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# Thermodynamics of a liquid-metal model from high-temperature series expansions 

Y S Yangt, C J Thompson $\dagger$ and J Oitmaa $\ddagger$<br>$\dagger$ Department of Mathematics, The University of Melbourne, Parkville, Victoria 3052, Australia<br>$\ddagger$ School of Physics, University of New South Wales, Kensington, NSW 2033, Australia

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#### Abstract

A lattice model for liquid metals proposed by Nara, Ogawa and Matsubara is studied using high-temperature series expansions. The grand-canonical potentials are expanded exactly to order $\beta^{9}$ and the susceptibilities are expanded to order $\beta^{11}$ on two-, three-, and fourdimensional hypercubic lattices. It is conjectured that, for fixed values of the fermion hopping energy and fermion chemical potential, the system goes critical only at particular values of the lattice-gas chemical potential. The critical values of the lattice-gas chemical potential and the critical temperature are calculated self-consistently and the critical exponent of the inverse isothermal compressibility is estimated using Pade approximants. It is concluded that the critical behaviour of the model is not affected by the presence of the fermions. This conclusion is consistent with the exact soiution on a one-dimensional lattice by Thompson, Matsubara and Yang.


## 1. Introduction

In a previous publication, a lattice model for metal-non-metal transitions proposed by Nara, Ogawa and Matsubara (NOM) [1] was solved by Thompson, Matsubara and Yang (TMY) [2] on a one-dimensional lattice. The model is composed of spinless fermions on a background of lattice gas atoms with nearest-neighbour atomic interactions and electronic hopping. It was found that, near the critical point ( $T \rightarrow 0^{+}$), the thermodynamic and cluster-size properties of the model were not affected by the presence of the fermions. However, properties of the model in higher dimensions are still unknown. This paper studies high-temperature series expansions for the problem on two-, three- and four-dimensional hypercubic lattices.

The model is defined by the Hamiltonian

$$
\begin{equation*}
\mathcal{H}=-J \sum_{\langle i j\rangle} \sigma_{i} \sigma_{j}-t \sum_{\langle i j\rangle} \sigma_{i} \sigma_{j}\left(a_{i}^{\dagger} a_{j}+a_{j}^{\dagger} a_{i}\right) \tag{1.1}
\end{equation*}
$$

where $\sigma_{i}=0,1$, represents the absence and presence of a lattice gas atom at site $i$, and $a_{i}$ ( $a_{i}^{\dagger}$ ) are fermion annihilation (creation) operators at site $i$. Equation (1.1) is defined on an $N$-site regular lattice and the other notations are standard.

The grand partition function is defined as

$$
\begin{align*}
Z_{\mathrm{G}} & =\operatorname{Tr} \exp \left[-\beta \mathcal{H}+\beta \mu_{l} \mathcal{N}_{i}+\beta \mu_{f} \mathcal{N}_{f}\right] \\
& =\operatorname{Tr} \exp \left[\beta J \sum_{\langle i j\rangle} \sigma_{i} \sigma_{j}+\beta t \sum_{(i j\rangle} \sigma_{i} \sigma_{j}\left(a_{i}^{\dagger} a_{j}+a_{j}^{\dagger} a_{j}\right)+\beta \mu_{t} \sum_{i=1}^{N} \sigma_{i}+\beta \mu_{f} \sum_{i=1}^{N} n_{i}\right] \tag{1.2}
\end{align*}
$$

where $\mu_{l}$ and $\mu_{f}$ are the chemical potentials of a lattice gas atom and of a spinless fermion, respectively. $\mathcal{N}_{l} \equiv \sum_{i=1}^{N} \sigma_{i}$ and $\mathcal{N}_{f} \equiv \sum_{i=1}^{N} n_{i}$ are their respective total number operators, and $n_{i}=a_{i}^{\dagger} a_{i}$ is the fermion number operator at site $i$.

When (1.2) is expanded as a power series, each term can be associated with a unique graph. In this paper, (1.2) is expanded to order of $\beta^{10}$. The critical properties are obtained by analysing the derived susceptibility series.

## 2. High-temperature series expansions

Following our work on the strongly correlated Hubbard model [3-5] and the strongly correlated Falicov-Kimball model [6], we define

$$
\begin{equation*}
Z_{0} \equiv \operatorname{Tr} z_{l}^{\mathcal{N}_{i}} z_{f}^{\mathcal{N}_{f}}=\prod_{i=1}^{N} \sum_{\left\{\sigma_{l}=0,1\right\}} z_{l}^{\sigma_{l}} \prod_{j=1}^{N} \sum_{\left\{n_{j}=0,1\right\}} z_{f}^{n_{j}}=\left(1+z_{l}\right)^{N}\left(1+z_{f}\right)^{N} \tag{2.1}
\end{equation*}
$$

where $z_{l}=\mathrm{e}^{\beta \mu_{l}}$ and $z_{f}=\mathrm{e}^{\beta \mu_{f}}$ are the fugacities of a lattice gas atom and a fermion, respectively. The grand partition function $Z_{G}$ can then be written as

$$
\begin{equation*}
Z_{\mathrm{G}}=Z_{0}\left\langle\mathrm{e}^{\beta J \mathcal{H}_{0}}\right\rangle=Z_{0}\left[1+\sum_{n=1}^{\infty} \frac{(\beta J)^{n}}{n!}\left\langle\mathcal{H}_{0}^{n}\right\rangle\right] \tag{2.2}
\end{equation*}
$$

where

$$
\begin{equation*}
\langle A\rangle \equiv \frac{1}{Z_{0}} \operatorname{Tr} z_{f}^{N_{1}} z_{f}^{\mathcal{N}_{f}} A \tag{2.3}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathcal{H}_{0} \equiv \sum_{\langle i j\rangle}\left[1+\frac{t}{J}\left(a_{i}^{\dagger} a_{j}+a_{j}^{\dagger} a_{i}\right)\right] \sigma_{i} \sigma_{j} \tag{2.4}
\end{equation*}
$$

If we associate $\left\langle\sigma_{i} \sigma_{j}\right\rangle$ with a bond connecting the two nearest-neighbour sites $i$ and $j$, and associate $\left\langle\sigma_{i} \sigma_{j} a_{i}^{\dagger} a_{j}\right\rangle$ with a fermion walk from site $j$ to site $i$ along the bond, $\left\langle\mathcal{H}_{0}^{n}\right\rangle$ can be represented by fermion walks of up to $n$ steps on graphs of up to $n$ edges embedded in the lattice.

As far as the partition function is concerned, the relevant configurations are those which leave the state of the system unchanged. In the graphical representation, fermions must return to their initial position at the completion of the walk. This implies an equal number of fermion creation and annihilation operators at any lattice site. Using the anti-commutation relation of the fermions, and noting that the spin operators commute with each other and with the fermion operators, those operators which operate at the same lattice site can be brought together. If we also notice the fact that $\left\langle\sigma^{2}\right\rangle=\langle\sigma\rangle$ and $\left\langle n^{2}\right\rangle=\langle n\rangle$, the magnitude of the weight of a graph is composed of the following factors:

$$
\begin{align*}
& \langle\sigma\rangle=\frac{1}{\left(1+z_{l}\right)\left(1+z_{f}\right)} \sum_{\sigma=0, l} \sum_{n=0,1} \sigma z_{l}^{\sigma} z_{f}^{n}=\frac{z_{l}}{1+z_{l}} \equiv p_{l} \\
& \left\langle\sigma a^{\dagger} a\right\rangle=\frac{1}{\left(1+z_{l}\right)\left(1+z_{f}\right)} \sum_{\sigma=0,1} \sum_{n=0,1} \sigma n z_{l}^{\sigma} z_{f}^{n}=\frac{z_{l}}{1+z_{l}} \frac{z_{f}}{1+z_{f}} \equiv p_{l} p_{f}  \tag{2.5}\\
& \left\langle\sigma a a^{\dagger}\right\rangle=\frac{1}{\left(1+z_{l}\right)\left(1+z_{f}\right)} \sum_{\sigma=0,1} \sum_{n=0,1} \sigma(1-n) z_{l}^{\sigma} z_{f}^{n}=\frac{z_{l}}{1+z_{l}} \frac{1}{1+z_{f}} \equiv p_{l} q_{f} \\
& \quad=p_{l}\left(1-p_{f}\right) .
\end{align*}
$$

All graphs of up to $n$ edges contribute to $\left\langle\mathcal{H}_{0}^{n}\right\rangle$. The rules for calculating the weights can be summarized as follows.
(i) The power of $p_{l}$ is equal to the number of lattice sites a graph occupies.
(ii) The power of $p_{f}$ is equal to the number of fermions. All fermions must be moved and the initial fermion configuration must be restored at the completion of the walk.
(iii) The power of $q_{f}$ is equal to the number of lattice sites visited and left unoccupied by any fermions at the completion of the walk.
(iv) The power of $t / J$ is equal to the total number of step movements of the fermions.
(v) The sign of the weight is determined by the number of permutations of the fermion operators required to bring together the operators at the same lattice site.

For instance, on the square lattice, the three-site graph $\bullet-$ has six embeddings. For $\left\langle\mathcal{H}_{0}^{3}\right\rangle$ on this graph, there can be no more than one fermion. The fermion could initially be at either end of the graph with a two-step movement, or it could initially be at the middle site with two two-step movements. The weight of the graph can therefore be calculated as
$6 p_{l}^{3}\left[K_{3200}+\left(2 \times 1 K_{3211}+1 \times 2 K_{3211}\right)\left(\frac{t}{J}\right)^{2} p_{f} q_{f}\right]=36 p_{l}^{3}+72 p_{l}^{3}\left(\frac{t}{J}\right)^{2} p_{f} q_{f}$
where the combinatorial factor $K_{n m u v}$ is associated with $\left\langle\mathcal{H}_{0}^{n}\right\rangle$ on an $m$-edge graph with a $2 u$-step fermion movement which visited $v$ edges. It is calculated through

$$
\begin{align*}
& K_{n 100}=1 \\
& K_{n n 00}=n! \\
& K_{n m 00}=0 \quad \text { when } n<m \text { or } n, m<0 \text { or } n>0 \text { and } m=0 \\
& K_{n+1, m, 0,0}=m K_{n m 00}+m K_{n, m-1,0,0}  \tag{2.7}\\
& K_{n m u v}=C_{2 u}^{n} \sum_{i=m-v}^{\min (n-2 u, m)} C_{i-m+v}^{v} K_{n-2 u, i, 0,0} \text { when } u, v \neq 0
\end{align*}
$$

where $C_{j}^{i}=i!/(i-j)!j!$.
The grand-canonical potential per lattice site $g$ is the $N$-coefficient of the $Z_{G}$ expansion

$$
\begin{equation*}
g=-\frac{1}{N \beta} \ln Z_{\mathrm{G}}=\frac{1}{\beta} \ln \left(q_{l} q_{f}\right)-\frac{1}{\beta} \sum_{n=1}^{\infty} \frac{(\beta J)^{n}}{n!}\left\langle\mathcal{H}_{0}^{n}\right\rangle_{\mathrm{l}} \tag{2.8}
\end{equation*}
$$

where $\left\langle\mathcal{H}_{0}^{n}\right\rangle_{1}$ is the $N$-coefficient of $\left\langle\mathcal{H}_{0}^{n}\right\rangle$ and $q_{l}=1-p_{l}$.
For instance, the grand-canonical potential of the model on the square lattice is expanded as

$$
\begin{aligned}
g=\frac{1}{\beta} \ln \left(q_{l} q_{f}\right) & -\frac{1}{\beta}\left\{\frac{\beta J}{1!} 2 p_{l}^{2}+\frac{(\beta J)^{2}}{2!}\left[2 p_{l}^{2}+4 p_{l}^{2}\left(\frac{t}{J}\right)^{2} p_{f} q_{f}+12 p_{l}^{3}-14 p_{l}^{4}\right]\right. \\
& +\frac{(\beta J)^{3}}{3!}\left[2 p_{l}^{2}+12 p_{l}^{2}\left(\frac{t}{J}\right)^{2} p_{f} q_{f}+36 p_{l}^{3}+72 p_{l}^{3}\left(\frac{t}{J}\right)^{2} p_{f} q_{f}+90 p_{l}^{4}\right. \\
& \left.\left.-84 p_{l}^{4}\left(\frac{t}{J}\right)^{2} p_{f} q_{f}-360 p_{l}^{5}+232 p_{l}^{6}\right]\right\}+\mathrm{O}\left((\beta J)^{4}\right)
\end{aligned}
$$

$$
\begin{align*}
= & \frac{1}{\beta} \ln \left[\left(1-p_{l}\right)\left(1-p_{f}\right)\right] \\
& -\frac{p_{l}^{2}}{\beta}\left\{\frac{\beta J}{1!} \times 2+\frac{(\beta J)^{2}}{2!}\left[2+4\left(\frac{t}{J}\right)^{2} p_{f}-4\left(\frac{t}{J}\right)^{2} p_{f}^{2}+12 p_{l}-14 p_{l}^{2}\right]\right. \\
& +\frac{(\beta J)^{3}}{3!}\left[2+12\left(\frac{t}{J}\right)^{2} p_{f}-12\left(\frac{t}{J}\right)^{2} p_{f}^{2}+36 p_{l}+72 p_{l}\left(\frac{t}{J}\right)^{2} p_{f}\right. \\
& \left.\left.-72 p_{l}\left(\frac{t}{J}\right)^{2} p_{f}^{2}+90 p_{l}^{2}-84 p_{l}^{2}\left(\frac{t}{J}\right)^{2} p_{f}+84 p_{l}^{2}\left(\frac{t}{J}\right)^{2} p_{f}^{2}-360 p_{l}^{3}+232 p_{l}^{4}\right]\right\} \\
& +\mathrm{O}\left((\beta J)^{4}\right) . \tag{2.9}
\end{align*}
$$

In general, on hypercubic lattices, $g$ has the expansion form

$$
\begin{align*}
& g=\frac{1}{\beta} \ln \left[\left(1-p_{l}\right)\left(1-p_{f}\right)\right] \\
&-\frac{p_{l}^{2}}{\beta} \sum_{n=1}^{\infty} \frac{(\beta J)^{n}}{n!} \sum_{i=0}^{2 n-2} \sum_{j=0}^{\min [[n / 2][(2 n-i-2) / 2]]} \sum_{k=1-\delta_{0 j}}^{\min (2 j, i+2)} a_{i j k}^{(n)} p_{l}^{i}\left(\frac{t}{J}\right)^{2 j} p_{f}^{k} \tag{2.10}
\end{align*}
$$

where $[n / 2]$ is the integer part of $n / 2$ and $\delta_{i j}$ is the Kronecker delta.
On the square lattice, comparing (2.9) with (2.10), we have $a_{000}^{(1)}=2 ; a_{000}^{(2)}=2, a_{011}^{(2)}=4$, $a_{012}^{(2)}=-4, a_{100}^{(2)}=12, a_{200}^{(2)}=-14 ; a_{000}^{(3)}=2, a_{011}^{(3)}=12, a_{012}^{(3)}=-12, a_{100}^{(3)}=36, a_{111}^{(3)}=72$, $a_{112}^{(3)}=-72, a_{200}^{(3)}=90, a_{211}^{(3)}=-84, a_{212}^{(3)}=84, a_{300}^{(3)}=-360, a_{400}^{(3)}=232 \ldots$ The expansions are carried out to order of $\mathcal{H}_{0}^{10}$ on two-, three- and four-dimensional hypercubic lattices for general values of $t, \mu_{l}$ and $\mu_{f}$ and to order of $\mathcal{H}_{0}^{12}$ for $t=0 \dagger$.

Expansions of the thermodynamic quantities can be calculated using standard thermodynamic relations [7]. For instance, the lattice-gas and the fermion densities are calculated as

$$
\begin{align*}
& \rho_{l}=-\frac{\partial g}{\partial \mu_{l}}=-\frac{\partial g}{\partial p_{l}} \frac{\partial p_{l}}{\partial \mu_{l}}=-\beta p_{l}\left(1-p_{l}\right) \frac{\partial g}{\partial p_{l}} \\
& \rho_{f}=-\frac{\partial g}{\partial \mu_{f}}=-\frac{\partial g}{\partial p_{f}} \frac{\partial p_{f}}{\partial \mu_{f}}=-\beta p_{f}\left(1-p_{f}\right) \frac{\partial g}{\partial p_{f}} \tag{2.11}
\end{align*}
$$

It is easily proved using the particle-hole symmetry properties for lattice gas atoms and for the fermions that

$$
\begin{array}{ll}
\rho_{l}=\frac{1}{2} & \text { when } t=0 \text { and } \mu_{I}=-d J \\
\rho_{f}=\frac{1}{2} & \text { when } \mu_{f}=0 . \tag{2.12}
\end{array}
$$

Our high-temperature series-expansion data are consistent with (2.12).
The critical behaviour is obtained by analysing the susceptibility series. In particular, the lattice-gas susceptibility has the same critical behaviour as the isothermal compressibility and is given by
$\chi_{l}=-\frac{\partial^{2} g}{\partial \mu_{l}^{2}}=-\beta^{2} p_{l}\left(1-p_{l}\right)\left[\left(1-2 p_{l}\right) \frac{\partial g}{\partial p_{l}}+p_{l}\left(1-p_{l}\right) \frac{\partial^{2} g}{\partial p_{l}^{2}}\right]$

[^0]\[

$$
\begin{align*}
= & \beta p_{l}\left(1-p_{l}\right)+\beta p_{l}^{2}\left(1-p_{l}\right) \sum_{n=1}^{\infty} \frac{(\beta J)^{n}}{n!} \sum_{i=0}^{2 n-2} \sum_{j=0}^{\min \{[n / 2],[(2 n-i-2) / 2]\}} \\
& \times \sum_{k=1-\delta_{0 j}}^{\min \left(2 j_{j} i+2\right)}\left[(i+2)\left(1-2 p_{l}\right)+(i+2)(i+1)\left(1-p_{l}\right)\right] a_{i j k}^{(n)} p_{l}^{i}\left(\frac{t}{J}\right)^{2 j} p_{f}^{k} . \tag{2.13}
\end{align*}
$$
\]

Without loss of generality, in the following an arbitrary unit of energy is chosen so that $J=1$. The susceptibility in (2.13) can then be expanded as a power series in $\beta, \mu_{l}, t$ and $\mu_{f}$. Explicitly, we have

$$
\begin{equation*}
\chi_{l}=\beta \sum_{n=0}^{\infty} \beta^{n} \sum_{i=0}^{n} \sum_{j=0}^{[(n-i) / 2]} \sum_{k=0}^{(n-i-2 j)\left(1-\delta_{j 0}\right)} u_{i j k}^{(n)} \mu_{l}^{i} t^{2 j} \mu_{f}^{k} \tag{2.14}
\end{equation*}
$$

For example, we have on the square lattice that $u_{000}^{(0)}=\frac{1}{4}, u_{000}^{(1)}=\frac{1}{4}, u_{100}^{(1)}=0, u_{000}^{(2)}=-\frac{1}{16}$, $u_{010}^{(2)}=\frac{1}{16}, u_{100}^{(2)}=-\frac{1}{4}, u_{200}^{(2)}=-\frac{1}{16}, u_{000}^{(3)}=-\frac{83}{96}, u_{010}^{(3)}=-\frac{1}{32}, u_{011}^{(3)}=0, u_{100}^{(3)}=-1$, $u_{110}^{(3)}=-\frac{1}{16}, u_{200}^{(3)}=-\frac{1}{4}, u_{300}^{(3)}=0, \ldots$. Higher-order exansion coefficients can be derived from the expansion coefficients for the grand-canonical potential given in the appendix.

## 3. Series analysis

From the lattice-gas-Ising-model equivalence, it follows that, when $t=0$, there is only one value for $\mu_{l}(=-d J)$ at which the system goes critical. The model with the above parameter values corresponds to the Ising model in a zero external field. It is easily seen from the last section that, when $t=0$, the critical behaviour is independent of the fermion chemical potential $\mu_{f}$ or fermion density $\rho_{f}$. This suggests that the model with $t=0$, $\mu_{l}=-d J\left(\rho_{l}=\frac{1}{2}\right)$ for any value of $\mu_{f}\left(\rho_{f}\right)$ should have the Ising critical behaviour.

When $t=0$, the relevant expansion coefficients for $g$ are $a_{i 00}^{(n)}$. Two extra terms are obtained for those coefficients to order $n=12$. Standard methods [8] for series analysis are applied to the series. The results compare favourably with the known values for the Ising model in two and three dimensions. The value of $\gamma$ is known to be $\frac{7}{4}$ exactly [9] in two dimensions and $1.2390 \pm 0.0025$ in three dimensions $[8,10,11]$.

The upper critical dimension of the Ising model is 4 . Therefore, it is expected that $\gamma=1$ in four dimensions. However, the numerical analysis indicates a higher value. It is often the case that logarithmic corrections occur at the critical dimension [12]. The logarithmic correction terms will account for the apparent inaccuracy of the Pade analysis in four dimensions.

It is observed numerically from our high-temperature series expansions that

$$
\begin{equation*}
\left.\frac{\partial \chi_{l}}{\partial \mu_{l}}\right|_{\mu_{l}=-d, t=0}=0 \quad \text { for any } \beta \text { and } \mu_{f} \tag{3.1}
\end{equation*}
$$

Equation (3.1) is confirmed on two-, three- and four-dimensional hypercubic lattices to order of $\beta^{13}$, which is the highest order of our expansion. From (2.14), equation (3.1) is equivalent to

$$
\begin{equation*}
\sum_{i=0}^{n} i u_{i 00}^{(n)}(-d)^{i-1}=0 \quad \text { for } \quad 0 \leqslant n \tag{3.2}
\end{equation*}
$$



Figure 1. The lattice-gas chemical potential $\mu_{\max }$ at which $\chi_{1}$ is a maximum, calculated with $\chi_{1}$ expanded to order of $\beta^{11}(n=10)$ and for $\mu_{f}=0:(a)$ on the square lattice; $(b)$ on the simple cubic lattice; ( $c$ ) on the four-dimensional hypercubic lattice.

It is also established numerically that, for any fixed $\beta$ and $t=0, \chi_{l}$ takes its maximum value at $\mu_{l}=-d$.

Therefore, when $t=0$, the critical behaviour of the system can be determined by first finding the value of $\mu_{l}=\mu_{\max }$ at which $\chi_{l}$ takes its maximum value with fixed temperature, then analysing $\chi_{l}$ as a power series in $\beta$ at $\mu_{l}=\mu_{\max }$.

When $t \neq 0$, it is not expected that a similar exact relation exists. One needs to analyse a true multi-variable series to determine the critical behaviour of the system. Unfortunately, there is not a generally accepted reliable method. The partial differential approximation (PDA) method [8] might be of possible assistance but the authors were unable to apply it to the present series.

When $t \neq 0$, in a wide temperature range ( $\beta \geqslant \beta_{\mathrm{c}}$ ), for fixed $\beta, t$ and $\mu_{f}$, the value


Figure 2. The lattice-gas chemical potential $\mu_{\max }$ at which $\chi_{1}$ is a maximum, calculated with $\chi_{1}$ expanded to order of $\beta^{11}(n=10)$ and for $\mu_{\mathrm{f}}=1:(a)$ on the square lattice; $(b)$ on the simple cubic lattice; (c) on the four-dimensional hypercubic lattice.
of $\mu_{l}=\mu_{\max }$ at which $\chi_{l}$ takes its maximum is insensitive to the actual value of the temperature, as shown in figures 1 and 2 . From the figures, it is seen that $\mu_{\max }$ changes by a few per cent when $\beta$ changes by an order of magnitude. On the other hand, the value of $\chi_{l}$ changes rapidly with $\beta$.

From the above discussions and by analogy with the pure lattice gas or $t=0$ case, it is conjectured that for each value of $t>0$ and $\mu_{f}>0$, there is only one value for $\mu_{I}$ at which the system goes critical. Therefore, by fixing values for $t$ and $\mu_{f}$, the problem reduces to a two-variable series. Regarding $t$ and $\mu_{f}$ as parameters, (2.14) can be rewritten as

$$
\begin{equation*}
\chi_{l}=\beta \sum_{n=0}^{\infty} \sum_{i=0}^{n} U_{n i}\left(J=1, t, \mu_{f}\right) \beta^{n} \mu_{l}^{i} \tag{3.3}
\end{equation*}
$$



Figure 3. $\mu_{1}^{(c)}(n)$ versus $1 / n$ for $\mu_{\mathrm{f}}=0$ and various values of $t$. The values of $\beta$ are best estimates from the self-consistent method discussed in the text. $\mu_{i}^{(c)}$ values are extrapolated with straight lines which agree most closely with the large $n(n \geqslant 5)$ portions of the curves. (a) On the square lattice. (b) On the simple cubic lattice. (c) On the four-dimensional hypercubic lattice.
where

$$
\begin{equation*}
U_{n i}=\sum_{j=0}^{[(n-i) / 2]} \sum_{k=0}^{(n-i-2 j)\left(1-\delta_{j 0}\right)} u_{i j k}^{(n)} t^{2 j} \mu_{f}^{k} . \tag{3.4}
\end{equation*}
$$

It is assumed that $\chi_{t}$ behaves near the critical point as

$$
\begin{equation*}
\chi_{l} \sim\left[\beta_{\mathrm{c}}\left(\mu_{l}^{(c)}, t, \mu_{f}\right)-\beta\right]^{-\gamma\left(\mu_{l}^{(c)}, t, \mu_{f}\right)} \tag{3.5}
\end{equation*}
$$

where $\mu_{l}^{(c)}\left(t, \mu_{f}\right)$ is the value of $\mu_{l}$ at which the system goes critical.
The critical behaviour of the system is obtained self-consistently as follows.


Figure 4. $\beta_{c}$ versus $1 / n$ for $\mu_{\mathrm{f}}=0$ and various values of $t$. The values of $\mu_{\mathrm{i}}$ are best estimates from the self-consistent method discussed in the text. $\beta_{c}$ values are extrapolated with straight lines which agree most closely with the large $n$ ( $n \geqslant 5$ ) portions of the curves. (a) On the square lattice. (b) On the simple cubic lattice. (c) On the four-dimensional hypercubic lattice.
(i) For a given value of $t$ and $\mu_{f}$, choose a value $\beta \simeq \beta_{c}$.
(ii) Calculate $\mu_{\max }^{(n)}$ as discussed previously for $n<N$, where $N$ is the highest order of expansion, then extrapolate graphically to $n \rightarrow \infty$ to get $\mu_{l}^{(c)}$ (cf figure 3).
(iii) Analyse $\chi_{l}$ as a power series of $\beta$ using a ratio method with $\mu_{l}=\mu_{l}^{(c)}$. Specifically, $\beta_{c}^{(n)}$ is calculated as

$$
\begin{equation*}
\beta_{c}^{(n)}=\frac{\sum_{i=0}^{n-1} U_{n-1, i} \mu_{l}^{i}}{\sum_{i=0}^{n} U_{n, i} \mu_{l}^{i}} \quad n \geqslant 1 . \tag{3.6}
\end{equation*}
$$

The extrapolation $\beta_{\mathrm{c}}^{(n)}$ to $n \rightarrow \infty$ is shown in figure 4, where $\beta_{\mathrm{c}} \equiv \beta_{\mathrm{c}}^{(\infty)}$.
(iv) Compare the $\beta_{\mathrm{c}}$ with the chosen value of $\beta$ in step (i). If they are different, set $\beta=\beta_{\mathrm{c}}$ and repeat.

It is also observed that $\beta_{\mathrm{c}}$ is not sensitive to small changes of $\mu_{i}$. The weak correlation between $\mu_{l}^{(c)}$ and $\beta_{c}$ permits a relatively accurate estimate of critical parameters. Results for various values of $\mu_{f}$ and $t$ are listed in table 1 .

For the pure lattice-gas case, $\beta_{\mathrm{c}}$ is inversely proportional to $J$ and $\mu_{l}^{(c)}$ is proportional to $J$. Consequently $\beta_{c} \mu_{l}^{(c)}$ is a quantity independent of $J$. Since $t$ and $\mu_{f}$ in essence produce an effective lattice-gas interaction, we would then expect the quantity $\beta_{\mathrm{c}} \mu_{l}^{(c)}$ to be weakly dependent on $t$ and $\mu_{f}$. This quantity is also listed in table 1. It is tentatively concluded that $-\beta_{c} \mu_{l}^{(c)}=3.53,2.66$ and 2.40 on two-, three- and four-dimensional hypercubic lattices for small values of $t$. When $t$ is larger, the value of $-\beta_{c} \mu_{l}^{(c)}$ tends to become larger.

Having determined the value $\mu_{l}^{(c)}$, the series (3.3) becomes an ordinary single variable power series. The critical exponent as defined in (3.5) is then determined using the standard Dlog Padé method [8]. The Pade method gives estimates of both $\beta_{c}$ and $\gamma$. The estimated $\beta_{\mathrm{c}}$ from the Pade method is compared with the previous estimate for further fine corrections. The series is also analysed using the ratio method and the results are consistent with the Padé estimate but with a larger error bar. Physical singularities from the Pade analysis are listed in tables 2 and 3 and the results for $\gamma$ are summarized in table 1 .

Table 1. Summary of the critical parameters.

| $\mu_{\mathrm{f}}$ | $d$ | $t$ | $\beta_{\mathrm{c}}$ | $\mu_{1}^{(c)}$ | $-\beta_{\mathrm{c}} \mu_{1}^{(c)}$ | $\gamma$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 2 | 0.0 | 1.763 (exact) | -2 (exact) | 3.526 (exact) | 1.75 (exact) |
|  |  | 0.2 | $1.73 \pm 0.02$ | $-2.030 \pm 0.005$ | $3.51 \pm 0.04$ | $1.75 \pm 0.05$ |
|  |  | 0.4 | $1.69 \pm 0.03$ | $-2.11 \pm 0.01$ | $3.57 \pm 0.06$ | $1.75 \pm 0.1$ |
|  |  | 0.6 | $1.67 \pm 0.05$ | $-2.225 \pm 0.01$ | $3.72 \pm 0.11$ | $1.75 \pm 0.1$ |
|  | 3 | 0.0 | $0.887 \pm 0.001^{1}$ | -3 (exact) | $2.661 \pm 0.003$ | $1.252 \pm 0.003^{\dagger}$ |
|  |  | 0.2 | $0.875 \pm 0.01$ | $-3.025 \pm 0.005$ | $2.65 \pm 0.03$ | $1.25 \pm 0.01$ |
|  |  | 0.4 | $0.86 \pm 0.01$ | $-3.09 \pm 0.01$ | $2.66 \pm 0.03$ | $1.25 \pm 0.01$ |
|  |  | 0.6 | $0.835 \pm 0.01$ | $-3.19 \pm 0.01$ | $2.66 \pm 0.03$ | $1.22 \pm 0.07$ |
|  |  | 0.8 | 0.82 $\pm 0.02$ | $-3.325 \pm 0.01$ | $2.73 \pm 0.07$ | $1.24 \pm 0.05$ |
|  |  | 1.0 | $0.80 \pm 0.03$ | $-3.465 \pm 0.02$ | $2.8 \pm 0.1$ | $1.22 \pm 0.08$ |
|  | 4 | 0.0 | $0.6000 \pm 0.0002$ | -4 (exact) | $2.4000 \pm 0.0008$ | $1.105 \pm 0.003{ }^{\dagger}$ |
|  |  | 0.2 | $0.5965 \pm 0.0005$ | $-4.020 \pm 0.005$ | $2.398 \pm 0.008$ | $1.105 \pm 0.005$ |
|  |  | 0.4 | $0.587 \pm 0.002$ | $-4.08 \pm 0.01$ | $2.395 \pm 0.008$ | $1.08 \pm 0.02$ |
|  |  | 0.6 | $0.573 \pm 0.002$ | $-4.18 \pm 0.01$ | $2.395 \pm 0.008$ | $1.10 \pm 0.02$ |
|  |  | 0.8 | $0.560 \pm 0.004$ | $-4.31 \pm 0.01$ | $2.41 \pm 0.02$ | $1.10 \pm 0.02$ |
|  |  | 1.0 | $0.548 \pm 0.005$ | $-4.46 \pm 0.02$ | $2.44 \pm 0.03$ | $1.08 \pm 0.02$ |
| 1 | 2 | 0.2 | $1.74 \pm 0.02$ | $-2.022 \pm 0.002$ | $3.52 \pm 0.04$ | $1.7 \pm 0.1$ |
|  |  | 0.4 | $1.70 \pm 0.04$ | $-2.083 \pm 0.005$ | $3.54 \pm 0.08$ | $1.7 \pm 0.1$ |
|  | 3 | 0.2 | $0.88 \pm 0.01$ | $-3.020 \pm 0.005$ | $2.66 \pm 0.03$ | $1.24 \pm 0.01$ |
|  |  | 0.4 | $0.865 \pm 0.01$ | $-3.085 \pm 0.01$ | $2.67 \pm 0.03$ | $1.25 \pm 0.02$ |
|  |  | 0.6 | $0.845 \pm 0.01$ | $-3.18 \pm 0.01$ | $2.69 \pm 0.03$ | $1.25 \pm 0.02$ |
|  |  | 0.8 | $0.82 \pm 0.02$ | $-3.30 \pm 0.02$ | $2.71 \pm 0.07$ | $1.27 \pm 0.03$ |
|  |  | 1.0 | $0.795 \pm 0.03$ | $-3.43 \pm 0.02$ | $2.73 \pm 0.1$ | $1.2 \pm 0.1$ |
|  | 4 | 0.2 | $0.596 \pm 0.002$ | $-4.020 \pm 0.005$ | $2.396 \pm 0.008$ | $1.11 \pm 0.01$ |
|  |  | 0.4 | $0.588 \pm 0.002$ | $-4.08 \pm 0.01$ | $2.399 \pm 0.008$ | $1.10 \pm 0.01$ |
|  |  | 0.6 | $0.575 \pm 0.003$ | $-4.17 \pm 0.01$ | $2.40 \pm 0.01$ | $1.10 \pm 0.01$ |
|  |  | 0.8 | $0.561 \pm 0.004$ | $-4.29 \pm 0.01$ | $2.41 \pm 0.01$ | $1.10 \pm 0.02$ |
|  |  | 1.0 | $0.55 \pm 0.01$ | -4.44 $\pm 0.03$ | $2.44 \pm 0.04$ | $1.10 \pm 0.03$ |

[^1]Table 2. Pade analysis of the inverse compressibility series on two-, three- and four-dimensional lattices for $\mu_{\mathrm{f}}=0, \mu_{1}=\mu_{1}^{(c)}$. In the table, $D$ and $N$ denote the order of the denominator and numerator of the Padé approximants. $\beta_{\mathrm{c}}^{*}$ is the real pole closest to the origin and $\gamma^{*}$ is the corresponding residue.

| $t$ | $N / D$ | 2D |  | 3D |  | 4D |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\beta_{c}^{*}$ | $\gamma^{*}$ | $\beta_{\mathrm{c}}^{*}$ | $\gamma^{*}$ | $\beta_{\mathrm{c}}^{*}$ | $\gamma^{*}$ |
| 0.2 | 2/3 | 1.7493 | 1.7855 | 0.8777 | 1.2420 | 0.5970 | 1.1111 |
|  | $3 / 3$ | 1.7008 | 1.5470 | 0.8718 | 1.2348 | 0.5940 | 1.0425 |
|  | 4/3 | 1.7161 | 1.6330 | 0.8808 | 1.2623 | 0.5966 | 1.1066 |
|  | 2/4 | 1.7176 | 1.6468 | 0.8723 | 1.2341 | 0.5960 | 1.0979 |
|  | 3/4 | 1.7263 | 1.6913 | 0.8789 | 1.2478 | 0.5966 | 1.1062 |
|  | 4/4 | 1.7411 | 1.7793 | 0.8800 | 1.2554 | 0.5963 | 1.1026 |
|  | 2/5 | 1.7358 | 1.7540 | 0.8807 | 1.2624 | 0.5966 | 1.1065 |
|  | 3/5 | Nil | Nil | 0.8800 | 1.2555 | 0.5964 | 1.1036 |
|  | 2/6 | 1.7497 | 1.8604 | 0.8739 | 1.1611 | 0.5968 | 1.1084 |
| 0.4 | 2/3 | 1.7312 | 1.8919 | 0.8614 | 1.2540 | 0.5840 | 1.0589 |
|  | 3/3 | 1.5933 | 1.1747 | 0.8607 | 1.2492 | 0.5846 | 1.0691 |
|  | 4/3 | 1.6575 | 1.5327 | 0.8610 | 1.2510 | 0.5867 | 1.1008 |
|  | 2/4 | 1.6691 | 1.6112 | 0.8608 | 1.2495 | 0.5846 | 1.0691 |
|  | 3/4 | 1.6814 | 1.6752 | 0.8628 | 1.2555 | 0.5840 | 1.0579 |
|  | 4/4 | 1.6906 | 1.7310 | 0.8622 | 1.2556 | 0.5866 | 1.0990 |
|  | $2 / 5$ | 1.6884 | 1.7208 | 0.8608 | 1.2499 | 0.5868 | 1.1011 |
|  | 3/5 | 1.7085 | 1.8969 | 0.8622 | 1.2556 | 0.5866 | 1.0992 |
|  | 2/6 | 1.6993 | 1.8019 | 0.8647 | 1.2541 | 0.5869 | 1.1023 |
| 0.6 | 2/3 | 1.7665 | 2.1053 | 0.8445 | 1.2851 | 0.5798 | 1.1455 |
|  | $3 / 3$ | 1.6647 | 1.6405 | 0.8258 | 1.1459 | 0.5699 | 1.0479 |
|  | 4/3 | 1.7267 | 1.9940 | 0.8302 | 1.1835 | 0.5727 | 1.0821 |
|  | 2/4 | 1.6910 | 1.7781 | 0.8301 | 1.1863 | 0.5712 | 1.0650 |
|  | 3/4 | 1.7021 | 1.8329 | 0.8351 | 1.2274 | 0.5746 | 1.1054 |
|  | 4/4 | Nil | Nii | 0.8341 | 1.2180 | 0.5736 | 1.0927 |
|  | 2/5 | 1.7045 | 1.8476 | 0.8262 | 1.1602 | 0.5729 | 1.0844 |
|  | 3/5 | 1.6873 | 1.7644 | 0.8342 | 1.2189 | 0.5737 | 1.0938 |
|  | 2/6 | 1.8140 | 2.8739 | 0.8394 | 1.2818 | 0.5747 | 1.1106 |
| 0.8 | 2/3 |  |  | 0.8349 | 1.3401 | 0.5702 | 1.1728 |
|  | $3 / 3$ |  |  | 0.8085 | 1.1693 | 0.5568 | 1.0532 |
|  | 4/3 |  |  | 0.8225 | 1.2864 | 0.5711 | 1.2459 |
|  | 2/4 |  |  | 0.8130 | 1.2047 | 0.5588 | 1.0759 |
|  | 3/4 |  |  | 0.8168 | 1.2327 | 0.5612 | 1.1007 |
|  | 4/4 |  |  | 0.8181 | 1.2444 | 0.5603 | 1.0903 |
|  | 2/5 |  |  | 0.8180 | 1.2430 | 0.5627 | 1.1197 |
|  | 3/5 |  |  | 0.8185 | 1.2478 | 0.5605 | 1.0920 |
|  | 2/6 |  |  | 0.8184 | 1.2473 | 0.5590 | 1.0725 |
| 1.0 | $2 / 3$ |  |  | 0.8204 | 1.3710 | 0.5611 | 1.1997 |
|  | 3/3 |  |  | 0.7903 | 1.1896 | 0.5455 | 1.0688 |
|  | 4/3 |  |  | 0.7864 | 1.1605 | 0.5478 | 1.0937 |
|  | 2/4 |  |  | 0.7943 | 1.1218 | 0.5475 | 1.0895 |
|  | 3/4 |  |  | 0.7858 | 1.1550 | 0.5475 | 1.0894 |
|  | 4/4 |  |  | 0.7895 | 1.1841 | 0.5482 | 1.0980 |
|  | $2 / 5$ |  |  | 0.7881 | 1.1755 | 0.5475 | 1.0894 |
|  | 3/5 |  |  | 0.7917 | 1.2022 | 0.5475 | 1.0895 |
|  | 2/6 |  |  | 0.7976 | 1.2592 | 0.5480 | 1.0957 |

Results in table 1 indicate that the critical exponent is not affected by the electrons, while the critical temperature, as expected, is dependent on the electronic parameters. The

Table 3. Padé analysis of the inverse compressibility series on two-, three- and four-dimensional lattices for $\mu_{f}=1, \mu_{i}=\mu_{1}^{(c)}$. In the table, $D$ and $N$ denote the order of the denominator and numerator of the Pade approximants. $\beta_{c}^{*}$ is the real pole closest to the origin and $\gamma^{*}$ is the corresponding residue.

|  | $N / D$ | 2D |  | 3D |  | 4D |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $t$ |  | $\beta_{c}^{*}$ | $\gamma^{*}$ | $\beta_{\mathrm{c}}^{*}$ | $\gamma^{*}$ | $\beta_{\mathrm{c}}^{*}$ | $\gamma^{*}$ |
| 0.2 | 2/3 | 1.7776 | 1.7855 | 0.8796 | 1.2483 | 0.5973 | 1.1106 |
|  | 3/3 | 1.6158 | 1.5470 | 0.8797 | 1,2484 | 0.5941 | 1.0535 |
|  | 4/3 | 1.7034 | 1.6330 | 0.8814 | 1.2584 | 0.5969 | 1.1065 |
|  | 2/4 | 1.7044 | 1.6468 | 0.8797 | 1.2484 | 0.5954 | 1.0829 |
|  | 3/4 | 1.7340 | 1.6913 | 0.8796 | 1.2483 | 0.5968 | 1.1053 |
|  | 4/4 | 1.7539 | 1.7793 | 0.8810 | 1.2552 | 0.5967 | 1.1047 |
|  | 2/5 | Nil | Nii | 0.8814 | 1.2584 | 0.5969 | 1.1066 |
|  | $3 / 5$ | 1.7765 | 1.7793 | 0.8810 | 1.2552 | 0.5967 | 1.1047 |
|  | 2/6 | Nil | Nil | 0.8750 | 1.1413 | 0.5969 | 1.1070 |
| 0.4 | 2/3 | 1.7785 | 1.9720 | 0.8690 | 1.2771 | 0.5940 | 1.1463 |
|  | 3/3 | 1.3876 | 0.5580 | 0.8506 | 1.1244 | 0.5836 | 1.0458 |
|  | 4/3 | 1.4243 | 0.6539 | 0.8611 | 1.2242 | 0.5875 | 1.0985 |
|  | 2/4 | 1,6058 | 1.3453 | 0.8555 | 1.1777 | 0.5840 | 1.0519 |
|  | 3/4 | 1.6940 | 1.6831 | 0.8646 | 1.2526 | 0.5900 | 1.1258 |
|  | 4/4 | 1.7198 | 1.8040 | 0.8649 | 1.2554 | 0.5880 | 1.1045 |
|  | 2/5 | Nil | Nil | 0.8608 | 1.2218 | 0.5876 | 1.0995 |
|  | 3/5 | 1.7276 | 1.8519 | 0.8649 | 1.2554 | 0.5880 | 1.1050 |
|  | $2 / 6$ | 1.6583 | 1.4622 | 0.8957 | 1.9849 | 0.5897 | 1.1376 |
| 0.6 | 2/3 |  |  | 0.8564 | 1.3206 | 0.5828 | 1.1585 |
|  | 3/3 |  |  | 0.8195 | 1.0777 | 0.5689 | 1.0296 |
|  | 4/3 |  |  | 0.7912 | 0.8914 | 0.5706 | 1.0485 |
|  | 2/4 |  |  | 0.8290 | 1.1530 | 0.5711 | 1.0570 |
|  | 3/4 |  |  | 0.8429 | 1.2491 | 0.5765 | 1.1128 |
|  | 4/4 |  |  | 0.8436 | 1.2544 | 0.5753 | 1.0996 |
|  | 2/5 |  |  | Nil | Nil | 0.5693 | 1.0395 |
|  | 3/5 |  |  | 0.8436 | 1.2545 | 0.5753 | 1.1005 |
|  | 2/6 |  |  | 0.8303 | 1.1407 | 0.5671 | 1.0246 |
| 0.8 | 2/3 |  |  | 0.8417 | 1.3563 | 0.5726 | 1.1828 |
|  | 3/3 |  |  | 0.8025 | 1.1273 | 0.5556 | 1.0402 |
|  | 4/3 |  |  | 0.8357 | 1.3762 | 0.5701 | 1.2029 |
|  | 2/4 |  |  | 0.8092 | 1.1739 | 0.5582 | 1.0671 |
|  | 3/4 |  |  | 0.8202 | 1.2447 | 0.5623 | 1.1063 |
|  | 4/4 |  |  | 0.8226 | 1.2631 | 0.5612 | 1.0946 |
|  | 2/5 |  |  | 0.8277 | 1.3081 | 0.5650 | 1.1385 |
|  | 3/5 |  |  | 0.8228 | 1.2652 | 0.5613 | 1.0958 |
|  | 2/6 |  |  | 0.8215 | 1.2529 | 0.5592 | 1.0694 |
| 1.0 | 2/3 |  |  | 0.8203 | 1.3621 | 0.5629 | 1.2044 |
|  | 3/3 |  |  | 0.7845 | 1.1165 | 0.5452 | 1.0636 |
|  | 4/3 |  |  | 0.7924 | 1.2189 | 0.5508 | 1.1199 |
|  | 2/4 |  |  | 0.7889 | 1.1935 | 0.5473 | 1.0844 |
|  | 3/4 |  |  | 0.7911 | 1.2078 | 0.5494 | 1.1037 |
|  | 4/4 |  |  | 0.7652 | 1.1377 | 0.5494 | 1.1036 |
|  | 2/5 |  |  | 0.7913 | 1.2094 | 0.5498 | 1.1082 |
|  | 3/5 |  |  | 0.7881 | 1.1901 | 0.5494 | 1.1036 |
|  | 2/6 |  |  | 0.8026 | 1.3087 | 0.5493 | 1.1027 |

higher $\gamma$ value than the mean-field value of 1 for $t \neq 0$ is almost certainly caused by the logarithmic correction terms, as discussed previously.

## 4. Summary

A lattice model for liquid metals proposed by Nara, Ogawa and Matsubara is studied using exact high-temperature series expansions. The grand-canonical potential is expanded to order $\beta^{8}$ on two-, three- and four-dimensional lattices exactly. Thermodynamic quantities are calculated from the grand-canonical potential using the usual thermodynamic relations. In particular, the lattice-gas susceptibility series is calculated exactly to order $\beta^{10}$.

Our series data satisfy the relation that, when the fermion hopping energy $t=0$ and the lattice-gas chemical potential $\mu_{l}=-d J$, where $J$ is the nearest-neighbour atomic interaction for the lattice gas and $d$ is the dimensionality, the lattice-gas atomic density $\rho_{l}$ is $\frac{1}{2}$. Our series data are also consistent with the relation that when the fermion chemical potential $\mu_{f}=0$, the fermion density $\rho_{f}$ is $\frac{1}{2}$.

When the fermion hopping energy $t$ is zero, the critical behaviour is independent of the fermion chemical potential $\mu_{f}$. In this case, the system goes critical only at a single value for the lattice-gas atomic chemical potential $\mu_{i}=-d J$. The susceptibility takes its maximum value as a function of $\beta$ at this value of the lattice-gas chemical potential.

For fixed positive values of the fermion hopping energy and the fermion chemical potential, it is conjectured that the system also goes critical at a single value of the latticegas chemical potential. The critical value of the lattice-gas chemical potential is taken to be the value at which the susceptibility takes its maximum as a function of $\beta$. When $t>0$, this value is weakly dependent on estimates of the critical temperature. The values of $\mu_{l}^{(c)}$ and $\beta_{c}$ are estimated self-consistently. It is observed that when $t$ or $\mu_{f}$ increase, $\chi_{l}^{(c)}$ decreases and that $\mu_{l}^{(c)}$ has a very weak dependence on the fermion chemical potential. The values of $-\beta_{c} \mu_{l}^{(c)}$ are almost constant and depend only on the dimensionality. For small $t$, the values are $3.53,2.66$ and 2.40 for two w, three- and four-dimensional lattices, respectively.

The critical exponent of the susceptibility is calculated using a self-consistent Pade analysis. It is found that the critical exponent is independent of the values of $t$ and $\mu_{f}$, and is estimated to be $1.75,1.25$ and 1.10 on two-, three- and four-dimensional lattices, respectively, in accordance with the corresponding values for the pure lattice-gas. For the lattice-gas model, the upper critical dimension is 4 . Therefore, the susceptibility exponent should be exactly 1 . The higher value of the numerical estimate is presumably due to logarithmic correction terms which normally appear at critical dimensions.

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[^0]:    $\dagger$ The additional expansion coefficients are available at the British Library, reference number SUP 70052.

[^1]:    $\dagger$ Value obtained by analysing of the lattice-gas compressibility expansion to order of $\beta^{13}(n=12)$.

