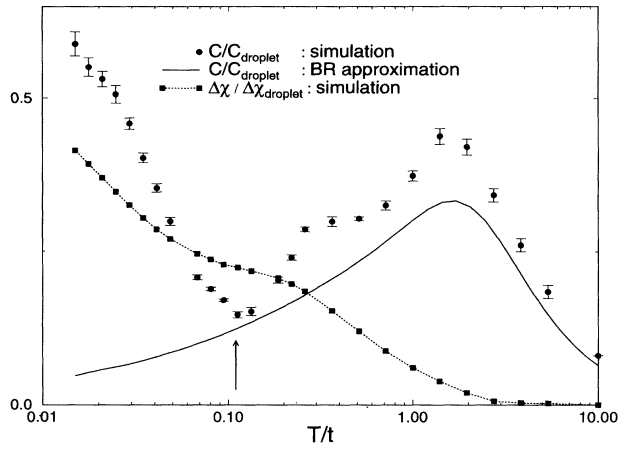

FIG. 3. Rescaled heat capacity C and excess susceptibility $\Delta\chi$ for one polaron on the bcc lattice. The transition to a ferromagnetic droplet occurs at T_0, shown by the arrow. The error bars for $\Delta\chi$ are smaller than the symbols.

rives at the following interpretation: Above T_0 the paths are diffuse and grow in size with decreasing temperature; however, as T_0 is approached, the paths suddenly begin to "ball up," forming a compact cluster below T_0. The droplet description is thus valid below T_0. Indeed, the asymptotic forms given above are consistent with the behavior of the simulation data at our lowest temperatures.

The two regimes are also reflected in the heat capacity data. At the highest temperatures the data follow the Brinkman-Rice approximation and then begin to deviate strongly as the hairless component of the paths grows. As the paths begin to ball up, the heat capacity decreases and reaches a minimum at T_0. The second maximum thus formed corresponds to diffuse paths having the greatest spatial extent. At this temperature we find that $|\partial\Delta\chi/\partial T|$ also has a maximum. Below T_0 the heat capacity grows in accordance with the droplet model. Departures from the asymptotic forms are probably due to surface effects. We note that droplet condensation would not have been noticed by Lanczos [10] and exact enumeration techniques [8] since the corresponding path lengths involved ($n_p \approx 78$) are too large.

In the millikelvin range, but well above the nuclear-spin ordering temperature, solid ^{3}He with vacancies may be modeled by the $U = \infty$ Hubbard Hamiltonian [11]. We predict that experiments in this temperature range with *artificially trapped* vacancies would show the behavior of Fig. 3. If the transfer matrix element t is taken to be 50 mK [12], we see that the ferromagnetic droplet will begin forming below 5 mK ($T_0 \approx 0.1t$ for the bcc lattice). Growth of the droplet below this temperature would be very limited, due to the onset of spin-exchange antiferromagnetism near 1 mK. So far, experiments have not been able to control the vacancy concentration at low temperatures and the data have been inconclusive [13–17]. Given the small value of T_0, it is unlikely that explanations based just on the droplet model [12,18,19] could be successful. The thermodynamic signature of polarons above the droplet condensation temperature (T_0) might be more accessible. For a 1% vacancy concentration, our calculations show that the heat capacity signal of polarons is at least as large as the spin-exchange contribution for $T > T_0$.

In summary, we have studied the $U = \infty$ model of the spin-polaron in two bipartite lattices by sampling the important paths in the partition function sum. All self-retracing paths are summed over exactly, and there are no finite-size effects. The simulation method enabled the exploration of a temperature regime that was inaccessible from either the droplet approach or the Brinkman-Rice approximation. In going from high to low temperatures in both two and three dimensions, the heat capacity shows structure that could not have been predicted by previous approaches. Experiments on solid ^{3}He with trapped vacancies should exhibit this behavior.

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