Table I. Energies of terms of $(2sns)\,^1S$ series in helium.

n	$E_{\text{expt.}}$ (eV)	E_{calc}[a] (eV)	E_{calc}[b] (eV)
2	57.82	57.87	57.824
3	62.95	62.99	62.952
4	64.22	64.22	
5	64.71	64.70	

[a]See P. G. Burke, D. D. McVicar, and K. Smith, Phys. Rev. Letters 11, 559 (1963); P. G. Burke and D. D. McVicar, to be published.
[b]See reference 2.

Table II. Energies of terms of the $(2snp)\,^3P$ series in helium.

n	$E_{\text{expt.}}$ (eV)	E_{calc}[a] (eV)	E_{calc}[b] (eV)
2	58.34	58.36	58.296
3	63.08	63.14	63.141
4	64.22	64.26	64.320
5	64.71	64.71	

[a]See P. G. Burke, D. D. McVicar, and K. Smith, Phys. Rev. Letters 11, 559 (1963); P. G. Burke and D. D. McVicar, to be published.
[b]See reference 2.

of the $n = 5$ terms of both series. A summary of the measured and calculated values of the energies of the two series appears in Tables I and II.

Identification of the two series was aided by the fact that triplet levels are not excited by proton bombardment but show up strongly under H_2^+ bombardment. This is due to the fact that in order to conserve spin the triplet levels must be excited by a projectile bearing an electron to exchange with one in the target atom. With the proton beam the terms of the $(2snp)\,^3P$ series did not appear.

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HARD-SQUARE LATTICE GAS*

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Exact statistical calculations of thermodynamic properties of two- or three-dimensional fluids with realistic interactions have never been obtained over the entire density range. Presented here are the results of rigorous calculations for a two-dimensional lattice model of a fluid of hard molecules, the system being of infinite length and relatively large finite width. The results provide strong evidence for the existence of a second-order phase transition for a system infinite in both directions.

The "hard-square lattice gas" investigated is illustrated in the inset of Fig. 1; the only forces present are the infinite repulsions corresponding to the nonzero area of the molecules. Mathematically, this is the Ising model with interaction $+\infty$ for two adjacent sites AA and interaction zero for two adjacent sites AB or BB. This is an extremely simple model of a fluid which yet retains the excluded-volume effect and reasonable lattice topology. Since the interactions are either zero or infinity, temperature enters into the problem in a trivial way, allowing attention to be focused on variable density.

Onsager[1] obtained the partition function for the two-dimensional Ising model of arbitrary size in vanishing field (in the original magnetic formulation). Yang and Lee[2] showed that for the ferromagnetic case (corresponding to attractions between neighboring molecules of area one) there can be only the one transition found by Onsager at zero field (or density one-half for the lattice gas). There has remained speculation about the existence of an antiferromagnetic transition at some nonvanishing field,

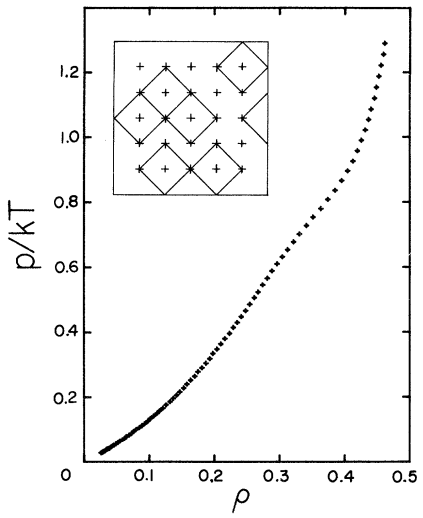

FIG. 1. Equation of state of the hard-square lattice gas, circumference 14.

which would correspond to a phase transition of the lattice gas with repulsive interactions. The well-known molecular dynamics calculations[3] for a continuum gas of rigid spheres and disks support the view that geometrical factors alone, in the absence of attractive forces, can lead to a phase transition.

The present model has been investigated previously by various authors. Burley[4] used a "ring approximation" for the combinatorics, which predicted a finite discontinuity in the compressibility at density 0.317 (where 0.5 is the close-packed density). Gaunt and Fisher[5] obtained high- and low-density expansions and concluded that the transition, apparently third order, is at density 0.37. Chesnut[6] has independently arrived at essentially the same method used by the author and has obtained many of the same conclusions.

The method reported here consists of obtaining exact solutions for lattices of infinite length and a series of finite circumferences N (cylinder convention of Onsager). Kramers and Wannier[7] set the precedent for this approach by solving the magnetic Ising model for infinite strips of circumference up to six sites, correctly inferring the linear dependence on $\log N$ of the specific heat at the transition point. Even earlier,[8] another well-known problem of statistical mechanics—the entropy of dimers on a plane lattice[9]—was investigated by studying infinite strips of circumference up to eight. In both cases, the exact result for the infinite lattice was anticipated remarkably well and better than by any approximate treatments of the infinite lattice.

The matrix method[10] was used to obtain the solutions for the hard-square lattice gas. For a given finite circumference N, all permissible states of a ring of N sites were determined, a state i being permissible if none of its m_i ($\leq N/2$) molecules occupy adjacent sites. If the length L of the cylinder is large, the grand ensemble partition function for $B = LM$ sites, temperature T, and chemical potential μ is

$$\Xi(B, T, \mu) = \exp(pB/kT) = \lambda_1^M, \tag{1}$$

where λ_1 is given by

$$\lambda_1 = \max_{uu^T = 1} uPu^T = vPv^T \tag{2}$$

and is the largest eigenvalue of the matrix $P_{ij} = \epsilon_{ij} \exp[\frac{1}{2}(m_i + m_j) \ln x]$; here $x = \exp(\mu/kT)$ and ϵ_{ij} is unity if states i and j can describe adjacent rows of the lattice with no molecules overlapping, and zero otherwise. (Superscript T denotes the transpose.) Because of the extremum property of λ_1 shown by Eq. (2), the eigenvector v gives, in addition to the pressure, the fractional density $\rho = (\delta p/\delta \mu)_T$ by the relationship

$$\rho = (x/N\lambda) v P' v^T, \tag{3}$$

where

$$P_{ij}' = (\delta P_{ij}/\delta x)_T = \tfrac{1}{2}(m_i + m_j) P_{ij}/x. \tag{4}$$

The symmetry of the model can be exploited to simplify the computations. Letting ω_i denote the degeneracy of state i—the number of states equivalent to state i under the operations of the dihedral group D_N—and replacing v_i by $(\omega_i)^{1/2} v_i$, P_{ij} by $(\omega_i \omega_j)^{1/2} P_{ij}$, the above equations remain valid if the matrix products are evaluated by summing over only nonequivalent states. This procedure greatly reduces the size of the matrices involved and yields the correct result since the largest eigenvalue must belong to the totally symmetric representation of the group D_n.

The entire analysis just described was carried out by Louisiana State University's IBM 7040 (32K) computer. The MAP program (essentially machine language) made extensive use of the logical machine operations and optimized efficiency by "packing" matrix elements

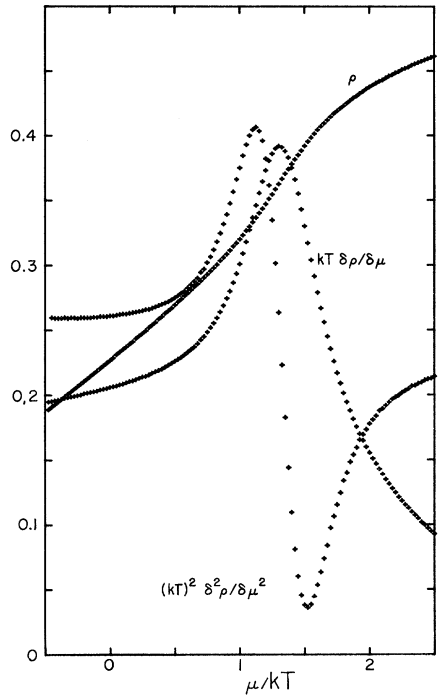

FIG. 2. Density isotherm for hard-square lattice gas, circumference 16. Vertical scale shown is for the density curve; scale and displacement vary for the derivative curves.

and transferring data between the central processing unit and tape drives on two channels simultaneously. An iterative process[11] was used to determined λ_1 and v, and hence ρ, for a series of incremented values of μ/kT. To find the second derivative of the pressure directly would require knowledge of all eigenvectors; a more expedient approach for second and third derivatives was to obtain them from finite-difference tables generated from the chemical potential changes.[12] The calculated thermodynamic properties were displayed graphically using a Calcomp 563 X-Y plotter driven by an IBM 1620. (The data points of Figs. 1 and 2 were plotted in this way.) Lattices with (even) circumference of 6 to 22 sites (3 to 11 molecules) have been studied. The matrix P for circumference 22 is 1022 square; had it not been reduced by symmetry as mentioned above, it would have been 39 603 square. Machine capacity extends to circumference 24, but since execution would be lengthy and the results already obtained seem to indicate well enough all of the trends, it was decided not to run 24 for the present. About 40 min. of running time are required to sweep the entire density range for a circumference of 14. Thereafter, running time increases by a factor of four for an increase in circumference of two.

Figure 1 shows the equation of state obtained in this way, for $N=14$. Although a bump in the curve is clearly visible, no singularity is evident. In fact, it can be shown easily that there can be no singularity for a lattice of finite circumference, using a slight modification of an argument given by Onsager[13] based on Frobenius's theorem. Any singularity for the infinitely wide lattice must then be approached as a limit of analytic functions.

In Fig. 2 is shown in a different form the results obtained for $N=16$. (For the larger problems only the interesting transition region was studied; away from this region, the results are independent of N for $N>10$.) Since the density is given by $\rho=(\delta p/\delta\mu)_T$, the first derivative curve of Fig. 2 is the second derivative of p with respect to μ. This function can be shown to be proportional to the heat capacity

Table I. Transition point.

N	μ^*/kT ±0.003	p^*/kT ±0.001	ρ^*/kT ±0.0005	$C=(\delta^2 p^*/\delta\mu^{*2})_T$ ±0.005	$\Delta C/\Delta \ln N$ $\pm 0.05\times10^{-2}$
6	1.162	0.7374	0.3472	0.120 09	•••
8	1.235	0.7597	0.3548	0.130 41	3.59×10^{-2}
10	1.268	0.7703	0.3586	0.138 72	3.72
12	1.287	0.7762	0.3609	0.145 64	3.80
14	1.298	0.7799	0.3624	0.151 56	3.84
16	1.306	0.7824	0.3634	0.156 73	3.87
18	1.311	0.7839	0.3640	0.161 31	3.89
20	1.316	0.7858	0.3648	0.165 41	3.89
22	1.319	0.7865	0.3652	0.169 15	3.92
∞	1.35 ± 0.01	0.796 ± 0.004	0.369 ± 0.002	∞	•••

at constant pressure, or to the compressibility. (The constant-area specific heat is identically zero.) The curve appears to be of the lambda type and is found to have a sharper maximum with increasing N.

Table I contains information about the maximum point (denoted by *) for all values of N studied. Remembering the Kramers and Wannier discovery about the heat capacity of the finite Ising ferromagnet, the height of the maximum was plotted versus $\log N$. A linear relationship is approached for $N > 8$, as indicated by the last column of Table I. (There is a slight amount of wobble for the last points, attributable to the increasing error accumulation in the numerical operations for the larger problems.) The finite thermodynamic properties at the transition point were obtained from extrapolation of plots versus N^{-1}.

There does appear to be, then, a transition of order no greater than second. While it is impossible to state unequivocally that the transition is not first order, the results obtained give little cause to suspect a discontinuity in the density curve at the transition point. The evidence favors a second-order transition of the logarithmic type, with transition point characterized by $\mu^*/kT = 1.35$, $p^*/kT = 0.796$, $\rho^* = 0.369$, and $(\delta p^*/\delta \rho^*)_T = 0$.

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ACOUSTIC ATTENUATION IN A TYPE-II SUPERCONDUCTOR*

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In this Letter we give a brief outline of the theory of the response of a type-II superconductor, in a static magnetic field $H > H_{c1}$, to an externally applied sound wave. We show that the detailed information on the structure of the mixed state of type-II superconductivity can be obtained by examining the nature of ultrasonic attenuation in type-II material.

For simplicity, we have restricted ourselves to the case of a longitudinal sound wave and have neglected impurity effects. Although the theory can, in principle, be carried out in a gauge-invariant manner,[1] here we consider only the dominant effects of a longitudinal wave, namely, the charge fluctuations induced in the system. Transverse currents, which arise in the presence of a static magnetic field and collective modes,[2] will be neglected.

The charge response of a superconductor is given in the thermal Green's-function formulation[3]:

$$\rho(1,\omega_n) = \sum_n \{G(1,\bar{2};\omega_n-\omega_m)G(\bar{2},1;\omega_n) - F(1,\bar{2};\omega_n)\bar{F}(1,\bar{2};-(\omega_n-\omega_m))\}\varphi(\omega_m,\bar{2}) = P(1,\bar{2};\omega_m)\varphi(\bar{2},\omega_m). \quad (1)$$

In Eq. (1), G and F are solutions of the Gor'kov equations,[4]

$$G(1,2) = G^0(1,2) - \Delta(\bar{2})\bar{F}(\bar{2},2)G^0(1,\bar{2}),$$
$$F(1,2) = \Delta(\bar{2})G(2,\bar{2})G^0(1,\bar{2}); \quad (2)$$

$\varphi(\bar{2},\omega_m)$ is the scalar potential induced by the sound wave; and

$$\omega_m = 2m\pi/\beta, \quad \omega_n = (2n+1)\pi/\beta \quad (n,m \text{ integer}).$$