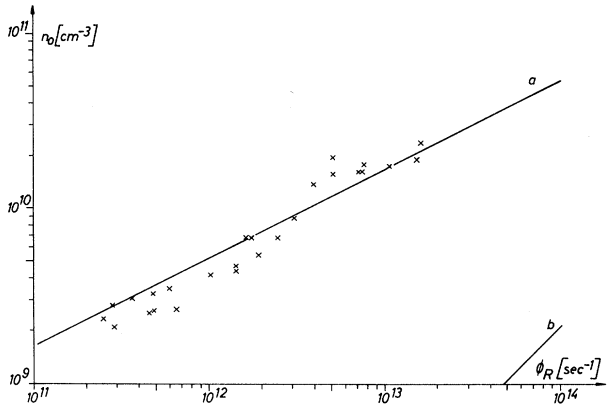

FIG. 3. Relationship between central particle density and flux of diffusing particles for $B = 11$ kG and $\iota = 0.3\pi$. Crosses indicate measured values determined from probe current and particle detector, respectively. Curve (a) is calculated assuming resistive diffusion, curve (b), from pump-out losses.

losses become excessively large for too small values of ι.

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PHASE TRANSITION IN A LATTICE GAS WITH EXTENDED HARD CORE

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Phase transitions in lattice models of "hard molecules" (i.e., molecules occupying one lattice site and excluding other molecules from certain neighboring sites) have been investigated by several authors. For planar square and triangular lattices occupied by molecules with an exclusion core covering first-neighboring sites only, the situation seems clear as a result of recent works of Gaunt and Fisher,[1] Runnels and Combs,[2] and Ree and Chesnut[3,4]: Both cases most likely exhibit a second-order continuous transition (with a horizontal inflection in the pressure-versus-density curve). Little work has been devoted to more extended hard cores. For the square lattice, Bellemans and Nigam[5,6] worked out the cases of hard-square molecules with exclusion ranges extending up to second- and third-neighboring sites, respectively. Using different techniques (low- and high-density series, matrix method, generalized Bethe approximation) they concluded that first-order and even second-order continuous transitions are excluded in the first case,

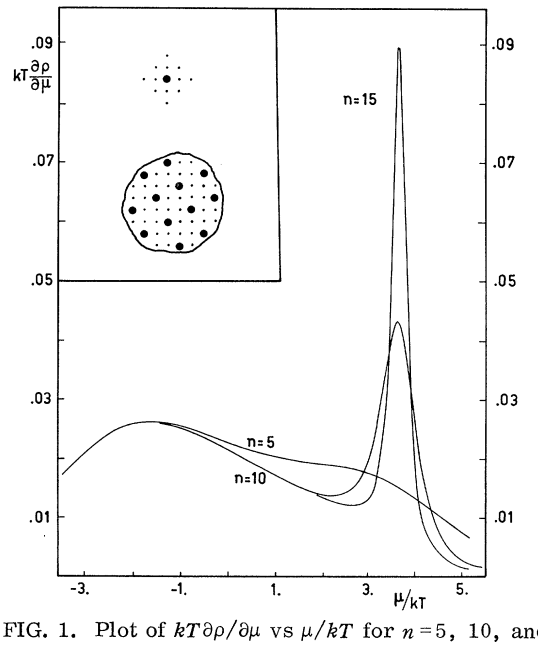

FIG. 1. Plot of $kT\partial\rho/\partial\mu$ vs μ/kT for $n = 5$, 10, and 15. The upper left part of the figure shows the exclusion neighborhood of a molecule and the close-packing configuration.

Table I. Number of configurations and symmetry classes for single and double rings of n sites.

n	Single ring Configurations	Classes	Double ring Configurations	Classes
5	6	2	21	4
10	46	6	441	34
15	309	19	9327	353

while the second case unquestionably exhibits a phase change, presumably first order. It is this particular case we wish to comment on here. The exclusion range of these molecules is shown on the upper left part of Fig. 1, as well as their close-packing configuration.

Perhaps the neatest argument for a transition in this system was obtained by considering the thermodynamic properties of semi-infinite cylindrical lattices with circumference of n sites, which can be handled exactly by the matrix method of Kramers-Wannier. In order to allow the system to reach close packing, n ought to be a multiple of 5; further, on account of the rather extended hard core, the appropriate matrix must be based upon the permissible configurations on a double ring of n sites. In view of this, and despite an enormous reduction of the matrix owing to symmetries of rotation and reflection, only the cases $n=5$ and $n=10$ could be studied by Bellemans and Nigam, the relevant matrices being constructed by hand. The case $n=10$ showed a sharp compressibility peak, leaving no doubt about the existence of a phase transition for $n\to\infty$.

Leaving aside the other methods used by Bellemans and Nigam for discussing this same system,[6] we thought it worthwhile to work out the next case, $n=15$. As it was out of question to construct the appropriate matrix by hand, a computer program was set up which successively (a) enumerates the allowed configurations on one ring of n sites and subdivides them into symmetry classes (with respect to rotation and reflection), (b) enumerates the allowed configurations on a double ring of n sites and subdivides them in symmetry classes, (c) constructs the matrix itself, and (d) calculates its largest eigenvalue and deduces all relevant thermodynamic properties from it. The numbers of configurations and classes are given in Table I. The calculations were made on a IBM 7040(16k); the case $n=15$ needed a few hours (matrix 353×353); all the next ones are far beyond the possibilities of this computer.

The results for all three cases, $n=5$, 10, and 15, are shown on Figs. 1 and 2 (p, ρ, μ denote pressure, density, and chemical potential, respectively). The peak in $kT\partial\rho/\partial\mu$ (i.e., essentially the compressibility) previously observed for $n=10$, is still located near the same abscissa for $n=15$, but it has grown up considerably while narrowing simultaneously. This is precisely the expected behavior for getting a first-order transition as $n\to\infty$. The curve p vs ρ of Fig. 2 shows a progressive flattening over a wide density range as n increases, in agreement with the idea of a first-order change.

The position of the peaks and the corresponding thermodynamic properties are given in Table II. The exact location of the transition is certainly very close to $\mu/kT=3.70$ and $p/kT=0.745$, in view of the small changes on going from $n=10$ to 15. Approximate calculations based on a generalization of the Bethe method[6] lead to a first-order transition, the character-

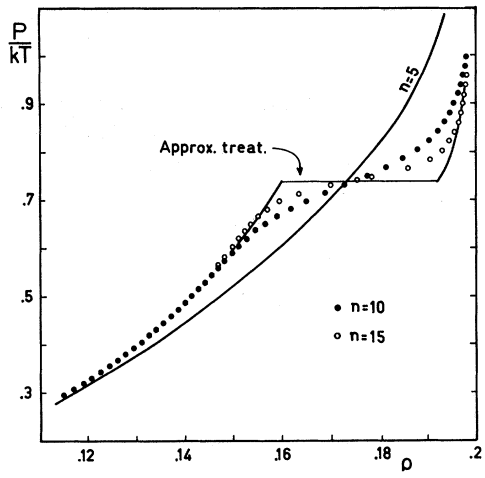

FIG. 2. Plot of p/kT vs ρ for the cases $n=5$, 10, and 15, and from the generalized Bethe method of Ref. 6.

Table II. Position of the compressibility peak and values of the corresponding thermodynamic properties (the maximum value of ρ is 0.20).

n	μ/kT	p/kT	ρ	$kT\partial\rho/\partial\mu$
5	...	...	...	...
10	3.635 ±5	0.740 ±1	0.1746 ±2	0.0431 ±2
15	3.665 ±5	0.742 ±1	0.1755 ±2	0.089 ±1
Approximate method	3.640 ±5	0.738 ±1	Density gap ($\rho = 0.160$ to 0.192)	

istics of which are given in the last line of Table II; they agree remarkably well with the results of the matrix method. This is also clear from Fig. 2, where the corresponding curve p vs ρ is shown. To conclude, the occurrence of a first-order phase change in the system considered here seems very likely. Further work based on low- and high-density series is progressing.

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[6]A. Bellemans and R. K. Nigam, to be published.

HIGHER ORDER BEHAVIOR IN THE BOLTZMANN EXPANSION OF THE BOGOLIUBOV-BORN-GREEN-KIRKWOOD-YVON HIERARCHY

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The purpose of this Letter is to indicate the form of equations governing "divergent" many-body behavior[1,2] within the spatially homogeneous Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy in the Boltzmann approximation for cut-off potentials, the nondivergent nature of the solutions which results from a linearization around a Maxwellian velocity distribution, and the strong analogy between this behavior and the structure of the BBGKY hierarchy in the plasma approximation.

To second order in ϵ ($=nr_0^3$, n = density, r_0 = range of binary potential) the single-particle distribution function $g_1(v,t)$ and the binary correlation function $g_2(x_{12},v_1,v_2,t)$ are of the form

$$g_s = g_s^0 + \epsilon g_{s0}^1 + \epsilon^2 \ln\epsilon g_{s1}^1 + \epsilon^2 g_{s|1}^2 + \epsilon^2 g_{s|2}^2.$$

The contributions up to and including order $\epsilon^2 \ln\epsilon$ have been studied in earlier work.[3-9] The contributions in $g_{1|1}^2$ and $g_{2|1}^2$ correspond to the "divergent" many-body behavior.

The behavior for $g_{1|1}^2$ and $g_{2|1}^2$ over times of order of the mean time (τ_m) and lengths of order of the mean free path (λ_m) is given by the equations[10]

$$\frac{\partial g_{1|1}^2}{\partial t} = \int_{|\vec{x}_{12}|=r_0} \vec{v}_{21}\cdot d\vec{\sigma}_2 d\vec{v}_2 \exp(-H_2^0\tau)(g_1^0 g_{1|1}^2 + g_{1|1}^2 g_1^0 + g_{2|1}^2) \tag{1}$$

and

$$\frac{\partial g_{2|1}^2}{\partial t} + \vec{v}_{12}\cdot\frac{\partial g_{2|1}^2}{\partial \vec{x}_{12}} + \sum_{i=1}^{2}(\nu_i + L_i) g_{2|1}^2 = S(\vec{x}_{12},\vec{v}_1,\vec{v}_2,t), \tag{2}$$

with

$$\nu_i = -\int_{|\vec{x}_{i3}|=r_0,\ \vec{x}_{3i}\cdot\vec{v}_{3i}<0} \vec{v}_{3i}\cdot d\vec{\sigma}_3 d\vec{v} g_1^0(3) \tag{3a}$$