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# Fluid–solid transitions of the lattice gases

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Received 6 August 1974

**Abstract.** Phase transitions of the soft-core lattice gas (finite repulsion at the first neighbour), and of the hard-core lattice gas (infinite repulsion at the first neighbour) with finite attraction at the second neighbour, are treated in the Bethe approximation (exact solution of infinite Bethe lattices). In the former two second-order transitions of fluid  $\rightarrow$  solid  $\rightarrow$  fluid and the phenomena of the melting point maximum are found. In the latter second- and first-order transitions of fluid (gas)  $\rightarrow$  solid are found above and below the tricritical point, respectively. The gas–liquid transition is masked by the gas–solid transition and is not realized.

## 1. Introduction

The phase transition between gaseous and liquid phases is understood by analogy with the ferromagnetic transition, and that between fluid and solid phases with the anti-ferromagnetic transition. As for the hard-core lattice gas (Temperley 1959, 1961, Burley 1960, 1972, Runnels 1972) results of closed-form approximations give a second- or first-order fluid–solid transition. Such a fluid–solid transition is also suggested from the results of numerical experiments (Alder and Wainwright 1962), using the method of the eigenvalue problem (Runnels and Combs 1966, Runnels *et al* 1970), and the series expansion method (Gaunt and Fisher 1965). The effect of attraction in the hard-core lattice gas is also discussed (Orban *et al* 1968, Runnels *et al* 1970).

In this paper, firstly, the soft-core lattice gas (first neighbour finite repulsion), and secondly, the hard-core lattice gas (first neighbour infinite repulsion) with second neighbour interaction, are discussed in the Bethe approximation (an exact solution of the infinite Bethe lattice, Katsura and Takizawa 1974). In the former, two second-order transitions (fluid phase  $\rightarrow$  solid phase  $\rightarrow$  fluid phase) and the phenomena of the melting point maximum, which are not realized in the hard-core lattice gas, are observed. In the latter, the gas–solid transition is second- and first-order, above and below the tricritical point, respectively. The gas–liquid transition is masked by the gas–solid transition.

## 2. Soft-core lattice gas

In this section we consider the fluid–solid transition of the soft-core lattice gas. The first-neighbour interaction is denoted by  $-2J_1$ . Positive and negative  $J_1$  refer to attraction and repulsion, respectively, and the latter is the case for a soft-core lattice gas. The model is treated by the Bethe approximation. In the case of repulsion, the possibility of a disordered phase (fluid phase) and that of an ordered phase (solid phase) is taken

into account, and the lattice is divided into  $\alpha$  and  $\beta$  sublattices. The result for the Bethe lattice (Katsura and Takizawa 1974, to be referred to as KT) is applied.

Let

$$x = e^{-J_1/kT},$$

$$u_{\alpha,\beta} \equiv x l_{\alpha,\beta}, \quad z \equiv x^q y = \text{fugacity},$$

then the densities of  $\alpha$  and  $\beta$  sublattices,  $\rho_\alpha$  and  $\rho_\beta$ , are given by

$$\rho_{\alpha,\beta} = \frac{z(1 + u_{\beta,\alpha}/x^2)^q}{(1 + \mu_{\beta,\alpha})^q + z(1 + u_{\beta,\alpha}/x^2)^q} = \frac{1 - \sigma_{\alpha,\beta}}{2} \quad (2.1a, 2.1b)$$

(see KT (3.4)). Here  $q$  is the coordination number and  $u_{\alpha,\beta}$  is determined by

$$u_{\alpha,\beta} = z \left( \frac{1 + u_{\beta,\alpha}/x^2}{1 + u_{\beta,\alpha}} \right)^{q-1} \quad (2.2a, 2.2b)$$

(see KT (3.2)). Evidently we have a solution in which  $u_\alpha = u_\beta = u$ , and it determines the disordered phase. Substituting

$$z = u \left( \frac{1 + u}{1 + u/x^2} \right)^{q-1}$$

into (2.1), we have

$$\rho = \frac{u + u^2/x^2}{1 + 2u + u^2/x^2}. \quad (2.3)$$

Then the pressure of the disordered phase  $p_f$  is given by

$$\frac{p_f}{kT} = \int_0^u \rho \frac{d \ln z}{du} du. \quad (2.4)$$

Expressing  $u$  in terms of  $\rho$  after the integration, we have

$$\frac{p_f}{kT} \equiv S_1(\rho) = (q-1) \ln(1-\rho) - \frac{q}{2} \ln \left( \frac{(1-2\rho) - 2x^{-2}(1-\rho) + [(1-2\rho)^2 + 4x^{-2}\rho(1-\rho)]^{1/2}}{2(1-x^{-2})} \right). \quad (2.5)$$

The equation of state (2.5) is equivalent to the one obtained by the method of quasi-chemical approximation (Cernushi and Eyring 1939). In the case of an attractive force, a first-order gas–liquid transition below  $T_c$  is known ( $x_c = \frac{1}{3}$ ,  $T_c/J_1 = 0.910239$ ,  $p_c/kT = \frac{5}{2} \ln 2 - \frac{3}{2} \ln 3 = 0.084949$ ). In the limit  $x \rightarrow \infty$  ( $T \rightarrow 0$  in the repulsive case) it gives one for the hard-core (first-neighbour infinite repulsion) lattice gas (Burley 1960).

Now the ordered phase for  $q = 3$  is considered. Multiplying the denominators of both (2.2a) and (2.2b), subtracting each other, and dividing by  $u_\alpha - u_\beta$ , we have

$$1 - u_\alpha u_\beta + \frac{2z}{x^2} + \frac{u_\alpha + u_\beta}{x^4} z = 0. \quad (2.6)$$

Substituting (2.2b) into (2.6), we have

$$\left(1 + \frac{z}{x^4}\right)^2 u_\alpha^2 + \left(-z + 2 + \frac{4z}{x^2} + \frac{z}{x^4} + \frac{2z^2}{x^6}\right) u_\alpha + \left(1 + \frac{z}{x^2}\right)^2 = 0. \quad (2.7)$$

The two solutions of (2.7) give  $u_\alpha$  and  $u_\beta$ .

The transition points between the disordered phase and the ordered phase are given by the condition that (2.7) has equal roots. Hence the values of the fugacity at the transition points are given by

$$\frac{z_{c1}}{z_{c2}} = \frac{8}{1 - 6x^{-2} - 3x^{-4} \pm [(1 - 6x^{-2} - 3x^{-4})^2 - 64x^{-6}]^{1/2}}, \quad (2.8)$$

where  $z_{c1}$  and  $z_{c2}$  are the values of the fugacity at which the ordered phase appears and ends, respectively. The value of  $x$  at which  $z_{c1} = z_{c2}$  gives the maximum melting temperature  $T_m$ , ie  $x_m = 3$ ,  $T_m/|J_1| = 0.910239$ .

Inserting  $z$  from (2.2a) into (2.1a), we express the density of the ordered phase as

$$\rho = \frac{1}{2}(\rho_\alpha + \rho_\beta) = \frac{1}{2} \frac{u_\alpha + u_\beta + 2u_\alpha u_\beta/x^2}{1 + u_\alpha + u_\beta + u_\alpha u_\beta/x^2}. \quad (2.9)$$

Using the relation between the roots and the coefficients in (2.7), we express  $\rho$  in terms of  $z$  instead of  $u_\alpha$  and  $u_\beta$ :

$$\rho = \frac{1}{2} \frac{2 - z(1 - 3x^{-2})}{1 - z(1 - 3x^{-2}) + x^{-6}z^2}. \quad (2.10)$$

From (2.10)

$$z = \frac{4(1 - \rho)}{(1 - 2\rho)(1 - 3x^{-2}) + [(1 - 2\rho)^2(1 - 3x^{-2}) + 16x^{-6}\rho(1 - \rho)]}. \quad (2.11)$$

The pressure of the ordered phase  $p_s$  is given by

$$\frac{p_s}{kT} = S_1(\rho_{c1}) + \int_{z_{c1}}^z \frac{\rho}{z} dz, \quad (2.12)$$

where  $S_1(\rho_{c1})$  is the value of the disordered phase at  $\rho(z_{c1})$  with (2.8) and (2.10). From (2.12), (2.5), (2.10) and (2.8),  $p_s$  is given by

$$\frac{p_s}{kT} = S_1(\rho_{c1}) + S_2(z(\rho)) - S_2(z_{c1}), \quad (2.13)$$

where

$$S_2(z) = -\frac{1}{2} \ln|x^2z^{-2} + (3 - x^2)z^{-1} + x^{-4}|, \quad (2.14)$$

and  $z(\rho)$  is given by (2.11).

At higher densities ( $\rho > \rho(z_{c2})$ ), the disordered phase again appears and the pressure is given by  $S_1(\rho)$  in (2.5) ( $= S_1(\rho_{c1}) + S_2(z_{c2}) - S_2(z_{c1}) + S_1(\rho) - S_1(\rho_{c2})$ ). At the hard-core limit  $x \rightarrow \infty$  ( $T \rightarrow 0$ ), the equation of state for the ordered state of the hard-core gas†

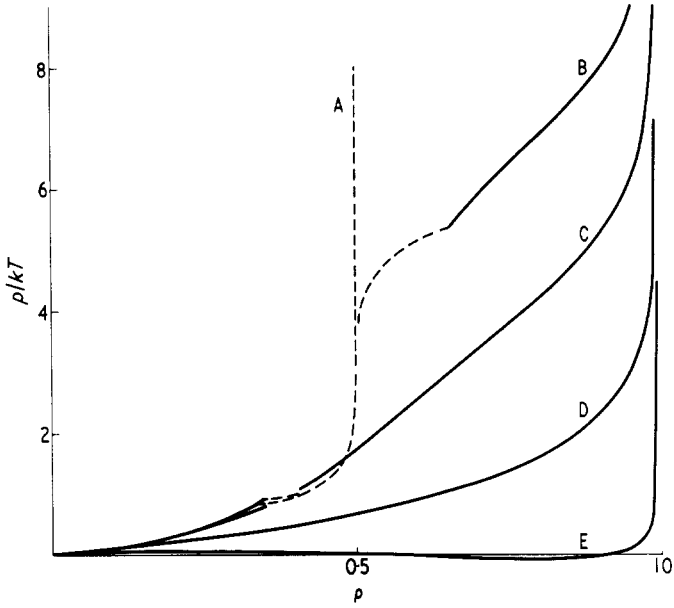
† Corresponding hard-core ordered-state equation for  $z = 4$  is given by Burley (1961) and shows second-order transitions.

(first-neighbour infinite repulsion, Runnels 1968)

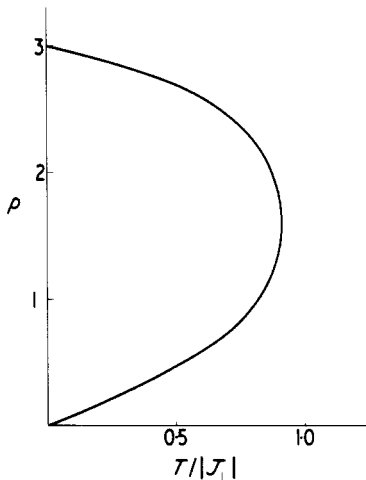
$$p_s/kT = \ln(1 - \rho) - \frac{1}{2} \ln(1 - 2\rho) + \ln 2, \tag{2.15}$$

is reproduced, and the part of the isotherm for  $\frac{1}{2} < \rho$  disappears.

The pressure–density characteristics are shown in figure 1. Two second-order fluid–solid transitions and the melting point maximum are observed. In figures 2 and 3 respectively are shown  $p$ – $T$  and  $\rho$ – $T$  phase diagrams for the soft-core lattice gas.



**Figure 1.** Isotherm of the soft-core lattice gas (first-neighbour interaction  $-2J_1$ ,  $J_1 > 0$ : attraction,  $J_1 < 0$ : repulsion). Full curves and broken curves represent the disordered (fluid) phase and the ordered (solid) phase, respectively. A,  $T/J_1 = 0$ ; B,  $T/J_1 = -0.5$ ; C,  $T/J_1 = -0.910239$  (maximum melting point); D,  $T/J_1 = \infty$ ; E,  $T/J_1 = 0.75$ .



**Figure 2.**  $p$ – $T$  phase diagram (melting point curves) of the lattice gas with soft core.

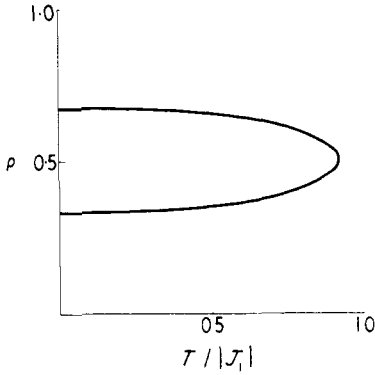


Figure 3.  $\rho$ - $T$  phase diagram of the lattice gas with soft core.

### 3. Hard-core lattice gas with attraction

Next the fluid–solid transition of the hard-core lattice gas with attraction  $-2J_2$  at the second neighbours is treated. Recently statistical mechanics of the infinite Bethe lattice with first- and second-neighbour interactions as shown in figure 4 ( $q = 3$ ) is developed

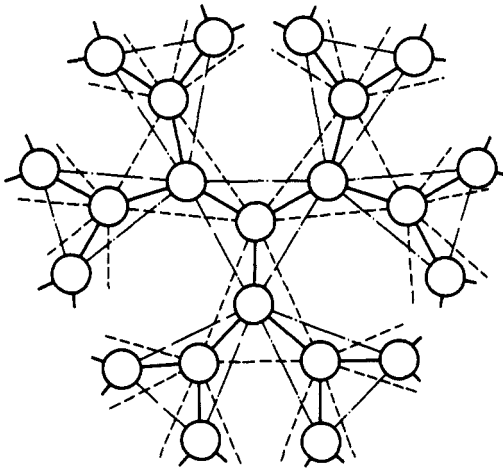


Figure 4. Bethe lattice with first- and second-neighbour interactions ( $q = 3$ ).

(Katsura and Takizawa 1974). The sublattice magnetizations  $\sigma_\alpha$  and  $\sigma_\beta$  are expressed in terms of four kinds of effective field in (KT (5.8')), and equations to determine the effective fields (KT (5.6a) and (5.6b)) are given. We transform these relations of the Ising model to the lattice gas language. Let

$$\begin{aligned}
 u_{\alpha+} &= x\eta^2 l_{\alpha+}, & u_{\alpha-} &= x\eta^2 l_{\alpha-}, \\
 u_{\beta+} &= x\xi^2 l_{\beta+}, & u_{\beta-} &= x\xi^2 l_{\beta-},
 \end{aligned}$$

where  $x = e^{-J_1/kT}$ ,  $\xi = \eta = e^{-J_2/kT}$ . Taking the hard-core limit  $x \rightarrow \infty$ ,  $l \rightarrow 0$  ( $u$  finite) in (KT (5.6))†, we have

$$\frac{l_{x-}}{l_{x+}} = \frac{u_{x-}}{u_{x+}} = \frac{1 + u_{\beta+}^2 \xi^{-2} + 2u_{\beta+}}{1 + u_{\beta+}^2 \xi^{-6} + 2u_{\beta+} \xi^{-2}}, \quad (3.1a)$$

$$\frac{l_{\beta-}}{l_{\beta+}} = \frac{u_{\beta-}}{u_{\beta+}} = \frac{1 + u_{\alpha+}^2 \eta^{-2} + 2u_{\alpha+}}{1 + u_{\alpha+}^2 \eta^{-6} + 2u_{\alpha+} \eta^{-2}}. \quad (3.1b)$$

After eliminating  $u_{x-}$  and  $u_{\beta-}$  by using (3.1), we represent  $u_{x+}$  and  $u_{\beta+}$  simply by  $u_x$  and  $u_\beta$ . Hereafter we consider the case  $\xi = \eta$ . From KT (5.6) we have

$$z = u_{x+} \frac{(1 + u_{\alpha+}^2 \eta^{-2} + 2u_{\alpha+})^2 (1 + u_{\beta+}^2 \xi^{-2} + 2u_{\beta+})}{(1 + u_{\alpha+}^2 \eta^{-6} + 2u_{\alpha+} \eta^{-2})^2} \quad (3.2a)$$

$$= u_{\beta+} \frac{(1 + u_{\beta+}^2 \xi^{-2} + 2u_{\beta+})^2 (1 + u_{\alpha+}^2 \eta^{-2} + 2u_{\alpha+})}{(1 + u_{\beta+}^2 \xi^{-6} + 2u_{\beta+} \xi^{-2})^2}, \quad (3.2b)$$

which determines  $u_x$  and  $u_\beta$  for given fugacity  $z$ . Evidently solution of the disordered phase,  $u_x = u_\beta = u$  exists. A solution for which  $u_x \neq u_\beta$  gives the ordered phase.

The density  $\rho$  and the sublattice density  $\rho_x$  are obtained from KT (5.8') by taking the hard-core limit as

$$\begin{aligned} \rho_x &= u_x (u_x^2 \xi^{-6} + 2u_x \xi^{-2} + 1) (u_\beta^2 \xi^{-2} + 2u_\beta + 1) \\ &\quad \times \{ (u_x^2 \xi^{-2} + 2u_x + 1) (u_\beta^2 \xi^{-2} + 1) [u_\beta^2 \xi^{-4} + (3 - \xi^{-2}) u_\beta + 1] \\ &\quad + u_x (u_x^2 \xi^{-6} + 2u_x \xi^{-2} + 1) (u_\beta^2 \xi^{-2} + 2u_\beta + 1) \}^{-1}. \end{aligned} \quad (3.3)$$

$$\rho = \frac{1}{2} (\rho_x + \rho_\beta), \quad (3.3')$$

$$\rho_\beta(u_x, u_\beta) = \rho_x(u_\beta, u_x).$$

In the disordered phase,  $\rho$ ,  $z$  and  $p_f/kT$  are given by

$$\rho = \frac{u(u^2 + 2u\xi^4 + \xi^6)}{2u^3 + 5u^2\xi^4 + 4u\xi^6 + \xi^6}, \quad (3.4)$$

$$z = u \frac{(1 + u^2\xi^{-2} + 2u)^3}{(1 + u^2\xi^{-6} + 2u\xi^{-2})^2},$$

$$\frac{p_f}{kT} = \int_0^u \frac{u(u^2 + 2u\xi^4 + \xi^6)}{2u^3 + 5\xi^4 u^2 + 4\xi^6 u + \xi^6} \left( \frac{1}{u} + 6 \frac{u + \xi^2}{u^2 + 2u\xi^2 + \xi^2} - 4 \frac{u + \xi^4}{u^2 + 2u\xi^4 + \xi^6} \right) du, \quad (3.5)$$

in a similar way as in § 2. When  $T < T_c$  ( $T_c/J_2 = 1.616$ ),  $p_f/kT$  shows van der Waals shape and gives gaseous and liquid phases.

† The second equation of (5.6a) and that of (5.6b) in KT should read

$$l_{x-} = y \frac{l_{\beta+}}{l_{\beta-}} \frac{x^2 + \xi^{-2} l_{\beta-}^2 + 2x l_{\beta-}}{1 + x^2 \xi^{-2} l_{\beta+}^2 + 2x l_{\beta+}},$$

$$l_{\beta-} = y \frac{l_{x+}}{l_{x-}} \frac{x^2 + \eta^{-2} l_{x-}^2 + 2x l_{x-}}{1 + x^2 \eta^{-2} l_{x+}^2 + 2x l_{x+}},$$

and the equation (5.8) for  $Z$  should be deleted.

Now we consider the ordered phase. We define

$$F(u) = u \frac{u^2 + 2u\xi^2 + \xi^2}{(u^2 + 2u\xi^4 + \xi^6)^2}. \quad (3.6)$$

Equation (3.2) gives  $F(u_\alpha) = F(u_\beta)$ . Multiplying the denominators to  $F(u_\alpha) - F(u_\beta) = 0$ , and dividing by  $u_\alpha - u_\beta$ , we have an equation for  $v \equiv u_\alpha u_\beta$  for given  $u = (u_\alpha + u_\beta)/2$ :

$$\begin{aligned} G(u, v) = & v^3 + (4\xi^2 u - 4\xi^8 + 6\xi^6 - \xi^2)v^2 \\ & + [4\xi^2 u^2 + (-8\xi^{10} + 8\xi^6)u - 7\xi^{12} + 4\xi^{10} + 2\xi^8]v \\ & + (-4\xi^{12} u^2 - 4\xi^{14} u - \xi^{14}) = 0. \end{aligned} \quad (3.7)$$

The real positive solution  $v$  of (3.7) together with

$$\begin{aligned} u_\alpha &= u \pm (u^2 - v)^{1/2} \\ u_\beta & \end{aligned} \quad (3.8)$$

determines  $u_\alpha$  and  $u_\beta$  for given  $u$ .

The fugacity  $z$  in the ordered phase (3.2) is transformed into

$$z = v^{1/2} \frac{[v^2 \xi^4 + 4vu\xi^6 + 4v\xi^8 + (4u^2 - 2v)\xi^6 + 4u\xi^8 + \xi^8]^{3/2}}{v^2 + 4vu\xi^4 + 4v\xi^8 + (4u^2 - 2v)\xi^6 + 4u\xi^{10} + \xi^{12}}. \quad (3.9)$$

The pressure  $p_s$  is given by

$$\frac{p_s}{kT} = \int_{u_c}^u \rho \frac{d \ln z}{du} du, \quad (3.10)$$

where  $\rho$  is given by (3.3') with  $u_\alpha$  and  $u_\beta$  in (3.7) and (3.8), and

$$\frac{d \ln z}{du} = \frac{\partial \ln z}{\partial u} + \frac{\partial \ln z}{\partial v} \frac{dv}{du}, \quad (3.11)$$

$$\frac{dv}{du} = - \frac{\partial G / \partial u}{\partial G / \partial v}, \quad (3.12)$$

using  $z$  in (3.9) and  $G$  in (3.7). The lower limit of (3.10),  $u_c$ , is the value of the limit  $u_\alpha \rightarrow u_\beta$ , in the solution of (3.7) and (3.8) for given  $\xi$ . It is a real positive solution of

$$u^4 + (4\xi^2 - 2\xi^4)u^3 + (3\xi^2 - 3\xi^6)u^2 + (2\xi^6 - 4\xi^8)u - \xi^8 = 0, \quad (3.13)$$

which is obtained by putting  $v = u^2$  in (3.7) and by factorizing by  $u^2 + 2\xi^4 u + \xi^6$ .

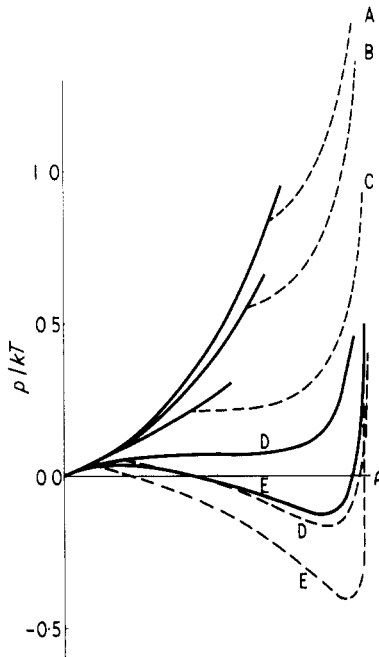
The inverse of the compressibility is given by

$$\frac{\partial p / kT}{\partial \rho} = \rho \frac{d \ln z}{du} \frac{du}{d\rho}. \quad (3.14)$$

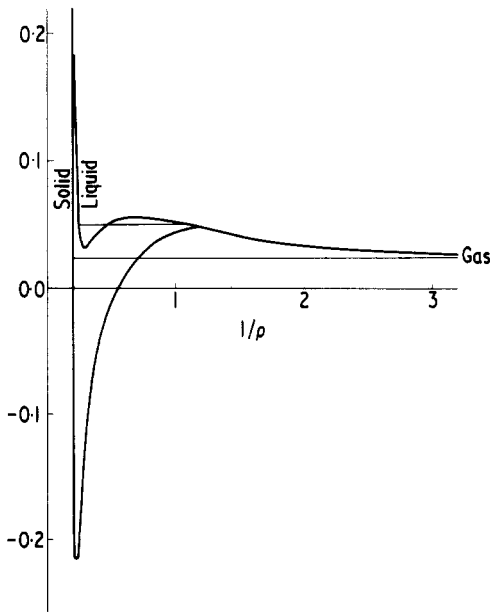
When  $(d \ln z / du)_{u_c} > 0$ ,  $u_c$  gives the point of the second-order transition ( $\rho = \rho(u_c)$  in (3.4)). When  $(d \ln z / du)_{u_c} < 0$ , the system has the first-order phase transition at some value of  $\rho$  ( $< \rho_c(u_c)$ ) which is determined by Maxwell's rule. The tricritical point  $T_t$  is shown to be  $T_t/J_2 = 3.4125$  which is determined by  $(d \ln z / du)_{u_c} = 0$ .

Figures 5 and 6 show the  $p/kT$ - $\rho$  characteristics. Figure 7 shows the  $p$ - $T$  phase diagram and figure 8 the  $\rho$ - $T$  phase diagram of the fluid-solid transition. The phenomenon of the melting point maximum is not observed. The gas-liquid transition is masked by the gas-solid transition in the range  $T < T_c < T_t$ .

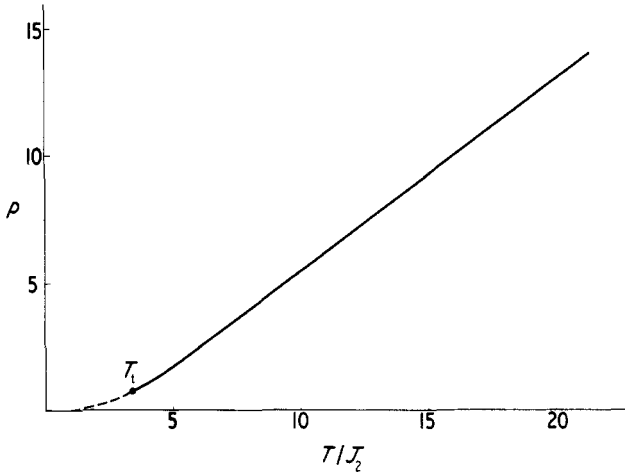




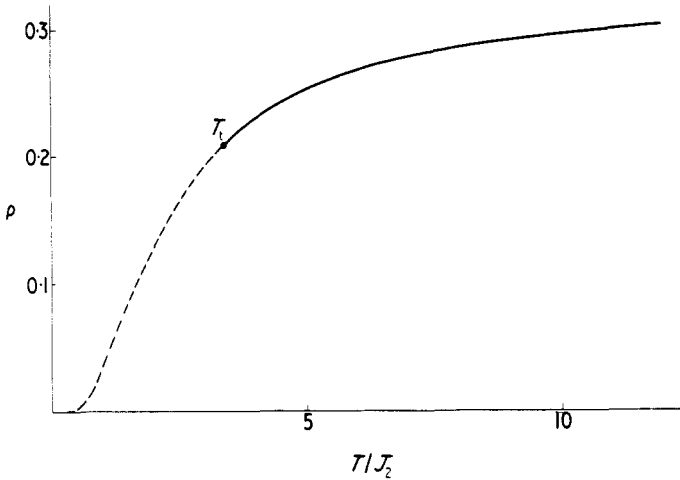
**Figure 5.** Isotherm of the hard-core lattice gas with finite interaction at the second neighbour,  $-2J_2$ . Full curves and broken curves represent the disordered (fluid) phase and the ordered (solid) phase, respectively. The full scale of the abscissa is  $\rho = 0.5$ . A,  $T/J_2 = \infty$ ; B,  $T/J_2 = 10$ ; C,  $T/J_2 = 3.4125$  (tricritical point); D,  $T/J_2 = 1.616$  (critical point between gas and liquid); E,  $T/J_2 = 1.25$ .



**Figure 6.** Maxwell construction of the isotherm of the hard-core lattice gas with finite attraction at the second neighbour:  $T = 1.5J_2$ . The gas–liquid transition is masked by the gas–solid transition, and only the gas–solid transition is realized.



**Figure 7.**  $p$ - $T$  phase diagram of the hard-core lattice gas with attraction at the second neighbour,  $-2J_2$ . The full curve represents the second-order transition and the broken curve its continuation. The first-order transition line locates below the broken curve.



**Figure 8.**  $\rho$ - $T$  phase diagram of the hard-core lattice gas with attraction at the second neighbour,  $-2J_2$ . The full curve represents the second-order transition and the broken curve its continuation.

#### 4. Conclusion and Discussions

In this paper, firstly, the soft-core lattice gas and secondly, the hard-core lattice gas with attraction at the second neighbours, are treated in the Bethe approximation, ie in the exact solutions of the infinite Bethe lattice<sup>†</sup>. The method has an advantage, compared to the series method or to the eigenvalue method, in that the transition point is given definitely. Main results for properties of the Bethe lattice gas will hold in general.

<sup>†</sup> In the finite Bethe lattice the surface effect is of the same order as the volume effect. The surface effect of the finite Bethe lattice which causes the disappearance of the fluid-solid transition was discussed by Runnels (1967) and that in connection with a Stanley-Kaplan type transition by Matsuda (1974).

In the soft-core lattice gas two second-order transitions, fluid  $\rightarrow$  solid  $\rightarrow$  fluid, exist for  $T < T_m$  and the melting point has a maximum ( $T_m = 0.910239|J_1|$ ). The latter transition disappears at the hard-core limit. For  $T > T_m$ , only the fluid phase is realized.

In the hard-core lattice gas with attraction at the second neighbours, two solutions describing the fluid (gas and liquid) phase and the solid phase exist. The former solution has a van der Waals type isotherm and the critical temperature  $T_c (= 1.616 J_2)$ . In the latter solution the tricritical point  $T_t (= 3.4125 J_2)$  exists and it divides the transition curve into the second-order part and the first-order part of the fluid-solid transition. Similar features are also reported in the results of the matrix method (Runnels *et al* 1970). At low temperatures the location of the starting point of the solid-phase solution is far in the low density side. The liquid phase does not appear because it is masked by the solid phase, and only the gas-solid transition is realized (see figure 5). In order for the two transitions, gas-liquid and liquid-solid, to appear together, the effect of the attraction should be stronger (for example, Kac potential or up to fifth neighbour interactions (Orban *et al* 1968)), or the repulsive interaction should be weaker.

In the hard-core lattice gas with finite repulsion at the second neighbours, the possibility of finding new phases other than the ones considered here is involved. It may correspond to another kind of solid and solid-solid transition will be found in such systems. It may be treated by considering three or four sublattices.

### Acknowledgments

The author thanks Professors S Inawashiro, Y Fukuda, T Morita and Dr F Matsubara for helpful discussions, and T Shibayama for numerical calculations using NEAC 2200/500 at the Computer Center of the Tohoku University.

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