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Thermodynamics of the attractive Hubbard chain

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Abstract. The thermodynamic Bethe *ansatz* equations for the attractive Hubbard chain are solved numerically. The entropy, specific heat, γ-values, band filling, spin and charge susceptibilities are obtained as a function of temperature, interaction strength and chemical potential in zero magnetic field. The dominant states at low temperatures are spin-paired electrons. The spin susceptibility is vanishingly small at low temperatures due to the spin gap.

1. Introduction and Bethe *ansatz* equations

The discovery of the high-T_c superconductors has renewed the interest in low-dimensional systems. In particular, the repulsive Hubbard model has been the focus of many authors since it is expected to describe the basic physics of these materials [1]. However, studies indicate that the purely 2D Hubbard model does not show superconductivity [2]. On the contrary, the attractive Hubbard model yields, by construction, superconductivity.

Even though the relevant physics is expected to occur in at least two dimensions, the study of the one-dimensional case is important since an exact solution is available via the Bethe *ansatz*. In this paper we consider this exact solution for the attractive Hubbard chain. The ground-state equations were obtained long ago [3] and the low-energy excitations have been studied [4]. The gap in the spin excitations and the lower critical field of the magnetization curve have also been considered [5].

The thermodynamic Bethe *ansatz* equations for this model have also been obtained [6, 7] extending previous results for the repulsive Hubbard chain [8, 9]. In the rest of this paper we solve numerically these equations. First, we present the thermodynamic Bethe *ansatz* equations [6] and briefly review the numerical method to solve them. In section 2 we present results for the entropy, specific heat, γ-values, band filling, spin and charge susceptibilities as a function of temperature, interaction strength and chemical potential in zero magnetic field. We conclude with section 3.

We consider the Hubbard chain described by the Hamiltonian

$$\hat{H} = -\sum_{i\sigma}\left(c^{\dagger}_{i\sigma}c_{i+1,\sigma} + c^{\dagger}_{i+1,\sigma}c_{i\sigma}\right) - U\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{1}$$

where $c^{\dagger}_{i\sigma}$ creates an electron of spin σ at site i and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ (with $U > 0$). It is well known that the repulsive and attractive models are related through unitary transformations like [9]

$$\Omega(U, T, A, H) = H - A + \Omega\left(-U, T, H - \frac{U}{2}, A - \frac{U}{2}\right) \tag{2}$$

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or

$$\Omega(-U,T,A,H)=H-A+\Omega\left(U,T,H+\frac{U}{2},A+\frac{U}{2}\right) \tag{3}$$

where Ω is the thermodynamic potential, A is the chemical potential and H is the magnetic field. In this paper we will solve the equations obtained directly for the attractive case. Using equation (3) we can obtain results for the repulsive Hubbard chain in a chemical potential $H+U/2$ and in a magnetic field $A+U/2$.

A convenient way to write the thermodynamic Bethe *ansatz* equations is the recursion sequence [8, 9, 6]

$$\ln\xi(k)=-\frac{2\cos k}{T}+\frac{4}{T}\int_{-\infty}^{+\infty}\mathrm{d}\Lambda\, s(\Lambda-\sin k)\mathrm{Re}\sqrt{1-\left(\Lambda-\mathrm{i}\frac{U}{4}\right)^2}$$
$$+\int_{-\infty}^{+\infty}\mathrm{d}\Lambda\, s(\Lambda-\sin k)\ln\frac{1+\eta_1'(\Lambda)}{1+\eta_1(\Lambda)} \tag{4}$$

$$\ln\eta_1(\Lambda)=s*\ln(1+\eta_2(\Lambda))+\int_{-\pi}^{\pi}\mathrm{d}k\, s(\Lambda-\sin k)\ln(1+\xi^{-1}(k))\cos k \tag{5}$$

$$\ln\eta_1'(\Lambda)=s*\ln(1+\eta_2'(\Lambda))+\int_{-\pi}^{\pi}\mathrm{d}k\, s(\Lambda-\sin k)\ln(1+\xi(k))\cos k \tag{6}$$

$$\ln\eta_n(\Lambda)=s*\ln(1+\eta_{n-1})(1+\eta_{n+1}) \tag{7}$$

$$\ln\eta_n'(\Lambda)=s*\ln(1+\eta_{n-1}')(1+\eta_{n+1}') \tag{8}$$

where $n=2,3,4,\ldots$ and where these functions satisfy the asymptotic conditions

$$\lim_{n\to\infty}\frac{1}{n}\ln\eta_n=\frac{2H}{T} \tag{9}$$

$$\lim_{n\to\infty}\frac{1}{n}\ln\eta_n'=\frac{-U-2A}{T}. \tag{10}$$

The star denotes convolution and

$$s(\Lambda)=\frac{1}{U}\frac{1}{\cosh(2\pi\Lambda/U)}. \tag{11}$$

The free energy per site is given by

$$\Omega=E_0-A-T\int_{-\pi}^{\pi}\mathrm{d}k\,\rho_0(k)\ln(1+\xi^{-1}(k))-T\int_{-\infty}^{+\infty}\mathrm{d}\Lambda\,\sigma_0(\Lambda)\ln(1+\eta_1') \tag{12}$$

where E_0 is the ground-state energy,

$$\sigma_0(\Lambda)=\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}s(\Lambda-\sin k) \tag{13}$$

and

$$\rho_0(k)=\frac{1}{2\pi}-\cos k\int_{-\infty}^{+\infty}\frac{\mathrm{d}\Lambda}{\pi}\frac{U/4}{(U/4)^2+(\Lambda-\sin k)^2}\sigma_0(\Lambda). \tag{14}$$

The functions ξ, η_n' and η_n are related to the potential functions of the three types of excitation of the model [6]: (i) real momenta corresponding to unpaired propagating electrons (charge degrees of freedom), (ii) complex momenta corresponding to a pair of electrons or bound states of pairs of electrons (pair degrees of freedom) and (iii) complex rapidities corresponding to spin-bound states forming so-called strings (spin degrees of freedom), respectively.

Since the local interaction is attractive (1), the ground state is formed of spin-singlet pairs of electrons of the Cooper-pair type. For a less than half-filled band at zero magnetic field all electrons are paired into these states, which move freely throughout the chain. The effect of a magnetic field is to break the singlet but a finite magnetic field (critical field) [5, 7] is needed to break the pairs. Therefore, at $T = 0$ a minimum magnetic field is needed to originate a magnetic response of the system.

For $T > 0$ the pairs tend to be promoted to higher-energy states where bound states of pairs appear as the dominant states: the Cooper pairs are not broken up at finite T [6]. Therefore the magnetic (spin) response is vanishingly small. The excitation spectrum resembles a degenerate Bose gas of Cooper pairs.

In summary, the three types of state of the system are [6]: (i) Cooper pairs and their collective excitations (analogous to magnons in the Heisenberg chain) having a charge $-2e$ and spin zero, (ii) unpaired electrons obeying Fermi statistics with a charge $-e$ and spin $\frac{1}{2}$ and (iii) spin excitations. Contrarily to the repulsive case, the spin excitations do not play a relevant role in the low-temperature limit [6] (due to the spin gap and at $H < H_c$, where H_c is the critical field). At high T the importance of the Cooper-pair-type excitations decreases gradually and as $T \to \infty$ the system behaves like a free-electron gas (if U is not very large).

Equations (4)–(14) can be solved in special limits [4–7]. (i) In the large-U limit all electrons are paired and in the ground state only free pairs exist. (ii) In the $U \to 0$ limit the free-electron case is recovered. (iii) In the $T \to \infty$ limit the three types of excitation decouple. (iv) In the $T \to 0$ limit the electrons are either spin paired or unpaired and no bound states of pairs of electrons contribute [6, 7]. (v) In the low-T limit the specific heat (for a less-than-half-filled band) is linear in T with a γ-value which shows a discontinuity as $U \to 0$ for all fillings, in contrast to the repulsive case which only shows a discontinuity at half filling. This is due to the excitation gap for the unpaired electron states. Hence, the limits $U \to 0$ and $T \to 0$ cannot be interchanged [4, 6, 7]. (vi) There is a critical field below which there are no unpaired electrons in the ground state and which grows with U (since the pairs are more tightly bound). (vii) The ground state magnetization vanishes for $H < H_c$ and saturates for $H > H_s$ [7]. (viii) The γ-value is constant for $H < H_c$, it diverges when H is slightly above (below) H_c (H_s) and is again constant (with zero value at half filling) for $H > H_s$ since the electron gas is fully polarized [7].

In the intermediate-temperature regime equations (4)–(14) have to be solved numerically. The procedure is standard [10, 11]. The infinite sequences are truncated to a finite number of equations n_c, and the integrals over the rapidity Λ truncated at $-\Lambda_c$ and Λ_c where the functions have reached their asymptotic values. The equations are then solved in a finite mesh of points and the convergence of the numerical derivatives of the free energy Ω is studied varying the parameters n_c, Λ_c and the density of points of the discrete mesh. The accuracy is expected to be better than a few per cent. Similar calculations were performed previously for the repulsive case [12, 13].

We obtain the free energy per site, equations (12)–(14), solving numerically equations (4)–(8) with the asymptotic conditions equations (9) and (10) as a function of U, T, A and for a small magnetic field, H. The first and second temperature derivatives yield the entropy, C/T and the specific heat (C). We also obtain the zero-field spin susceptibility (χ_s). The first and second chemical-potential derivatives yield the band filling (n) and the charge susceptibility (χ_c).

The limits $U \ll 1$ and $U \gg 1$ are difficult to obtain numerically. As stated above, due to the excitation gap for the unpaired electron states, the physical situations $U \to 0$ and $U = 0$ are qualitatively different [4, 6] for all band fillings. As a consequence, for instance

the γ-values show a discontinuity as $U \to 0$. This discontinuous behaviour requires a very high numerical accuracy which, with the method used here, is increasingly difficult to control as T is lowered. Also, as U becomes large ($U \sim 8$) the numerical method becomes unreliable at low T and therefore we do not include results for values of $U > 4$.

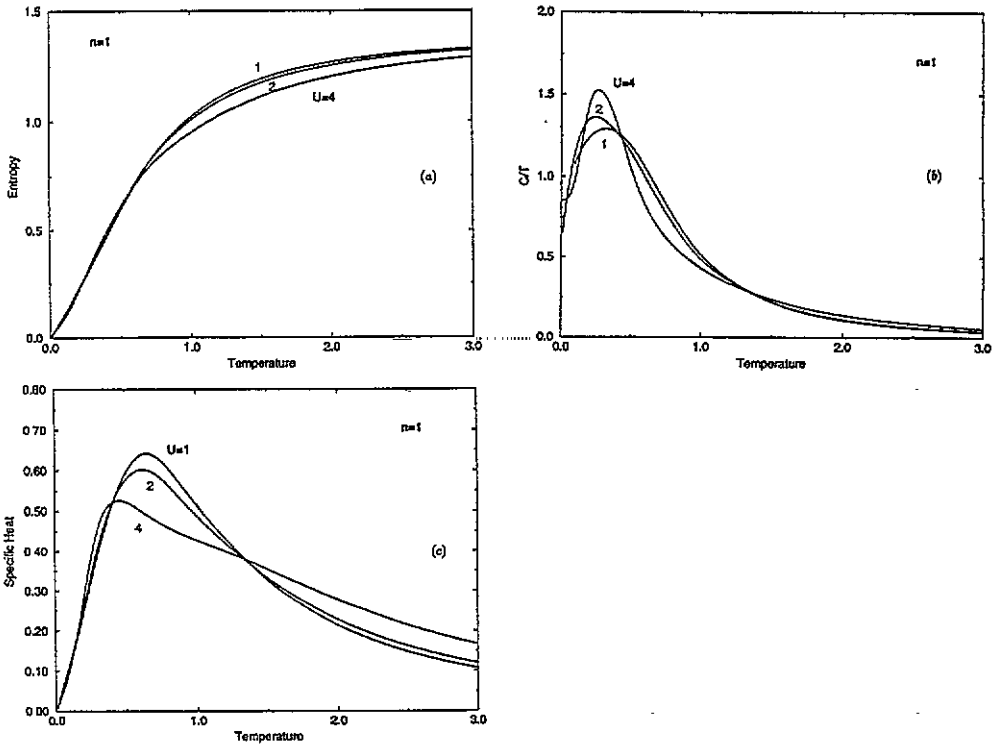

Figure 1. (a) Entropy, (b) C/T and (c) specific heat against T at half filling for $U = 1, 2, 4$.

2. Results

We consider first the temperature derivatives of the free energy. In figure 1 we show (a) the entropy, (b) C/T and (c) the specific heat, at half filling ($n = 1$ and $A = -U/2$), as a function of temperature for the values of the interaction $U = 1, 2, 4$. As $T \to \infty$ the entropy (figure 1(a)) tends to $\ln 4$ as in the repulsive case. As $T \to 0$ the entropy tends to zero showing that the ground state is a singlet. As T grows the Cooper-pair singlets are promoted to higher bound states of pairs or are broken and since the binding energy grows with U the entropy is smaller for higher values of U. In figure 1(b) we show C/T as a function of temperature for the same set of values of U at half filling. In the zero-T limit $\gamma = (C/T)(T \to 0)$ has been obtained before [6] and

$$\gamma = \frac{\pi}{6} \frac{I_0(2\pi/U)}{I_1(2\pi/U)} \tag{15}$$

where I_0 and I_1 are Bessel functions. For very small U, $\gamma \to \pi/6$ (as for the repulsive case [9]). However, at $U = 0$ (free-electron gas) $\gamma = \pi/3$. There is therefore a discontinuity around $U = 0$ which is due to the spin gap [4]. (15) shows that γ grows with U (linearly for large U). As T grows from zero C/T goes through a maximum which increases with

U. The specific heat at half filling as a function of T is shown in figure 1(c) for the same values of the interaction. The specific-heat peak decreases in height as U grows, in agreement with figure 1(a) for the entropy, and shifts towards lower T values.

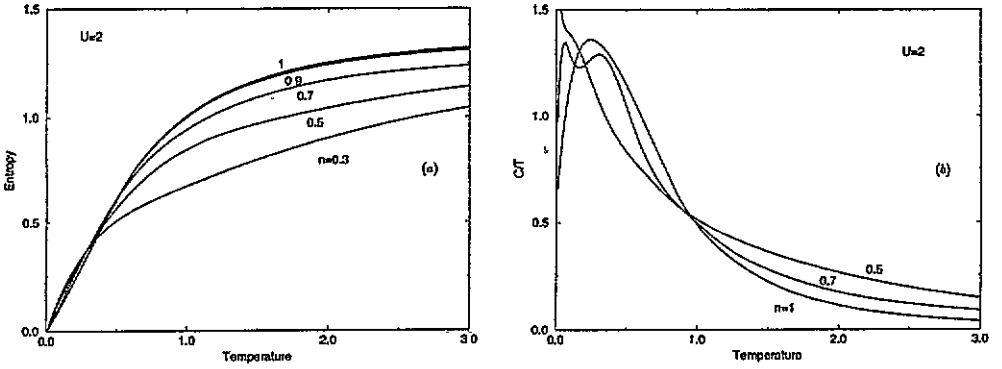

Figure 2. (a) Entropy and (b) C/T against T for several values of n for $U = 2$.

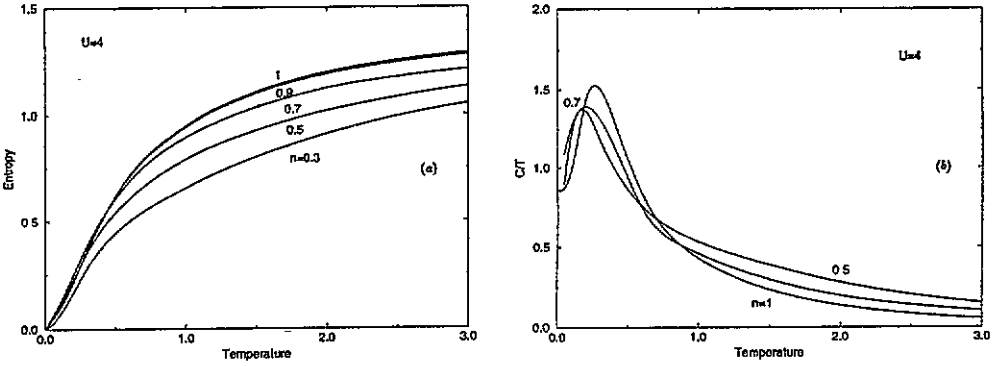

Figure 3. (a) Entropy and (b) C/T against T for several values of n for $U = 4$.

In figures 2 and 3 we show (a) the entropy and (b) C/T as a function of temperature for the values of $U = 2$ and $U = 4$, respectively, at constant band filling for several values of n. For the two values of U the entropy decreases as the the band filling decreases. The curve for $n = 0.9$ is very close to the one for the half-filled case. At low T the entropy is larger for smaller band fillings than for the half-filled case (for $U = 2$) but as U grows ($U = 4$) the ordering of the curves observed at high temperatures extends to lower T. (as clearly seen for $n = 0.3$ in figure 3(a).

In figures 2(b) and 3(b) we show C/T at constant band filling as a function of temperature for the values $U = 2$ and $U = 4$, respectively. At half filling the curve shows a maximum as discussed above. At zero T, γ increases as the band filling decreases (see figure 7 of [7]) and diverges in the empty-band limit as a consequence of the van Hove singularity in the density of states. For $U = 2$ the curves with $n < 1$ show a second peak at low T. For $U = 4$ this peak shifts to lower temperatures below the range where the numerical procedure used here is accurate ($T < 0.01$). The height of the second peak for $U = 2$ grows rapidly as n decreases.

The specific heat at constant band filling as a function of T is shown in figure 4 for $U = 1$ and for several band fillings. For n between half filling ($n = 1$) and quarter filling

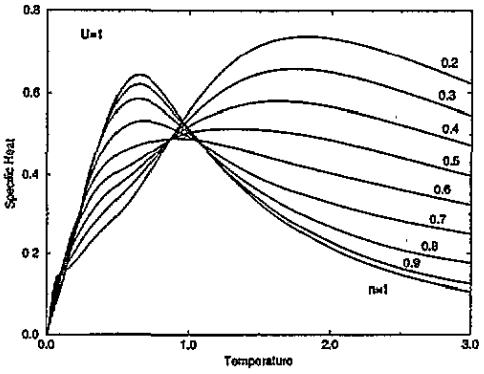

Figure 4. Specific heat against T for $U = 1$ for several values of the band filling.

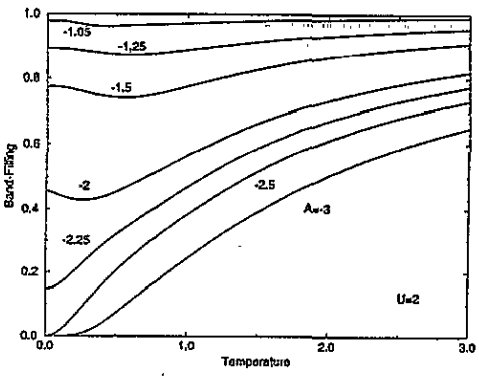

Figure 5. Band filling against T for $U = 2$ for several values of the chemical potential.

($n > 0.5$) the specific heat shows a peak around $T \sim 0.6$. For $n \leqslant 0.5$ the largest peak is now centred around $T \sim 1.7$. There is still some evidence of the lower-T peak for $n = 0.5$. For $n = 0.6$ the peak broadens considerably and centres around $T \sim 0.9$–1.

In figure 5 we show the band filling at constant chemical potential, as a function of T for the value $U = 2$. As T ($T \geqslant 1$) grows the band filling increases at constant A specially for the smaller band fillings. In the low-T limit the behaviour is not monotonic and the curves display a minimum at a temperature that decreases (tends to zero) as $|A|$ grows.

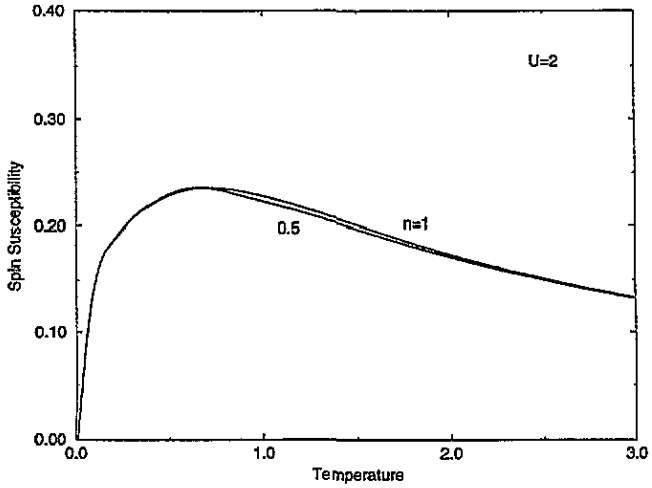

Figure 6. Spin susceptibility against T for $U = 2$ for $n = 1$ and 0.5.

In figure 6 we show the spin susceptibility as a function of T at constant band filling for $U = 2$. As $T \to 0$ the spin susceptibility is vanishingly small due to the spin gap [14]. At zero T there is no magnetic response to an external field and as T grows the magnetic response is still very small, since the dominant states are still the Cooper pairs promoted to bound states and therefore the spin excitations do not contribute at very low T [6]. As T grows further χ_s goes through a maximum. χ_s is very insensitive to n.

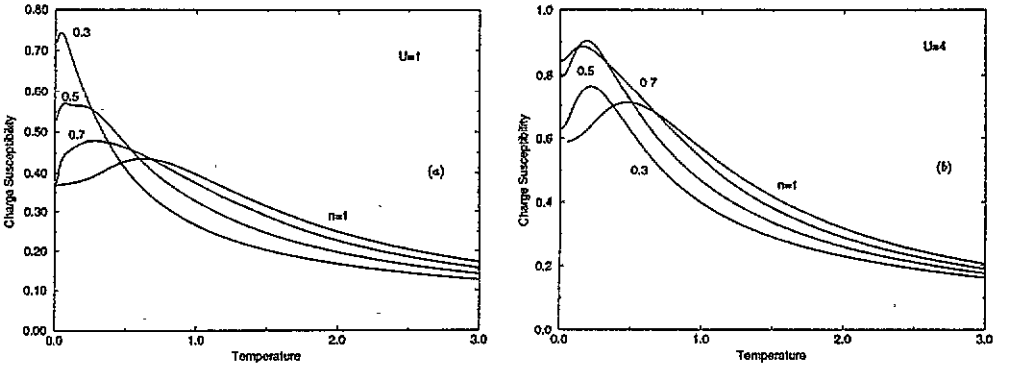

Figure 7. Charge susceptibility against T for (a) $U = 1$ and (b) $U = 4$ for $n = 1$, 0.7, 0.5, 0.3.

The charge susceptibility for (a) $U = 1$ and (b) $U = 4$ is shown in figure 7 as a function of T at constant band filling. As $T \to 0$ the charge susceptibility tends to a finite value which at half filling grows with the value of U [14]. As T grows, the curves at half filling develop a maximum that also grows with U. As n decreases from $n = 1$ the peak grows and shifts to lower temperatures for $U = 1$. For $U = 4$ the behaviour is not monotonic as for $U = 1$ and there is an inversion in the peak height and position when $n \sim 0.5$.

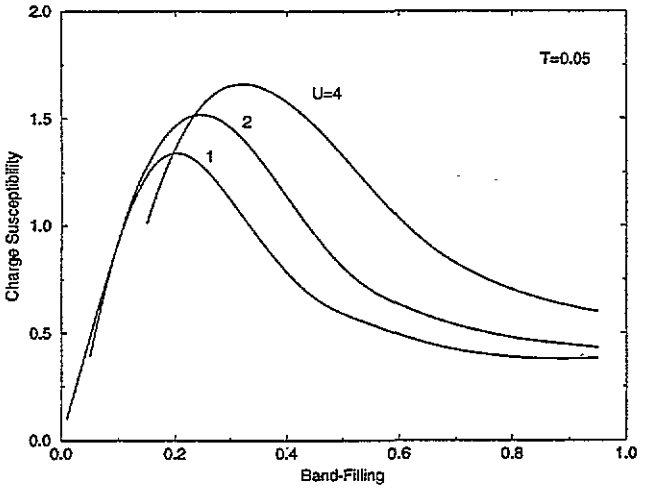

Figure 8. Charge susceptibility against band filling for $T = 0.05$ with U a parameter.

In figure 8 we present the charge susceptibility as a function of the band filling. We compare χ_c at constant $T = 0.05$ as a function of band filling for the three values of the interaction $U = 1, 2, 4$. It shows a maximum that grows with U and that shifts to higher values of the band filling also as U grows. For a fixed value of U the curves for χ_c show a maximum as a function of the band filling that grows as T decreases and shifts to lower values of the band filling [14].

3. Summary

We have presented exact results (within the accuracy of the numerical procedure) for the thermodynamics of the attractive Hubbard chain. Unitary transformations establish

relations between the repulsive and the attractive Hubbard chains. Roughly speaking in these transformations the roles of the spin and charge degrees of freedom are interchanged. In the repulsive case the spin degrees of freedom play an important role (in particular if U is large) and the ground-state charge fluctuations are strongly suppressed ($\chi_c = 0$) at half filling due to the Mott–Hubbard gap. Similarly, in the attractive case the ground-state spin susceptibility is zero due to the spin gap of the Cooper-pair singlets formed due to the local attractive interaction. As a consequence of the gap at half filling the limit $U \to 0$ in the repulsive case shows a discontinuous behaviour with respect to the exactly free-electron gas [4, 9]. Since the spin gap in the attractive case prevails for all band fillings (less than half filling) this discontinuous behaviour as $U \to 0$ is observed for all band fillings and $\chi_s \to 0$ as $T \to 0$. In the repulsive case both χ_s and γ are finite as $T \to 0$. It was also found previously that (at $T = 0$) χ_c and γ diverge close to half filling in the repulsive case [15]. Also, for finite and small T these quantities show anomalies close to half filling [12, 13]. The divergence in γ was interpreted as due to the charge contribution to the specific heat [13].

In this work we have presented results for the entropy, specific heat, C/T, n, χ_s and χ_c as a function of T. As expected, the entropy yielded a singlet ground state and a finite C/T as $T \to 0$. The spin susceptibility is vanishingly small at low T confirming that the dominant states for $T > 0$, although small, are still the Cooper-pair singlets, independent of the band filling and confirming that the spin excitations do not contribute significantly at low T [6, 7].

We found a double-peak structure in C/T for $n < 1$ which shifts to very low T as U grows. Also, we found a shift in the peak position of the specific heat as a function of temperature as n decreases from half filling through quarter filling and to the empty-band limit. As for C/T at constant and low band filling, χ_c peaks strongly (as compared to the half-filled case) at low n and low T. We also found that χ_c shows a maximum at low T as a function of band filling which peaks and shifts to lower values of n as T decreases [14]. For a specified value of T the height of the peak grows with U and appears at higher band fillings.

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