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High-temperature Thermodynamics of the Hubbard Model*

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Abstract

Recently derived 10th-order high-temperature expansions for the Hubbard model are used to obtain the ferromagnetic susceptibility and specific heat at high temperatures. Numerical results are obtained for the simple cubic and face-centred cubic lattices by using Padé approximants to sum the series. The results are compared with two solvable limiting cases, namely the non-interacting limit $U = 0$ and the strongly-correlated or atomic limit $t = 0$.

1. Introduction

One of the fascinating, only partially understood, areas of condensed matter physics is that of electron states in narrow bands, where correlations between the electrons play an essential part in the physics (see e.g. Moriya 1981). The Hubbard model (Hubbard 1963) provides a simple framework for discussing such phenomena. Initially proposed in connection with magnetism in transition metals, the model has recently again become the focus of much work in connection with theories of high temperature superconductivity (for reviews see e.g. Emery 1989; Fukuyama 1989).

The Hubbard Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

consists of two parts. The first term describes non-interacting electrons within a tight-binding picture and gives rise to the usual Bloch band description. The U-term is a simplified Coulomb repulsion which only acts between electrons of opposite spin at the same site. This model is clearly only a caricature of reality but one hopes, in the usual way, that some essential physics remains. This indeed appears to be the case.

Except in one dimension, where some exact results exist, the properties of the Hubbard model can only be deduced from approximate calculations. One such approach is via high-temperature expansions. Until very recently such expansions

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had only been computed to order $(\beta t)^4$ for the general case. Even then there were errors in the 4th-order term—an indication of the complexity of the calculation. Recent work by Pan and Wang (1991), ten Haaf and van Leeuwen (1992), and our group (Henderson *et al.* 1992; Oitmaa *et al.* 1993) has extended the series considerably.

We write the Hamiltonian in a more general form as

$$H = H_0 + V\,, \tag{2}$$

with

$$H_0 = U \sum_i n_{i\uparrow}\, n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) - h \sum_i (n_{i\uparrow} - n_{i\downarrow})\,, \tag{3}$$

$$V = -t \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma}\, c_{j\sigma} + c^\dagger_{j\sigma}\, c_{i\sigma})\,. \tag{4}$$

Here μ is the chemical potential and $h = \mu_B B$, with B the external magnetic field. We take H_0 to be the unperturbed Hamiltonian. This corresponds to the 'atomic limit' which can be solved exactly. Using rather standard diagrammatic perturbation theory, the details of which can be found in Henderson *et al.* (1992), we obtain an expansion for the logarithm of the grand partition function in the form

$$\frac{1}{N} \ln Z_g = \ln z_0 + \sum_{r=2}^{\infty} z_0^{-r}\, F_r(\beta U, x, y)\, (\beta t)^r\,. \tag{5}$$

In this expression z_0 is the partition function per site in the atomic limit

$$z_0 = 1 + x(y + y^{-1}) + x^2 \mathrm{e}^{-\beta U}\,, \tag{6}$$

where $x = e^{\beta\mu}$ is the fugacity and $y = e^{\beta h}$. The F_r are multinominal expressions in x, y, the coefficients being functions of βU. The first one is

$$F_2(\beta U, x, y) = \tfrac{1}{2} q \Big[(y + y^{-1})x + \frac{4}{\beta U}(1 - \mathrm{e}^{-\beta U})x^2 + \mathrm{e}^{-\beta U}\,(y + y^{-1})x^3 \Big]\,, \tag{7}$$

where q is the coordination number of the lattice. The subsequent expressions rapidly become too lengthy to write down explicitly. We have obtained the F_r terms through F_{10} for the standard lattices: square, triangular, simple cubic, body-centred cubic and face-centred cubic. This has been possible only through efficient computerisation of the whole procedure. Even then a few of the 10th-order diagrams required several weeks of CPU time on a DEC workstation. Without a significant breakthrough in the algorithm it would be impractical to extend the series further. For loose-packed lattices only even powers of βt occur in (5).

From the grand potential (5) standard thermodynamics relations can be used to obtain the internal energy,

$$E = -\left(\frac{\partial}{\partial\beta}\right)_x \left(\frac{1}{N}\ln Z_g\right), \tag{8}$$

and the specific heat $C = \partial E/\partial T$. The (dimensionless) magnetic susceptibility is given by

$$\bar{\chi} = \lim_{y\to 1}\left(y\frac{\partial}{\partial y}\right)^2\left(\frac{1}{N}\ln Z_g\right). \tag{9}$$

This is related to the real susceptibility χ by $\bar{\chi} = k_B T\chi/\mu_B^2$.

The resulting expressions have the form

$$E = E_0 + \sum_{r=2}^{\infty} z_0^{-r-1} E_r(\beta U, x)(\beta t)^r, \tag{10}$$

$$\bar{\chi} = \bar{\chi}_0 + \sum_{r=2}^{\infty} z_0^{-r-1} X_r(\beta U, x)(\beta t)^r, \tag{11}$$

where E_0, χ_0 are the zeroth-order or atomic-limit quantities, and the E_r, X_r are polynomials in x with coefficients dependent on βU. The atomic-limit internal energy and susceptibility are, with $\zeta = \mathrm{e}^{-\beta U}$,

$$E_0 = Ux^2\zeta/(1 + 2x + x^2\zeta), \tag{12}$$

$$\bar{\chi}_0 = 2x/(1 + 2x + x^2\zeta). \tag{13}$$

The expansions (10) and (11) are expressed in terms of the fugacity x. For most purposes it is more convenient to express the series in terms of the average number of electrons per site, which can be obtained from the grand potential as

$$\begin{aligned} n &= \left(x\frac{\partial}{\partial x}\right)\left(\frac{1}{N}\ln Z_g\right) \\ &= 2x(1 + x\zeta)/(1 + 2x + x^2\zeta) \\ &\quad + \sum_{r=2}^{\infty} z_0^{-r-1} Y_r(\beta U, x)\,(\beta t)^r. \end{aligned} \tag{14}$$

It is then necessary to invert this expression to obtain x in powers of (βt), with coefficients being functions of n, βU. In general this can only be done

numerically. Finally the fugacity is eliminated to obtain expansions in the form

$$E = \sum_{r=0}^{\infty} e_r\,(n, \beta U)\,(\beta t)^r\,, \tag{15}$$

$$C/k_{\mathrm{B}} = \sum_{r=0}^{\infty} a_r\,(n, \beta U)\,(\beta t)^r\,, \tag{16}$$

$$\bar{\chi} = \sum_{r=0}^{\infty} c_r(n, \beta U)\,(\beta t)^r\,. \tag{17}$$

The aim of most series studies of the Hubbard model (Henderson *et al.* 1992, and references therein) has been to locate the phase transition and hence determine the form of the phase diagram. This is done by looking for a mathematical singularity in χ, which will signal a transition from a paramagnetic to a ferromagnetic phase, or in the staggered susceptibility χ, which signals an antiferromagnetic phase. This is difficult to achieve in practice since the series are typically quite erratic. A less ambitious goal is to use the series to evaluate the thermodynamic quantities at high temperatures, well above any transition, where the series are well converged. This was done by Beni *et al.* (1973) using short series. The present work can be thought of as an extension of that calculation using our much longer series.

2. The Susceptibility

The susceptibility in the atomic limit is given by

$$\bar{\chi}_0 = 2x/(1 + 2x + x^2\zeta)\,,$$

where, in this limit, the fugacity is

$$x = \frac{n - 1 + [(1-n)^2 + n(2-n)\zeta]^{\frac{1}{2}}}{(2-n)\zeta}\,. \tag{18}$$

Analytic expressions can be obtained in the following special cases:

(i) $\beta U = 0$ (infinite-temperature limit)

$$\bar{\chi}_0 = \tfrac{1}{2}n(2-n)\,, \tag{19}$$

(ii) $\beta U = \infty$ (strong-correlation limit)

$$\bar{\chi}_0 = n\,, \tag{20}$$

(iii) $n = 1$ (half-filled band)

$$\bar{\chi}_0 = \mathrm{e}^{\beta U/2}/(1 + \mathrm{e}^{\beta U/2})\,. \tag{21}$$

Turning now to the general case, where

$$\bar{\chi} = \bar{\chi}_0 + \sum_{r=2}^{\infty} c_r(n, \beta U)\,(\beta t)^r\,,$$

we proceed as follows. For given values of n, βU we obtain the coefficients of the series numerically (up to $r = 10$). We then construct Padé approximants to the series,

$$\bar{\chi}_{K,L} \equiv P_K(\beta t)/Q_L(\beta t)\,, \tag{22}$$

where P_K and Q_L are polynomials in βt of degree K, L respectively, with $K+L \leq 10$. Evaluation of the Padé approximants thus provides estimates of χ. An estimate of the reliability of the result is obtained from the consistency between different approximants. This approach takes some account of the remaining unknown terms of the series and is far superior to simply summing the known terms.

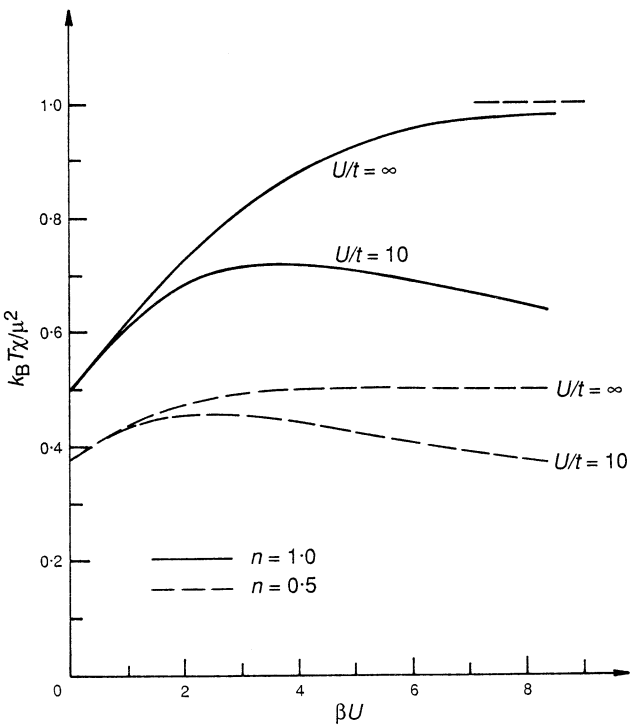

Fig. 1. Susceptibility versus βU for the simple cubic lattice, for $U/t = \infty$ (the atomic limit) and for $U/t = 10$. The full curves are for half-filling, the broken curves for quarter-filling.

In Figs 1 and 2 we show the susceptibility $k_B T\chi/\mu_B^2$, plotted as a function of βU, for the simple cubic and face-centred cubic lattices respectively. For each lattice we show results for $n = 1$ (half-filling) and $n = 0{\cdot}5$, for $U/t = \infty$

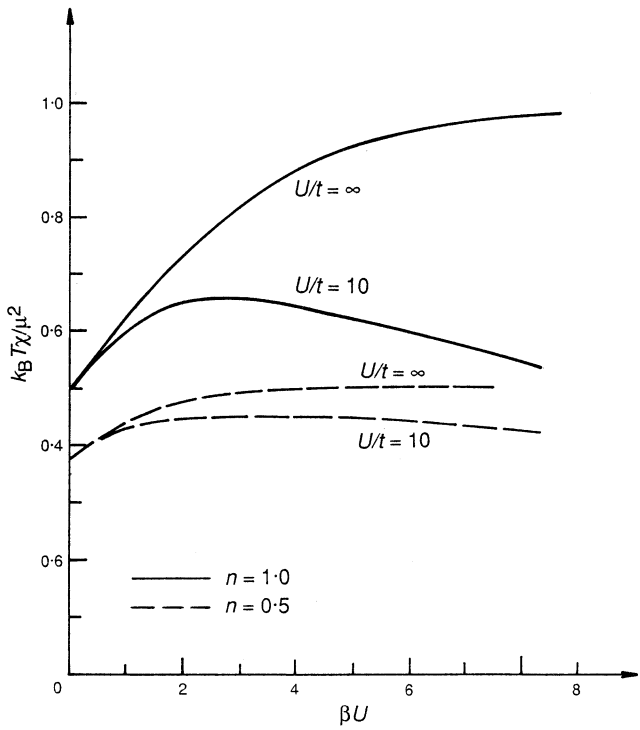

Fig. 2. Susceptibility versus βU for the face-centred cubic lattice.

and $U/t = 10$. The former case is the atomic limit and so comparison of the two curves shows the effect of increasing bandwidth (proportional to t) on the susceptibility. The results for the two lattices are broadly similar.

We note the following points:

(i) At high temperatures the susceptibility has the approximate form

$$\chi \sim \frac{A}{k_B T} + \frac{B}{(k_B T)^2} + \cdots, \tag{23}$$

with A, B dependent on n but independent of t.

(ii) At finite temperature and fixed U the effect of increasing t is to depress the susceptibility below the atomic limit result.

(iii) There is no indication of an upturn in the susceptibility for $n \leq 0{\cdot}5$ in the region $\beta U \sim 6$. Such a change in curvature was noted by Beni *et al.* (1973) but is presumably an artifact of their short series.

Presumably the susceptibility does diverge but at some much lower temperature where the series cannot effectively probe.

It is also of some interest to evaluate the susceptibility in the region of small U/t to compare the result with the uncorrelated limit ($U = 0$), where again the system is exactly solvable. Evaluation of the series for small βU (including

$\beta U = 0$) must be done with care to avoid serious roundoff problems (or divergences) which come from terms with negative powers of (βU) [see e.g. equation (7)]. In Fig. 3 we show the susceptibility for the fcc lattice, as a function of βt, for $n = 1$ and $n = 0{\cdot}5$, as before. For each n we show three curves for $U/t = 0, 1, 10$. The following features are apparent.

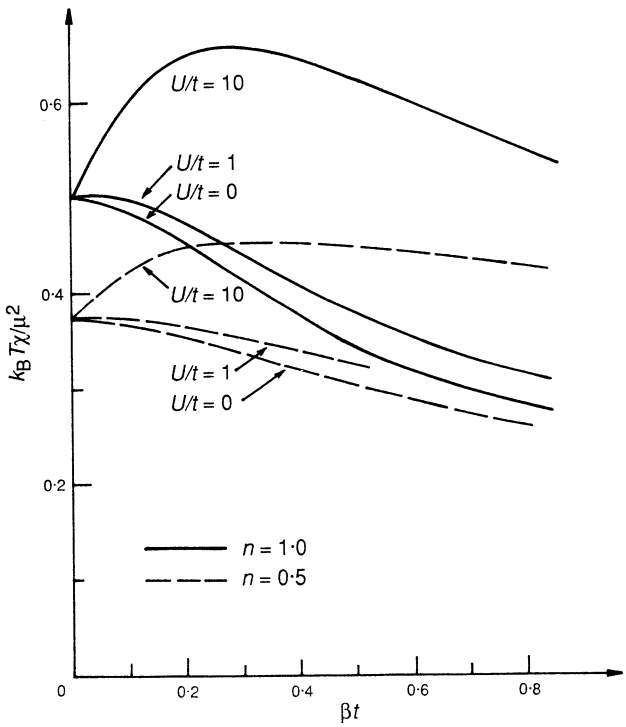

Fig. 3. Susceptibility versus βt for the face-centred cubic lattice, for $U/t = 10$, 1 and 0 (the non-interacting limit).

(iv) For fixed t the susceptibility is enhanced by the correlation term U, consistent with (ii) above.

(v) For $U/t \leq 1$ the curves approach the $\beta t = 0$ limit with zero slope, consistent with a strict Curie law $\chi = A/k_B T$ at high temperatures. At temperatures sufficiently high that the electrons are non-degenerate, a Curie-law behaviour is expected to hold even for non-interacting electrons. For larger U/t the curves have a finite positive slope consistent with the form (23).

3. The Specific Heat

We start again with the atomic limit. The internal energy in this limit is given by

$$E_0 = Ux^2\zeta/(1 + 2x + x^2\zeta)\,. \tag{24}$$

When differentiating this to obtain the specific heat it must be remembered that x is also temperature-dependent. After some algebra we obtain the result

$$C/k_B = (\beta U)^2 \frac{x(1+x)n\zeta[(1-n)^2 + n(2-n)\zeta]^{-\frac{1}{2}} - x^2\zeta}{(1+2x+x^2\zeta)^2}. \tag{25}$$

This can be simplified in the special cases
(i) $\beta U = 0$ (infinite-temperature limit)

$$C/k_B = \tfrac{1}{16} n^2 (2-n)^2 (\beta U)^2 + \ldots, \tag{26}$$

(ii) $\beta U = \infty$ (strong-correlation limit)

$$C/k_B = \frac{n^2}{4(1-n)} (\beta U)^2 \, \mathrm{e}^{-\beta U}, \tag{27}$$

(iii) $n = 1$ (half-filled band)

$$C/k_B = (\beta U)^2 \frac{\mathrm{e}^{\beta U/2}}{4(1+\mathrm{e}^{\beta U/2})^2}. \tag{28}$$

When the hopping term is included we use the same approach as for the susceptibility, i.e. we construct Padé approximants to the series, for fixed n, βU, and evalute these for the appropriate values of βt. There is, however, a minor technical difficulty. It is straightforward to compute the energy series (15)

$$E = \sum_{r=0}^{\infty} e_r(n, \beta U) \, (\beta t)^r,$$

from which we obtain the specific heat as

$$C/k_B = \sum_{r=0}^{\infty} \{-(\beta U)^2 e_r' - r(\beta U) e_r\} \, (\beta t)^r \tag{29}$$

with $e_r' = \partial e_r / \partial(\beta U)$. However, the e_r are not available as analytic expressions in βU, and hence the derivative in (29) must be evaluated numerically. Since the e_r are smooth functions of βU this can be done easily.

In Figs 4 and 5 we show the specific heat as a function of βU for the simple cubic and face-centred cubic lattices respectively. Again we consider the two cases $n = 1$ and $0{\cdot}5$ and for each n two values of U/t, namely $U/t = \infty$ (the atomic limit) and $U/t = 10$. Results for the two lattices are broadly similar.

We note the following points:

(i) In the atomic limit the specific heat has a single Schottky-type peak which moves to smaller βU, i.e. higher temperatures, as the electron density decreases. As noted by Beni *et al.* (1973) this peak is associated with the onset of significance excitation of doubly occupied sites.

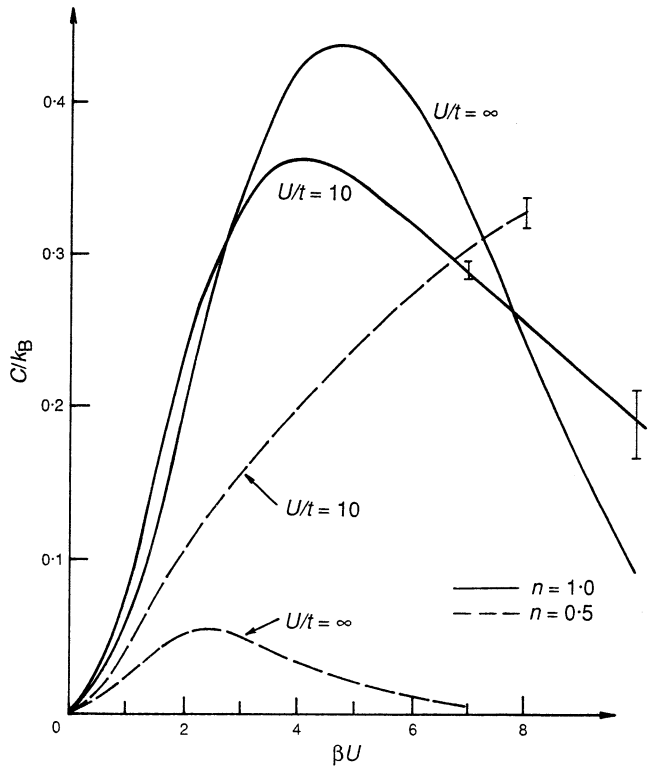

Fig. 4. Specific heat versus βU for the simple cubic lattice, for $U/t = \infty$ and $U/t = 10$. The error bars are subjective error estimates obtained from variations among different Padé approximants.

(ii) For half-filling, or near half-filling, the inclusion of finite hopping t does not destroy this peak, but the peak broadens, decreases in height, and moves to higher temperatures.

(iii) For lower electron density, and in particular for $n = 0{\cdot}5$ as shown, the effect of finite t is quite different and much more dramatic. The specific heat is increased above that in the atomic limit, indicating an enhancement in excitations of the system. The high-temperature peak is no longer present, and in the (βU) range shown the specific heat is monotonically increasing. A new peak, which we are unable to obtain from our series, must develop at lower temperatures.

Finally we plot the specific heat versus βt in Fig. 6, to allow comparison with the non-interacting limit $U = 0$, and note the following features:

(iv) For $n = 1$ there is a qualitative change in the specific heat on going from $U/t = 10$, where there is still a pronounced high-temperature peak, as in the atomic limit, to $U/t = 0$, where the specific heat is a monotonically increasing function of βt in the range shown. Of course there must be a maximum at some lower temperature, since when $U = 0$ it is well known that $C \sim \beta^{-1}$ in the low-temperature limit $\beta t \to \infty$. There is a

crossover temperature at $\beta t \sim 0{\cdot}4$, below which for fixed t the specific heat is depressed for increasing U.

(v) For $n = 0{\cdot}5$, in the range of βt values shown, the specific heat for $U/t = 10$ is everywhere greater than for the non-interacting limit.

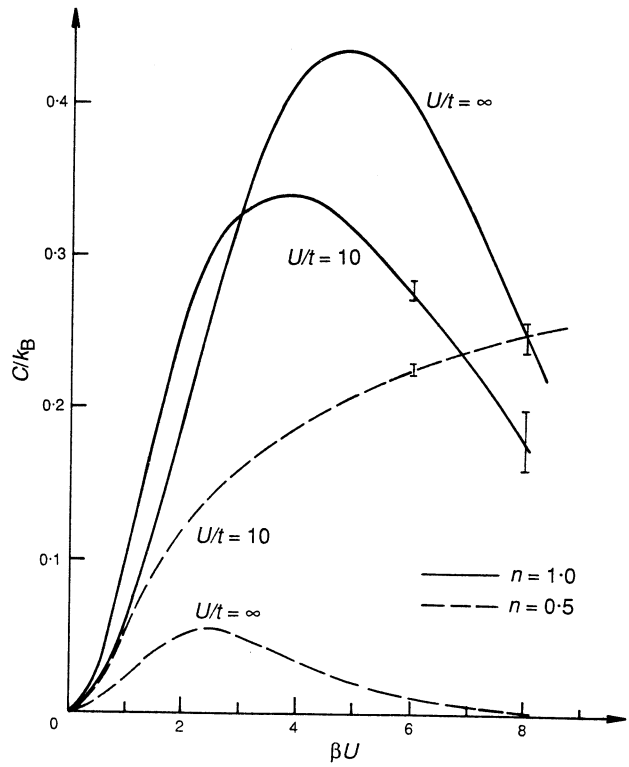

Fig. 5. Specific heat versus βU for the face-centred cubic lattice.

4. Conclusions

We have recently derived high-temperature expansions to 10th order for the Hubbard model on the standard 2- and 3-dimensional lattices. This is a substantial increase in order over previous series for this model. In the temperature range where phase transitions are to be expected, the series are erratic and difficult to analyse with precision. However, at higher temperatures the series are well converged and can be accurately summed using Padé approximants.

In this way we have computed both the ferromagnetic susceptibility and the specific heat for the simple cubic and face-centred cubic lattices. Results are presented for two values of the electon density, namely $n = 1$ (half-filled band) and $n = 0{\cdot}5$, and for various ratios U/t. The results are compared with the exactly solvable limiting cases; the non-interacting limit, $U/t = 0$, and the strongly-correlated or atomic limit, $U/t = \infty$. In most cases the results provide a smooth interpolation between these two limits.

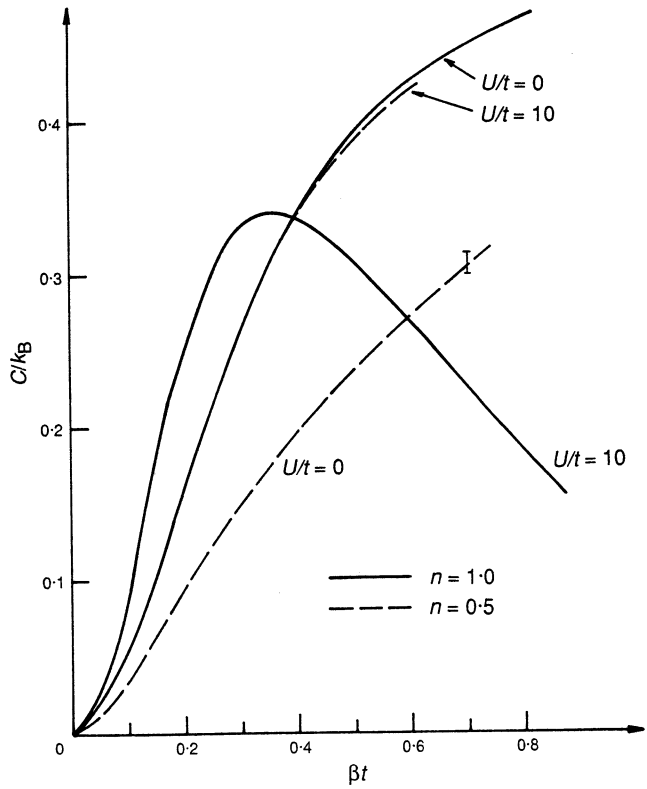

Fig. 6. Specific heat versus βt for the face-centred cubic lattice for $U/t = 0$ and 10. Results for $U/t = 1$ are virtually indistinguishable from the case $U/t = 0$.

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