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LETTER TO THE EDITOR

The estimation of the tricritical point of the interacting hard squares from the low-temperature series expansions

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Abstract. Using the low-temperature series expansions, the tricritical parameters for the interacting hard squares are estimated to be $t_{tc} = \exp(-\varepsilon/kT_{tc}) \simeq 5.45$, $y_{tc} \simeq 1.040$, values rather different from previous estimates derived from other methods.

The tricritical behaviour of the lattice gas with nearest-neighbour exclusion and next-nearest-neighbour finite attraction ε on the square lattice was treated previously using the closed-form approximations (Kaye and Burley 1974, Aksenenko and Shulepov 1978, 1982, 1984), the exact finite method (Runnels *et al* 1970), and renormalisation group calculations (Kinzel and Schick 1981); recently Baxter (1980), Huse (1982), Baxter and Pearce (1983) calculated the tricritical density $\rho_{tc} = \frac{1}{10}(5-\sqrt{5})$. Springgate and Poland (1979) conjectured the value $t_{tc} \sim 3.5$ for the lower bound on the temperature parameter $t = \exp(-\varepsilon/kT)$ in the tricritical point using the expansions in activity and in inverse activity. This value differs considerably from the renormalisation group result (Kinzel and Schick 1981, $t_{tc} \sim 5.0$) and from the extended cluster variation calculation result (Aksenenko and Shulepov 1984, $t_{tc} \sim 4.1$).

The more reliable estimate of this parameter is obtained here using the low-temperature expansions of the grand canonical potential (Aksenenko and Shulepov 1979, 1981) in the form

$$\Gamma(u, y_a, y_b) = \sum_k \psi_k(y_a, y_b) u^k,$$

$$\Gamma^*(u, y_a, y_b^{-1}) = \tfrac{1}{2}\left[\log(y_b) + \sum_k \psi_k^*(y_a, y_b^{-1}) u^k\right], \tag{1}$$

at low and high densities respectively; here the low-temperature variable $u = \exp(\varepsilon/kT)$, and the sublattice fugacities are related to the activities z_ν as follows: $y_\nu = z_\nu \exp(-2\varepsilon/kT)$, $\nu = a, b$. The coefficients of the polynomials ψ_k, ψ_k^* can be obtained combining the expansions in activity and inverse activity (Springgate and Poland 1975, 1979), the expansions for Ising model (Sykes *et al* 1965, 1973a, b) and the values at high powers of the fugacities,

$$\begin{aligned}
&\psi_8(v_{ij}) = -16v_{1,9} + \ldots, \\
&\psi_9(v_{ij}) = -40v_{1,12} - 152v_{1,11} - 40v_{2,9} - 540v_{1,10} - 40v_{4,6} - 228v_{2,8} - 1224v_{1,9} - \ldots, \\
&\psi_9^*(w_{i,j}) = 6w_{1,12} + 20w_{1,11} + 60w_{1,10} + \ldots, \\
&v_{ij} = \tfrac{1}{2}(y_a^i y_b^j + y_a^j y_b^i), \qquad w_{ij} = y_a^i y_b^{-j}
\end{aligned} \tag{2}$$

obtained in Aksenenko and Shulepov (1981).

The tricritical point was estimated as the value of the fugacity y_{tc} at which the series for the modified isothermal compressibilities $\chi_0(u, y) = \partial^2\Gamma(u, y)/(\partial \log y)^2$ and $\chi_0^*(u, y^{-1}) = \partial^2\Gamma^*(u, y^{-1})/(\partial \log y^{-1})^2$, $y = y_a = y_b$, both diverge simultaneously. This procedure is illustrated in figure 1(*a*) where the ratios of the successive coefficients of the Ising model series $\chi_{0\text{I}}^{1/\gamma'} \sim 1 + \Sigma_i a_i u^i$ are plotted against $1/i$; these ratios we expect to converge to the critical value $t_c = u_c^{-1}$. For the Ising model the exact critical values are known: $t_c = (1+\sqrt{2})^2 \simeq 5.828\ldots$, $y_c = 1$, $\gamma' = \frac{7}{4}$, and the low- and high-density expansions are related to each other: $\chi_{0\text{I}}^*(u, y^{-1}) = \chi_{0\text{I}}(u, y^{-1})$. One can assure from figures 1(*a*) and 1(*b*) that the values of the critical parameters y_c and t_c estimated from this procedure are good enough, and the variation in γ' gives rise to the variation of the slope of the extrapolating line but does not affect the estimated values.

The exact value of the critical exponent γ' for the interacting hard squares is not known; Kinzel and Schick (1981) conjectured for it the Ising value of $\frac{7}{4}$. From the Padé approximants to the logarithmic derivatives of the compressibilities we obtained

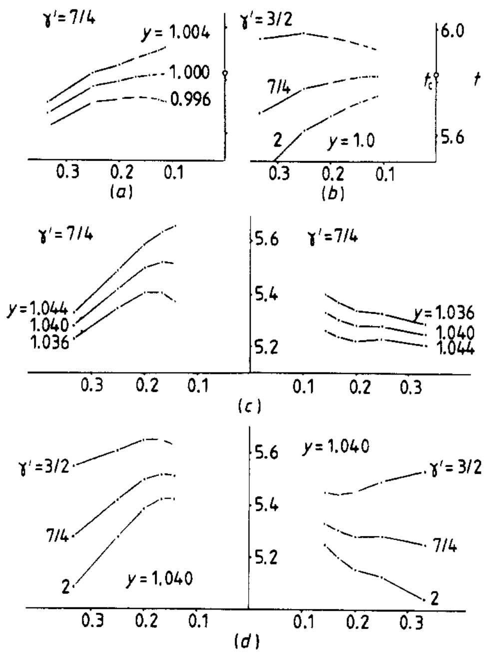

Figure 1. The ratios of the successive coefficients of (*a*, *b*) the Ising model modified compressibility $\chi_{0\text{I}}^{1/\gamma'}$ and (*c*, *d*) the interacting hard squares model $\chi_0^{1/\gamma'}$ (left) and $\chi_0^{*1/\gamma'}$ (right), for various values of y and γ'.

a rather surprising result: 1.2 and 1.9 for the low- and high-density series respectively, which may stem from the small number of terms in the series investigated. The behaviour of the series for χ_0 and χ_0^* is worse than that of the Ising model series; from figures 1(c) and 1(d) one can see however that a sufficiently large variation of γ' does not affect the estimate of the tricritical parameters. A similar behaviour is characteristic of the compressibility $\chi = \chi_0/\rho$.

It was alluring to verify the obtained values of t_{tc} and y_{tc} calculating the estimate for ρ_{tc}. It turned out however that in contradiction to the results of Springgate and Poland (1979) the partial sums of the density expansions increase rapidly with the number of terms involved and the estimate of ρ_{tc} depends strongly on the method of extrapolation.

The values $t_{tc} \simeq 5.45$ and $y_{tc} \simeq 1.040$ estimated here from the low-temperature expansions obviously differ from the earlier results obtained by Kinzel and Schick (1981).

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References

Aksenenko E V and Shulepov Yu V 1978 *Ukr. Fiz. J.* **23** 1510–5 (in Russian)
—— 1979 *Ukr. Fiz. J.* **24** 1192–201 (in Russian)
—— 1981 *Ukr. Fiz. J.* **26** 536–40 (in Russian)
—— 1982 *J. Phys. A: Math. Gen.* **15** 2515–22
—— 1984 *J. Phys. A: Math. Gen.* **17** 2111–4
Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61–70
Baxter R J and Pearce P A 1983 *J. Phys. A: Math. Gen.* **16** 2239–55
Huse D A 1982 *Phys. Rev. Lett.* **49** 1121–4
Kaye R D and Burley D M 1974 *J. Phys. A: Math., Nucl. Gen.* **7** 843–58
Kinzel W and Schick M 1981 *Phys. Rev.* B **24** 324–8
Runnels L K, Salvant J P and Streiffer H R 1970 *J. Chem. Phys.* **52** 2352–8
Springgate M W and Poland D 1975 *J. Chem. Phys.* **62** 680–9
—— 1979 *Phys. Rev.* A **20** 1267–84
Sykes M F, Essam J W and Gaunt D S 1965 *J. Math. Phys.* **6** 283–98
Sykes M F, Gaunt D S, Mattingly S R, Essam J W and Elliott C J 1973a *J. Math. Phys.* **14** 1066–70
Sykes M F, Gaunt D S, Martin J L, Mattingly S R and Essam J W 1973b *J. Math. Phys.* **14** 1071–4