Thermodynamics of the infinite-U Hubbard model

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I observe that the high-temperature expansions of the $U=\infty$ Hubbard model on two- and three-dimensional bipartite lattices are consistent with a strong separation of energy scales for spin and translational degrees of freedom at an electron density n near $\frac{8}{11}$. The high-temperature expansion of the specific heat is nearly identical with the high-temperature expansion of spinless fermionic holes of density $1-n$, while the expansion of the uniform magnetic susceptibility is nearly identical with the susceptibility of free spins. Previous finite-size calculations are also consistent with this result.

The single-band Hubbard model in the strong-correlation ($U=\infty$) limit is important theoretically if only because it is the simplest model of interacting fermions. Unfortunately, very little is understood about the ground state or thermodynamics of this model on lattices of more than one spatial dimension. In one dimension, the thermodynamics of the $U=\infty$ Hubbard model is very different from that of a conventional Fermi liquid. In a Fermi liquid, electrons fill up renormalized energy levels with one spin-up and one spin-down electron per level. Therefore, spin and translational (sometimes called "charge") degrees of freedom will freeze out of the entropy at the same basic temperature scale—the Fermi energy. At low temperatures, only the electrons near the Fermi energy can respond to a uniform magnetic field, so the susceptibility saturates to its Pauli value.

Consider, on the other hand, the $U=\infty$ Hubbard model on a one-dimensional chain with free boundary conditions. To establish notation, I write the standard single-band Hubbard Hamiltonian,

$$H=-t\sum_{(ij)\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where (ij) indicates that the sum is over nearest neighbors, σ is up or down spin, and the $c^{\dagger}$'s, c's, and n's are fermionic creation, annihilation, and density operators, respectively. The system consists of N_E electrons on N_L sites. The condition of $U=\infty$ corresponds to the constraint that no two electrons, even of opposite spin, be on the same site. Finally, we set our energy units such that $t=1$.

It is obvious that because of the $U=\infty$ constraint, spins on a one-dimensional chain cannot switch places so the order of up and down spins cannot change. In fact, the Hamiltonian matrix for a given spin configuration will clearly be identical to the Hamiltonian for N_L-N_E spinless fermionic holes. The spin degrees of freedom simply add an overall entropy of $N_E\ln 2$ and respond to a uniform magnetic field exactly like free spins—with a susceptibility which behaves like N_E/T. Thus, the spin and translational degrees of freedom of the $U=\infty$ Hubbard model on a one-dimensional chain are completely decoupled.[1] The specific heat consists of only the contribution from the spinless fermionic holes, while the uniform susceptibility is simply that of free spins, with no Pauli-like saturation at low temperatures.

A great deal of theoretical attention has recently focused on the single-band Hubbard model in two or three dimensions following Anderson's initial suggestion of its importance for understanding high-temperature superconductivity in cuprate materials.[2] Anderson has also argued that the behavior of the Hubbard model in two or three dimensions should display similarities with the behavior in one dimension—particularly with respect to the separation of translational ("holon") and spin ("spinon") degrees of freedom.[3] In this paper, I analyze the exact high-temperature expansion of the specific heat and uniform susceptibility of the $U=\infty$ Hubbard model on the square, simple cubic, and BCC lattices, and observe that near a hole concentration of about $\frac{3}{11}$, the energy scales for translational and spin degrees of freedom are indeed decoupled. To be more specific, near this hole concentration, the specific-heat expansion is almost exactly identical to the specific-heat expansion for spinless fermions with a concentration corresponding to the concentration of holes, and the uniform susceptibility expansion is almost exactly identical to the susceptibility expansion for free spins. I also show that these results are consistent with existing finite-size studies of the ground-state properties of this model.

Kubo and Tada[4] have constructed exact high-temperature expansions for the specific heat and uniform susceptibility at arbitrary filling $n\equiv N_E/N_L$ for various two- and three-dimensional lattices. Inspired by the exact results in one dimension, I have compared these expansions with the corresponding expansions obtained to the same order on the square, simple cubic, and bcc lattices for spinless fermions of density $n_H\equiv 1-n$ and free spins of density n. These expansions are simple to obtain in principle, but somewhat tedious to obtain in practice, so I present them later.

On a d-dimensional lattice the density of free spinless fermions is given by

TABLE I. The polynomial coefficients $C_k(n)$ in the expansion for the specific heat of spinless fermions.

Square

$C_2(n)=4n-4n^2$

$C_4(n)=-6n-6n^2+24n^3-12n^4$

$C_6(n)=\frac{20n}{3}+\frac{160n^2}{3}-200n^3+300n^4-240n^5+80n^6$

$C_8(n)=\frac{-77n}{12}-\frac{5215n^2}{36}+\frac{4487n^3}{9}-\frac{9779n^4}{18}-196n^5+980n^6-784n^7+196n^8$

Simple cubic

$C_2(n)=6n-6n^2$

$C_4(n)=-9n-45n^2+108n^3-54n^4$

$C_6(n)=10n+95n^2+450n^3-1875n^4+1980n^5-660n^6$

$C_8(n)=\frac{-77n}{8}-\frac{105n^2}{8}-\frac{5033n^3}{2}+\frac{7973n^4}{4}+14\,994n^5-31\,458n^6+22\,680n^7-5670n^8$

bcc

$C_2(n)=8n-8n^2$

$C_4(n)=12n-276n^2+528n^3-264n^4$

$C_6(n)=\frac{-320n}{3}+\frac{1040n^2}{3}+5600n^3-18\,000n^4+18\,240n^5-6080n^6$

$C_8(n)=\frac{399n}{2}+\frac{71\,575n^2}{18}-\frac{244\,006n^3}{9}-\frac{662\,977n^4}{9}+480\,200n^5-785\,960n^6+536\,480n^7-134\,120n^8$

$$n_H=\int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\cdots\int_{-\pi}^{\pi}\frac{dk_d}{2\pi}\frac{1}{1+\exp[\beta(\varepsilon_k-\mu)]}\,, \tag{2}$$

where $\beta\equiv 1/T$ is the inverse temperature, μ is the chemical potential, and

$$\varepsilon_k=\begin{cases}-2[\cos(k_1)+\cos(k_2)]\,,\\ -2[\cos(k_1)+\cos(k_2)+\cos(k_3)]\,,\\ -8\cos(k_1)\cos(k_2)\cos(k_3)\end{cases} \tag{3}$$

for square, simple cubic, and bcc lattices. By inverting the high-temperature expansion of the density, one obtains the corresponding expansion for the chemical potential. One can then substitute that into the equation for the energy of free spinless fermions:

$$E/N_L=\int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\cdots\times\int_{-\pi}^{\pi}\frac{dk_d}{2\pi}\frac{\varepsilon_k}{1+\exp[\beta(\varepsilon_k-\mu)]}\,. \tag{4}$$

Expanding around $\beta=0$ and then differentiating with respect to temperature one finally obtains the expansion

$$C/N_L=C_2(n_H)\beta^2+C_4(n_H)\beta^4+C_6(n_H)\beta^6+C_8(n_H)\beta^8+\cdots\,, \tag{5}$$

TABLE II. The polynomial coefficients $A_k(n)$ in the expansion of the deviation of the $U=\infty$ susceptibility from the susceptibility of free spins.

Square

$A_4(n)=\frac{n^2(1-n)(-8+11n)}{6}$

$A_6(n)=\frac{n^2(1-n)(256-496n+380n^2-219n^3)}{120}$

$A_8(n)=[n^2(1-n)(-216\,192+377\,336n+111\,216n^2-1\,156\,744n^3+1\,511\,040n^4-563\,045n^5)]/80\,640$

Simple cubic

$A_4(n)=\frac{n^2(1-n)(-8+11n)}{2}$

$A_6(n)=\frac{n^2(1-n)(256+3748n-8940n^2+4631n^3)}{120}$

$A_8(n)=[n^2(1-n)(43\,392-1\,284\,872n-2\,789\,392n^2+14\,279\,816n^3-14\,448\,064n^4+4\,310\,913n^5)]/26\,880$

bcc

$A_4(n)=n^2(1-n)(-16+22n)$

$A_6(n)=\frac{n^2(1-n)(-352+17\,204n-36\,780n^2+19\,177n^3)}{60}$

$A_8(n)=[n^2(1-n)(130\,464-153\,076n-7\,286\,142n^2+21\,511\,885n^3-20\,641\,036n^4+6\,476\,969n^5)]/1680$

TABLE III. The polynomial coefficients $B_k(n)$ in the expansion of the deviation of the $U=\infty$ specific heat from the specific heat of spinless fermionic holes.

Square

$$B_4(n)=n^2(1-n)(8-11n)$$

$$B_6(n)=\frac{n^2(1-n)(-512+992n-708n^2+381n^3)}{16}$$

$$B_8(n)=[n^2(1-n)(216\,192-233\,976n-774\,128n^2+2\,266\,620n^3-2\,373\,336n^4+842\,219n^5)]/2880$$

Simple cubic

$$B_4(n)=n^2(1-n)(24-33n)$$

$$B_6(n)=\frac{n^2(1-n)(-512-7496n+18\,452n^2-9889n^3)}{16}$$

$$B_8(n)=[n^2(1-n)(-43\,392+1\,714\,952n+1\,805\,840n^2-15\,419\,068n^3+17\,916\,120n^4-6\,060\,783n^5)]/960$$

bcc

$$B_4(n)=n^2(1-n)(96-132n)$$

$$B_6(n)\frac{n^2(1-n)(704-34\,408n+75\,484n^2-40\,463n^3)}{8}$$

$$B_8(n)=[n^2(1-n)(-260\,928+1\,166\,312n+12\,683\,788n^2-45\,099\,583n^3+47\,712\,480n^4-16\,241\,258n^5)]/120$$

where the polynomials $C_k(n_H)$ are listed in Table I for the square, simple cubic, and bcc lattices. Note that these expansions are symmetric around $n_H/2$, so we have replaced $n_H=(1-n)$ with n. Of course, as mentioned before, the susceptibility of free spins is simply

$$\chi/N_L=n/T\ . \tag{6}$$

Using Kubo and Tada's results for the susceptibility and specific heat of the $U=\infty$ Hubbard model, we can write the deviation of the true $U=\infty$ results from our model of spinless fermionic (SF) holes and free spins as

$$\chi T/N_L-n=A_4(n)\beta^4+A_6(n)\beta^6+A_8(n)\beta^8+\cdots \tag{7}$$

and

$$[C(U=\infty)-C(\mathrm{SF})]/N_L=B_4(n)\beta^4+B_6(n)\beta^6+B_8(n)\beta^8+\cdots\ , \tag{8}$$

where the polynomials $A_k(n)$ and $B_k(n)$ are given in Tables II and III for the square, simple cubic, and bcc lattices. In one dimension these polynomials are all strictly zero. Note that the deviations of the true $U=\infty$ expansions from the theory of spinless fermions plus free spins does not begin until order β^4 for both expansions—which is the order at which an electron can first hop around in a loop. The polynomials $A_k(n)$ and $B_k(n)$ are all of order n^2 for small n and of order n_H for small n_H. Note also that all the $A_4(n)$ and $B_4(n)$ are zero at precisely $n=\frac{8}{11}$. Clearly the $A_4(n)$ and $B_4(n)$ terms arise from the simple loop diagram, but it was not obvious *a priori* that they should vanish at the same density.

In Figs. 1 and 2 I plot the polynomials $A_k(n)$ and $B_k(n)$ for $k=4$, 6, and 8 for the square, simple cubic, and bcc lattices. The crucial point to notice here is that all these polynomials (especially in three dimensions) are nearly zero at an electron density of $n\approx\frac{8}{11}$. This is the main observation of this paper—that near $n=\frac{8}{11}$, the specific-heat expansion of the $U=\infty$ Hubbard model on the square, bcc, or simple cubic lattices is almost exactly the same as the specific-heat expansion of spinless fermions of density n_H, while the susceptibility expansion is almost exactly the same as the susceptibility of free spins.

The conclusions for nonbipartite lattices like the triangular or fcc lattices would be different. Looking at Kubo and Tada's expansions, we see that there exist low-order terms in the susceptibility expansion that never vanish.

If the $U=\infty$ Hubbard model at hole densities n_H near $\frac{3}{11}$ is indeed well described by spinless fermionic holes and free spins down to low temperatures, then the energies of the ground states with different S_z (total spin pointing in the z direction) should be roughly degenerate around this hole density. Finite-size studies of the ground-state properties of the $U=\infty$ Hubbard model are indeed consistent with this picture. Takahashi[5] considered various two- and three-dimensional clusters with free boundary conditions, while Riera and Young[6] studied square clusters with periodic boundary conditions. Examining their results for their largest square clusters, we notice that in Takahashi's 3×4 cluster, the ground states with different S_z when there are three holes are nearly degenerate. Specifically, the relative spread of the energies of the ground states with different S_z is only 0.6% (from $-6.710\,23$ to $-6.669\,10$), compared to a relative spread of 10.3% (from $-9.248\,97$ to $-8.300\,56$) when there are six holes. Similarly, we notice that for five holes in Riera and Young's 4×4 lattice, the relative spread of the energies of the ground states with different S_z is only 2.1% (from $-12.159\,13$ to $-11.908\,19$) compared to a relative spread of 16.4% (from $-14.060\,53$ to -12.0) for eight holes. It is also interesting to note that for the case of three holes in the 3×4 cluster or five holes in the 4×4 cluster, the energy is not a monotonic function of S_z, indicating that the energy is "trying" to remain as flat as possible as a function of S_z.

Given our current ignorance of the zero-temperature phase diagram of the $U=\infty$ Hubbard model as a func-

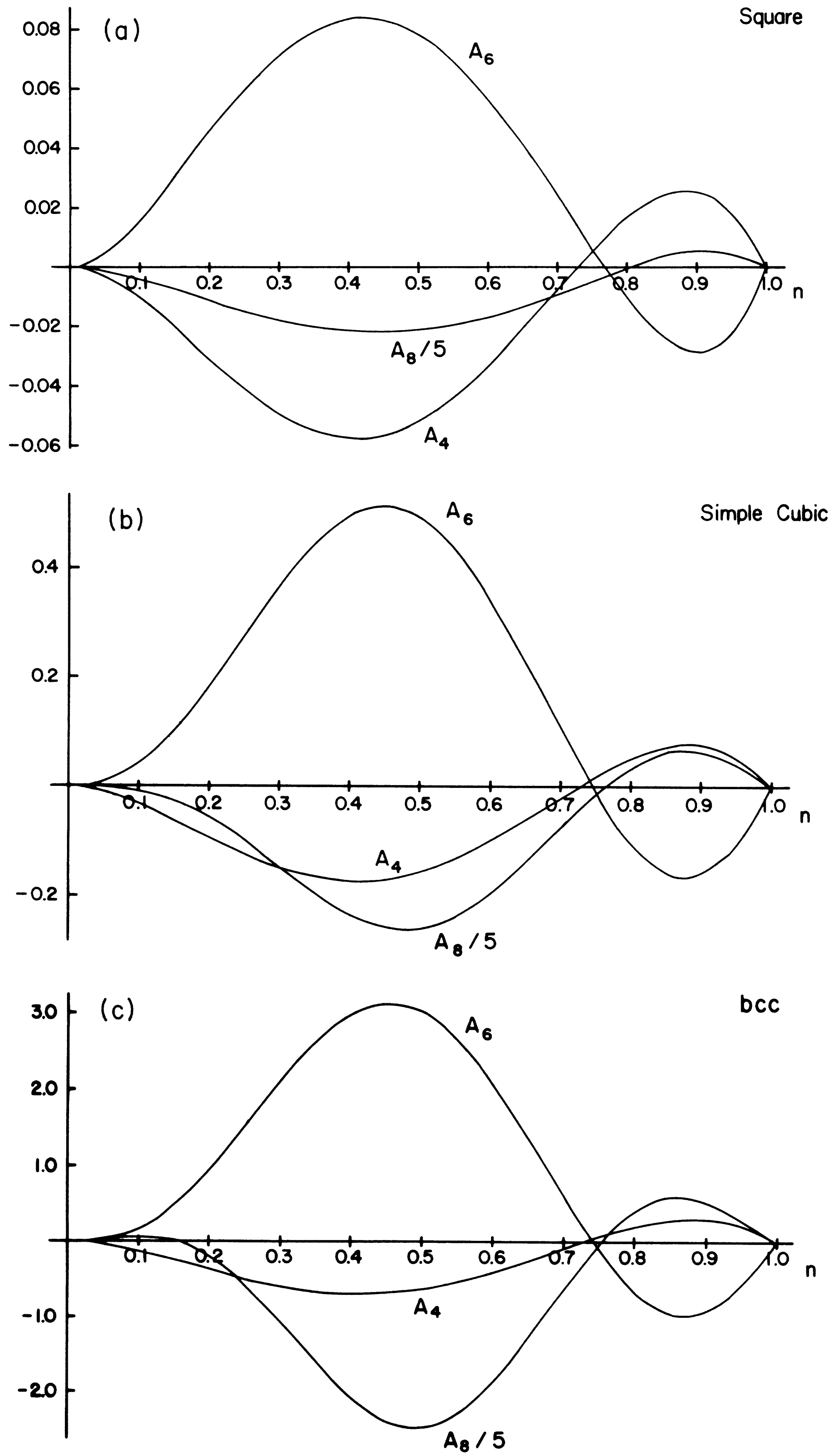

FIG. 1. $A_k(n)$ for $k=4$, 6, and 8 as functions of n. (a) Square, (b) simple cubic, (c) bcc.

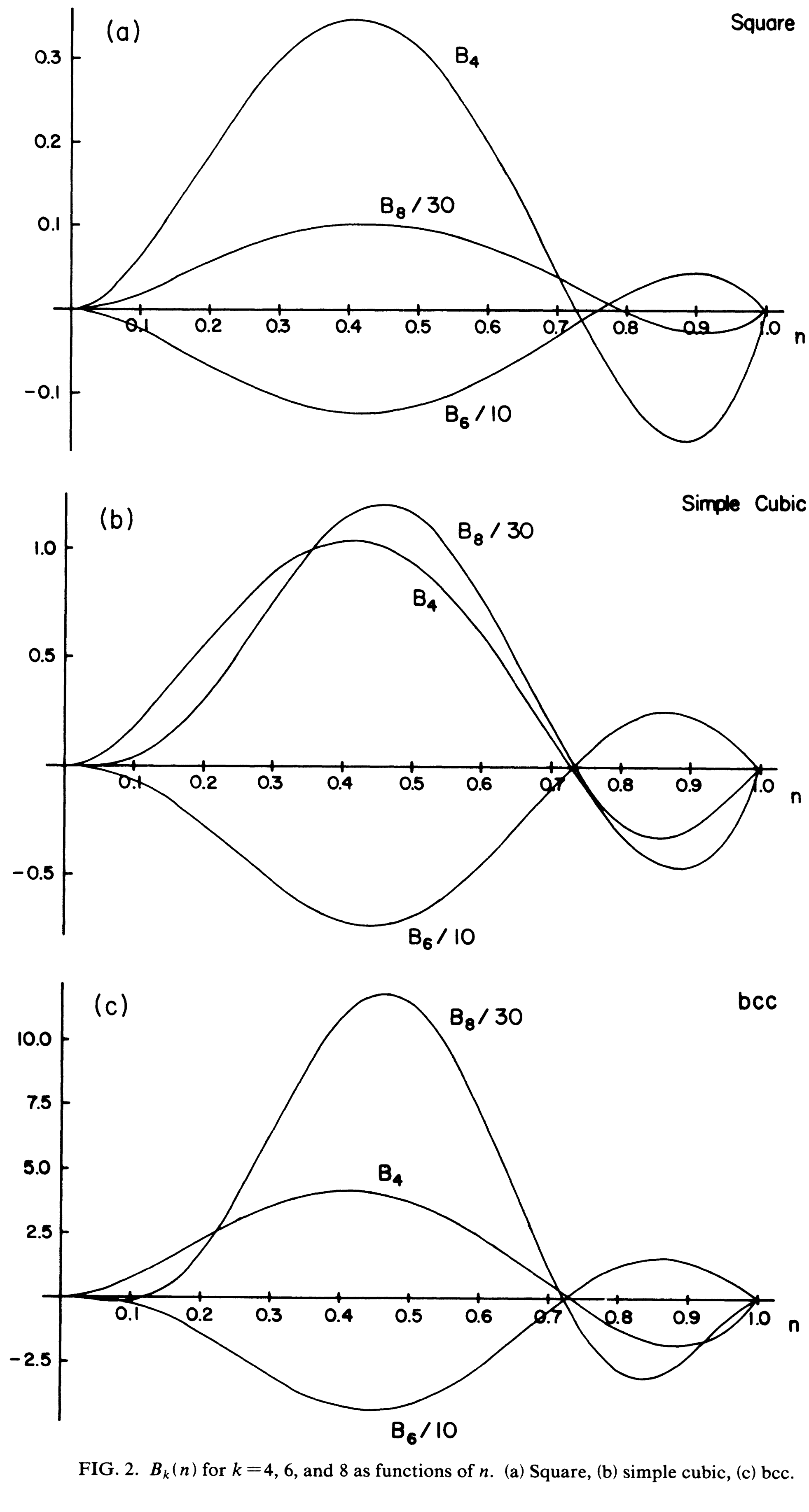

FIG. 2. $B_k(n)$ for $k=4$, 6, and 8 as functions of n. (a) Square, (b) simple cubic, (c) bcc.

tion of n in more than one dimension, there are several possible interpretations of the results presented here. One more or less "conventional" possibility is that the special density around $\frac{8}{11}$ that we are focusing on is the critical density separating a Nagaoka-like[7] ferromagnetic phase and a Fermi-liquid phase. Shastry, Krishnamurthy, and Anderson[8] have studied the stability of the fully saturated ferromagnetic state against a single spin flip and have constructed a trial wave function which has lower energy than the fully saturated ferromagnetic state at $n=0.51$ for the square lattice, $n=0.68$ for the simple cubic lattice, and $n=0.68$ for the bcc lattice. Since the true ground state with a single spin flip will have a lower energy than their trial state, the true critical density for instability of the fully saturated ferromagnetic state will be greater than these numbers. According to the picture described in this paper, the fully saturated ferromagnetic state should be marginally stable near $n=0.73$, so my results are completely consistent with those of Shastry *et al.* Given the closeness of my critical density and theirs in three dimensions, it may be that their trial wave function is very good for three dimensions.

If the critical density around $n=\frac{8}{11}$ is merely a transition point between ferromagnetism and Fermi-liquid behavior, it remains to be explained why this transition point should have such strong separation of energy scales for translational and spin degrees of freedom. A second possibility is that there is an entire resonating-valence-bond (RVB) phase centered around $n=\frac{8}{11}$ that extends to both greater and lesser densities and has other features that distinguish it from a Fermi liquid, such as an $n(k)$ distribution which is more like the $n(k)$ of the one-dimensional $U=\infty$ Hubbard model[9] than like a Fermi liquid.

One standard RVB picture is that holons are bosonic,[10] but in this paper I have compared the specific heat to the specific heat of spinless fermions. In one dimension spinless fermions are equivalent to hard-core bosons, so it would be interesting to compare the high-temperature expansion of the specific heat of the $U=\infty$ Hubbard model with the corresponding expansion of hard-core bosons of fixed density in more than one dimension. Another possibility is that holons are anyons.[11] Unfortunately, how to construct high-temperature expansions even for free anyons is an unsolved problem.

Various other extensions of this work are possible. In particular, it would be interesting to extend the $U=\infty$ expansions to higher order to see to what order these results persist. It would also be interesting to develop long expansions for arbitrary U (see Ref. 4 for expansions to order β^4). For large U, one would expect that the picture presented here would remain valid in the regime where $U \gg T \gg t^2/U$. Finally, one might wonder what happens as the spatial dimensionality is increased above three.

In conclusion, we have seen that for bipartite lattices (especially in three dimensions), the $U=\infty$ Hubbard model has a strong separation of energy scales for spin and translational degrees of freedom at a density near $n=\frac{8}{11}$. The high-temperature expansion of the specific heat is almost exactly identical to the high-temperature expansion of spinless fermions of density $1-n$, and the high-temperature expansion of the susceptibility is almost exactly identical to that of free spins.

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