Pressure and density of vacancies in solid ^{4}He

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Crystals of ^{4}He contain vacancies that move around by a quantum-mechanical hopping process. The density and pressure of these vacancies can be experimentally studied. The accuracy of the experiments is high enough to detect the effect of the Bose statistics of the vacancies. In this paper we examine the effect of the hard-core repulsion between the vacancies, which should also have a measurable effect on their behavior. We set up a virial expansion for a lattice gas of hard-core particles, and calculate the second virial coefficient. It turns out that the vacancies behave as ideal Bose particles at low temperatures, but that the hard-core interaction makes them behave more and more like fermions as the temperature increases.

I. INTRODUCTION

The thermodynamic behavior of vacancies in solid ^{4}He is an interesting experimental and theoretical problem.[1] Vacancies in helium are more mobile than in any other solid. At the temperatures where solid helium exists the motion of vacancies requires a quantum-mechanical description. They hop from site to site with a certain rate ν_v, leading to a band of states $\varepsilon(\mathbf{k})$, much like the electron motion in the tight-binding approximation. For ^{4}He the vacancies are obviously bosons, since the creation operator for a vacancy is the annihilation operator for a ^{4}He particle, which is a boson.[2] The fact that two vacancies cannot occupy the same lattice site has to be incorporated as a hard-core potential for the hopping bosons. So the simplest model for vacancies in ^{4}He is that of a gas of hard-core bosons on a lattice. In reality the strain fields around the vacancies produce a more complicated interaction between them than the simple on-site exclusion. However, we consider the hard-core boson approximation as a sufficiently realistic description of the vacancy motion to leave out these further refinements, in order not to complicate the model too much.

Experiments show that the percentage of vacancies in a crystal is at most of the order of 1%,[3] at least at temperatures of the order of 1 K, where the experiments take place. As a first approximation the vacancies thus behave as an ideal gas. However, present day experiments are sufficiently accurate that effects of Bose statistics can be detected. It is one of our points that then also effects of the hard-core interaction become detectable.

In this paper we present a systematic analysis of the vacancies using $\exp(-\Delta/k_BT)$ as a small parameter, Δ being the excitation energy, or band gap, required to create a vacancy. This is equivalent to a virial expansion[4] for the quantum lattice gas, and we work out the properties in detail up to the second virial coefficient. A general formula for the second virial coefficient of the hard-core Bose lattice gas is derived and evaluated for hypercubic lattices in one, two, and three dimensions. The case of the hcp lattice, which applies to real solid ^{4}He, will be treated elsewhere.

II. THE HARD-CORE BOSE LATTICE GAS

The vacancies are represented by Bose creation and annihilation operators $b_i^\dagger, b_i$ obeying the usual Bose commutation relations. The Hamiltonian for the vacancies is given by

$$\mathcal{H} = -t\sum_{\langle i,j\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + (\Delta + ct)\sum_i b_i^\dagger b_i + \frac{U}{2}\sum_i b_i^\dagger b_i^\dagger b_i b_i. \tag{2.1}$$

Here the transfer integral t is equal to $h\nu_v$, and the hops take place between all pairs of nearest neighbors $\langle i,j\rangle$ on the lattice. The coordination number of the lattice is c, and Δ is the energy required to create a vacancy. It functions as minus the chemical potential for the vacancies. The last term represents the vacancy-vacancy repulsion. We will let $U \to \infty$, or U is much larger than any other energy in the problem.

Without the potential term we have an ideal Bose lattice gas, the Hamiltonian of which is diagonal in momentum space,

$$\mathcal{H}_0 = \sum_k [\Delta + \varepsilon(\mathbf{k})] b^\dagger(\mathbf{k}) b(\mathbf{k}). \tag{2.2}$$

Here $b(\mathbf{k}) = \frac{1}{\sqrt{N}}\sum_j b_j e^{i\mathbf{k}\cdot\mathbf{r}_j}$ (N is the number of sites, and periodic boundary conditions are used), and the energy band $\varepsilon(\mathbf{k})$ is given by

$$\varepsilon(\mathbf{k}) = t\sum_\delta (1 - \cos\mathbf{k}\cdot\mathbf{r}_\delta), \tag{2.3}$$

where $\mathbf{r}_\delta$ is the set of the c nearest neighbor positions with respect to any site. Δ is the gap of the energy band, since we have $\varepsilon(\mathbf{0}) = 0$ as lowest energy in the center of the Brillouin zone. One sees that t is a measure for the bandwidth, which for a d-dimensional hypercubic lattice is $w = 4dt$.

The interaction is written in terms of $b^{(\dagger)}(\mathbf{k})$ as

$$V = \frac{U}{2N}\sum_{\mathbf{k}_i,\mathbf{G}} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4+\mathbf{G}} b^\dagger(\mathbf{k}_1)b^\dagger(\mathbf{k}_2)b(\mathbf{k}_3)b(\mathbf{k}_4), \tag{2.4}$$

where $\mathbf{G}$ is a vector of the reciprocal lattice. The matrix elements of the interaction have no other structure than the conservation of the total incoming and outgoing momentum (up to a reciprocal lattice vector), a feature which is of great advantage in solving the two-particle problem.

III. THE VIRIAL EXPANSION

The grand partition function of the vacancy system is given by

$$\Xi = \mathrm{Tr}\, e^{-\beta\mathcal{H}} = \sum_{n=0}^{\infty} Z_n e^{-n\beta\Delta}, \tag{3.1}$$

where $\beta = 1/k_BT$, Tr stands for the trace over all symmetrized states, and Z_n is the canonical partition sum for n vacancies excluding the contribution from the gap Δ. Of course, $Z_0 = 1$, and

$$Z_1 = \mathrm{Tr}_1\, e^{-\beta(\mathcal{H}_0-\Delta)} = \sum_{\mathbf{k}} e^{-\beta\varepsilon(\mathbf{k})}, \tag{3.2}$$

because for one vacancy no hard-core effects enter. Tr_n is the trace over n-vacancy states.

For $\ln\Xi$ we may deduce from (3.1)

$$\beta p N v_0 = \ln\Xi = N\sum_{\ell=1}^{\infty} b_\ell e^{-\ell\beta\Delta}, \tag{3.3}$$

where v_0 is the volume of the unit cell, p is the pressure of the vacancies, and the b_ℓ are the fugacity expansion coefficients. The first of these, b_1, reads

$$b_1(\beta) = \frac{1}{N}Z_1 = \frac{v_0}{(2\pi)^d}\int_{\mathrm{BZ}} d\mathbf{k}\, e^{-\beta\varepsilon(\mathbf{k})}, \tag{3.4}$$

where we have replaced the sum over $\mathbf{k}$ by an integral over the Brillouin zone. For temperatures so low that $\varepsilon(\mathbf{k})$ may be replaced by its low-momentum behavior, we find the familiar result for the continuum case,

$$b_1 = v_0/\lambda^d, \tag{3.5}$$

with the thermal wavelength $\lambda^2 = h^2/2\pi m^* k_BT$, and the effective mass $m^* = \hbar^2/2ta^2$.

The second term b_2 in (3.3) is our main concern in this paper. It can be written as the sum of two terms by adding and subtracting the contribution of the non-interacting two-vacancy system,

$$b_2 = \frac{1}{N}\left(Z_2 - \frac{Z_1^2}{2}\right) = b_2^0 + b_2^{\mathrm{int}}. \tag{3.6}$$

The two terms are given by

$$b_2^{\mathrm{int}} = \frac{1}{N}\mathrm{Tr}_2\left[e^{-\beta(\mathcal{H}-2\Delta)} - e^{-\beta(\mathcal{H}_0-2\Delta)}\right], \tag{3.7}$$

the contribution of the hard-core interaction, and

$$b_2^0 = \frac{1}{N}\left[\mathrm{Tr}_2\, e^{-\beta(\mathcal{H}_0-2\Delta)} - \frac{1}{2}\left(\mathrm{Tr}_1\, e^{-\beta(\mathcal{H}_0-\Delta)}\right)^2\right], \tag{3.8}$$

the effect of the Bose statistics of the vacancies.

The statistical effects are trivial to calculate, and we find for the unperturbed system that

$$b_\ell^0 = \frac{1}{N\ell}\sum_{\mathbf{k}} e^{-\ell\beta\varepsilon(\mathbf{k})} = \frac{1}{\ell}b_1(\beta\ell), \tag{3.9}$$

with $b_1(\beta)$ given by (3.4). Thus it suffices to focus our attention on the calculation of b_2^{int}. As a general observation we note that the two contributions in (3.6) will have opposite signs. To see this more clearly, we go over to a series in the density n of the vacancies,

$$n = \frac{1}{Nv_0}\left\langle\sum_i b_i^\dagger b_i\right\rangle = -\partial p/\partial\Delta = \frac{1}{v_0}\sum_{\ell=1}^{\infty} \ell b_\ell e^{-\ell\beta\Delta}. \tag{3.10}$$

Eliminating $e^{-\beta\Delta}$ from (3.3) and (3.10) we obtain a virial expansion for the pressure

$$\beta p = n - (b_2/b_1^2)v_0 n^2 + \cdots\ . \tag{3.11}$$

So at fixed density n the statistical effects lower the pressure as b_2^0 is positive according to (3.9). The hard-core repulsion can only increase the pressure, and so b_2^{int} must be negative.

IV. THE SECOND VIRIAL COEFFICIENT

The second virial coefficient (3.7) is evaluated as

$$b_2^{\mathrm{int}} = \frac{1}{N}\int dE\,\left[\rho_2(E) - \rho_2^0(E)\right] e^{-\beta(E-2\Delta)}, \tag{4.1}$$

where the level densities $\rho_2(E)$ can be obtained from the Green's function,

$$\rho_2(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}_2\,\mathcal{G}_+(E). \tag{4.2}$$

The states of the unperturbed two-vacancy Hamiltonian are denoted by two wave numbers $|\mathbf{k}_1\,\mathbf{k}_2\rangle$, and the two-vacancy energy band is given by

$$E_0(\mathbf{k}_1,\mathbf{k}_2) = 2\Delta + \varepsilon(\mathbf{k}_1) + \varepsilon(\mathbf{k}_2). \tag{4.3}$$

The matrix elements of V are obtained from (2.4),

$$\langle\mathbf{k}_1\,\mathbf{k}_2|V|\mathbf{k}_1'\,\mathbf{k}_2'\rangle = \frac{2U}{N}\sum_{\mathbf{G}} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_1'+\mathbf{k}_2'+\mathbf{G}}, \tag{4.4}$$

which shows that a representation in center-of-mass and relative coordinates will be advantageous. Thus we introduce

$$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2, \qquad \mathbf{k} = (\mathbf{k}_1 - \mathbf{k}_2)/2. \tag{4.5}$$

The sum over $\mathbf{G}$ is eliminated by choosing the Brillouin zone in such a way that no two points in it have values of $\mathbf{K}$ differing by a reciprocal lattice vector, so that only the term with $\mathbf{G} = \mathbf{0}$ contributes. The matrix element of V is then diagonal in $\mathbf{K}$. From now on we will assume that the Brillouin zone has been chosen in such a way, and drop the reference to $\mathbf{G}$. Since the total momentum $\mathbf{K}$ is conserved by $\mathcal{H}_0$ and V, $\mathcal{G}$ becomes diagonal in it, and we have

$$\langle \mathbf{K}\,\mathbf{k}|\mathcal{G}(z)|\mathbf{K}\,\mathbf{k}'\rangle = \langle \mathbf{K}\,\mathbf{k}|\left[\mathcal{G}_0(z) + \mathcal{G}_0(z)V\mathcal{G}(z)\right]|\mathbf{K}\,\mathbf{k}'\rangle = \frac{1}{z - E_0(\mathbf{K},\mathbf{k})}\left\{\delta_{\mathbf{k},\mathbf{k}'} + \frac{2U}{N}\sum_{\mathbf{k}''}\langle \mathbf{K}\,\mathbf{k}''|\mathcal{G}(z)|\mathbf{K}\,\mathbf{k}'\rangle\right\}. \tag{4.6}$$

The simplifying feature of (4.6) is that the general matrix element of $\mathcal{G}$ couples only to the total sum over the first entry of the matrix elements. For the latter we can obtain an expression by summing (4.6) over $\mathbf{k}$. The result is an algebraic equation for $\sum_{\mathbf{k}}\langle \mathbf{K}\,\mathbf{k}|\mathcal{G}(z)|\mathbf{K}\,\mathbf{k}'\rangle$. Using the solution of this equation in (4.6) one finds

$$\langle \mathbf{K}\,\mathbf{k}|\mathcal{G}(z)|\mathbf{K}\,\mathbf{k}'\rangle = \frac{1}{z - E_0(\mathbf{K},\mathbf{k})}\left\{\delta_{\mathbf{k},\mathbf{k}'} + \frac{2U/N}{1 - 2U\mathcal{R}(z,\mathbf{K})}\frac{1}{z - E_0(\mathbf{K},\mathbf{k}')}\right\}, \tag{4.7}$$

with $\mathcal{R}(z,\mathbf{K})$ given by

$$\mathcal{R}(z,\mathbf{K}) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{z - E_0(\mathbf{K},\mathbf{k})}. \tag{4.8}$$

Note that the off-diagonal elements of (4.7) are of order N^{-1} while the diagonal elements are of order 1.

From (4.7) we can now calculate the trace, leading to the compact expression

$$\mathrm{Tr}\,\mathcal{G}(z) = \mathrm{Tr}\,\mathcal{G}_0(z) + \frac{\partial}{\partial z}\sum_{\mathbf{K}}\ln\left[1 - 2U\mathcal{R}(z,\mathbf{K})\right], \tag{4.9}$$

which in turn yields for the difference $\rho_2 - \rho_2^0$

$$\rho_2(E) - \rho_2^0(E) = -\frac{1}{\pi}\,\mathrm{Im}\left[\frac{\partial}{\partial z}\sum_{\mathbf{K}}\ln\left(1 - 2U\mathcal{R}(z,\mathbf{K})\right)\right]_{z=E+i\epsilon}. \tag{4.10}$$

This expression holds generally for any on-site repulsion U. We may let $U \to \infty$, by which it will disappear from the formula as the U term under the logarithm starts to dominate the argument for any z and $\mathbf{K}$. Omitting the 1 in the argument of the logarithm, the term $\ln(-2U)$ drops out after differentiation with respect to z. So for (4.10) we have in the limit $U \to \infty$ the equivalent expression

$$\rho_2(E) - \rho_2^0(E) = -\frac{1}{\pi}\,\mathrm{Im}\left[\frac{\partial}{\partial z}\sum_{\mathbf{K}}\ln\mathcal{R}(z,\mathbf{K})\right]_{z=E+i\epsilon}. \tag{4.11}$$

Hereby the problem is essentially reduced to the evaluation of $\mathcal{R}(z,\mathbf{K})$ given by (4.8).

A few comments are in order about this expression. For bosons the state $|\mathbf{k}_1\,\mathbf{k}_2\rangle$ is the same as $|\mathbf{k}_2\,\mathbf{k}_1\rangle$. So the relative momenta $\mathbf{k}$ and $-\mathbf{k}$ should be identified with each other. Both $\mathbf{k}_1$ and $\mathbf{k}_2$ run through a Brillouin zone appropriate for the structure of the lattice, and this in principle defines the ranges of $\mathbf{K}$ and $\mathbf{k}$. But as was mentioned before, we have chosen the Brillouin zone such that there are no points whose values of $\mathbf{K}$ differ by a reciprocal lattice vector.

The expression (4.1) for the second virial coefficient can be further simplified by changing the integration variable so as to eliminate the shift 2Δ in the energy, and by making use of the fact that $\mathrm{Im}\ln z = \arg z$. The result is

$$b_2^{\mathrm{int}} = -\frac{1}{\pi}\int dE\left(\frac{\partial}{\partial E}F(E)\right)e^{-\beta E}, \tag{4.12}$$

with

$$F(E) = \frac{1}{N}\sum_{\mathbf{K}}\arg\mathcal{R}'(z,\mathbf{K})|_{z=E+i\epsilon}, \tag{4.13}$$

and where $\mathcal{R}'(z,\mathbf{K})$ is given by (4.8) with Δ set equal to zero.

From (4.13) one sees that only E values occur in (4.12) which lead to complex values of $\mathcal{R}'(z,\mathbf{K})$. These occur when $z = E + i\epsilon$ is a pole in the $\mathbf{k}$ integration in (4.8). Thus the combined bandwidth of $\varepsilon(\mathbf{K}/2+\mathbf{k}) + \varepsilon(\mathbf{K}/2-\mathbf{k})$ determines the range of E values. This is twice the bandwidth of $\varepsilon(\mathbf{k})$ just as in the ideal Bose contribution (3.9).

V. THE ONE-DIMENSIONAL CASE

We interrupt the general discussion for the treatment of the one-dimensional case of (4.12) and (4.13), as this case is interesting, completely analyzable, and elucidating for the structure of the functions occurring in (4.12) and (4.13).

Using the $d = 1$ band structure (2.3) (with a lattice constant $a = 1$) we find for $b_1(\beta)$ the expression

$$b_1(\beta) = \frac{1}{2\pi}\int_{-\pi}^{\pi}dk\,e^{-2\beta t(1-\cos k)} = e^{-2\beta t}I_0(2\beta t), \tag{5.1}$$

where $I_0(x)$ is a modified Bessel function of the first kind.

For the evaluation of $\mathcal{R}(z,K)$ we rearrange the Brillouin zone in such a way that its boundaries in K,k space are convenient, and also such that no reciprocal lattice vector G enters into the problem. In Fig. 1 we have divided the original Brillouin zone $-\pi < k_1 < \pi$, $-\pi < k_2 < \pi$ into four domains, I, II, III, and IV. Domains I and IV, as well as II and III, refer to the same states, as they are obtained from each other through interchanging $k_1 \leftrightarrow k_2$. So it suffices to take one of each, say, I and III. Now III is equivalent to III′, which follows from III by shifting k_1 over 2π. The combined domain I and III′ is given in K,k space by $0 < K < 2\pi$, $0 < k < \pi$.

Using this parameter space, and putting $z = 4t(\zeta+1+i\epsilon)$, one can write $\mathcal{R}$ explicitly as (dropping the primes)

$$\begin{aligned}\mathcal{R}(\zeta,K) &= \frac{1}{8\pi t}\int_0^\pi dk\,\frac{1}{\zeta+i\epsilon+\cos\frac{K}{2}\cos k}\\ &= \frac{1}{8\pi t}\mathcal{P}\int_0^\pi dk\,\frac{1}{\zeta+\cos\frac{K}{2}\cos k}\\ &\quad -\frac{i}{8t}\int_0^\pi dk\,\delta(\zeta+\cos\frac{K}{2}\cos k),\end{aligned}\tag{5.2}$$

for $\epsilon \downarrow 0$. $\mathcal{P}$ indicates a principal value integral. Two cases must be distinguished: For $|\zeta| > |\cos(K/2)|$, the imaginary part of $\mathcal{R}$ is zero, and for $|\zeta| < |\cos(K/2)|$ its real part is zero. The result for $\arg\mathcal{R}$ is

$$\arg\mathcal{R}(\zeta,K) = \begin{cases}-\pi & [\zeta < -|\cos(K/2)|],\\ -\pi/2 & [|\zeta| \le |\cos(K/2)|],\\ 0 & [\zeta > |\cos(K/2)|].\end{cases}\tag{5.3}$$

These values of $\arg\mathcal{R}$ are plotted in Fig. 2 in the $\zeta, K/2$ plane. Integrating in the K direction, we find for $F(\zeta)$

$$\begin{aligned}F(\zeta) &= \frac{1}{2\pi}\int_0^{2\pi} dK\,\arg\mathcal{R}(\zeta,K)\\ &= \begin{cases}-\pi & (\zeta < -1),\\ -\arccos\zeta & (-1 \le \zeta \le 1),\\ 0 & (\zeta > 1).\end{cases}\end{aligned}\tag{5.4}$$

Using ζ instead of E in (4.12) as integration variable we find

$$b_2^{\rm int} = -\frac{1}{\pi}\int_{-1}^1 d\zeta\,\frac{1}{\sqrt{1-\zeta^2}}e^{-4\beta t(\zeta+1)} = e^{-4\beta t}I_0(4\beta t).\tag{5.5}$$

We now compare this with the result for an ideal lattice gas, given by (3.9),

$$b_2^0 = \frac{1}{2}b_1(2\beta) = \frac{1}{2}e^{-4\beta t}I_0(4\beta t) = -\frac{1}{2}b_2^{\rm int}.\tag{5.6}$$

So the hard-core interaction giving rise to $b_2^{\rm int}$ changes the value of b_2 from b_2^0 into its opposite, or in other words, the Bose value is turned into the Fermi value. This is exactly what has to be expected from the well known fact that a hard-core Bose gas in one dimension is equivalent to an ideal Fermi gas (for all virial coefficients).

The picture shown in Fig. 2 for $\arg\mathcal{R}$ has some general validity, in the sense that for sufficiently negative ζ one has $\arg\mathcal{R} = -\pi$ while for ζ sufficiently positive $\arg\mathcal{R} = 0$. In the zone in between, one has for $d > 1$ a continuous transition from $-\pi$ to 0, in general, with eventually also zones with $\arg\mathcal{R} = -\pi/2$.

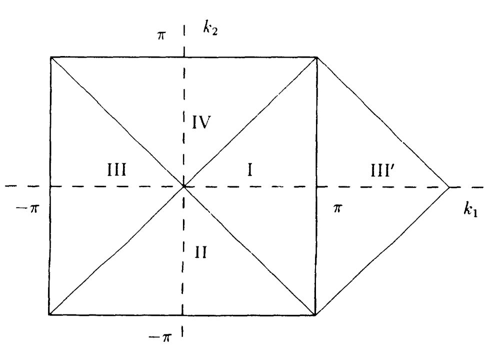

FIG. 1. The Brillouin zone for the one-dimensional problem. Domains I and III′ are the Brillouin zone used in the calculation.

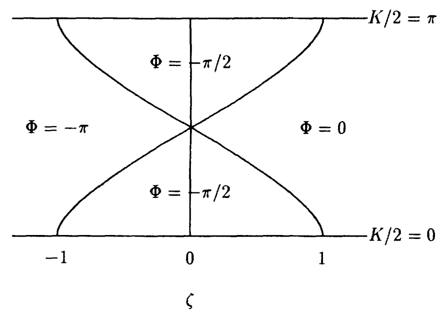

FIG. 2. The phase $\Phi(\zeta,K) = \arg\mathcal{R}(\zeta,K)$ in the $\zeta, K/2$ plane.

VI. THE TWO- AND THREE-DIMENSIONAL LATTICES

The calculation of b_2 for hypercubic lattices in higher dimensions runs along the same lines as what was done in Sec. V for one dimension. Using the one-vacancy band structure (2.3) with $a=1$ in d dimensions, $b_1(\beta)$ is simply found to be

$$\begin{aligned}b_1(\beta) &= \frac{1}{(2\pi)^d}\left[\int_{-\pi}^{\pi} dk\,e^{-2\beta t(1-\cos k)}\right]^d\\ &= e^{-2d\beta t}\left[I_0(2\beta t)\right]^d.\end{aligned}\tag{6.1}$$

As before, we rearrange the Brillouin zone such that its boundaries in $\mathbf{K},\mathbf{k}$ space are convenient. The different components of $\mathbf{K},\mathbf{k}$ are independent, and we have $0 \le K_i \le 2\pi$, $0 \le k_x \le \pi$, $-\pi \le k_y, k_z \le \pi$. The k_x interval is halved to avoid counting the same (symmetric) state twice. The two-vacancy energy bands are given by

$$E_0(\mathbf{K},\mathbf{k}) = 4t\left(2-\cos\frac{K_x}{2}\cos k_x - \cos\frac{K_y}{2}\cos k_y\right) \quad (d=2),$$

$$E_0(\mathbf{K},\mathbf{k}) = 4t\left(3-\cos\frac{K_x}{2}\cos k_x - \cos\frac{K_y}{2}\cos k_y - \cos\frac{K_z}{2}\cos k_z\right) \quad (d=3). \tag{6.2}$$

We scale the parameter z as

$$z = \begin{cases} 8t(\zeta+1+i\epsilon) & (d=2), \\ 12t(\zeta+1+i\epsilon) & (d=3), \end{cases} \tag{6.3}$$

so that in both cases the energy band runs from $\zeta=-1$ to $\zeta=1$.

In two dimensions we find with (5.2)

$$\mathcal{R}_2(\zeta,\mathbf{K}) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} dk_y \int_0^{\pi} dk_x \frac{1}{8t}\left[\zeta + i\epsilon + \frac{1}{2}\left(\cos\frac{K_x}{2}\cos k_x + \cos\frac{K_y}{2}\cos k_y\right)\right]^{-1}$$
$$= \frac{1}{32t\pi}\int_{-\pi}^{\pi} dk_y \frac{f(A,B)}{\sqrt{|A^2-B^2|}}, \tag{6.4}$$

where

$$A = \zeta + \frac{1}{2}\cos\frac{K_y}{2}\cos k_y, \quad B = \frac{1}{2}\cos\frac{K_x}{2}, \tag{6.5}$$

and

$$f(A,B) = \begin{cases} \operatorname{sgn}(A) & (A^2 > B^2), \\ -i & (A^2 < B^2). \end{cases} \tag{6.6}$$

The integral in (6.4) can be expressed in terms of complete elliptic integrals of the first kind (see the Appendix). This gives an analytic expression for $\mathcal{R}_2(\zeta,\mathbf{K})$.

This expression can also be used to find the result in three dimensions,

$$\mathcal{R}_3(\zeta,\mathbf{K}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_z \frac{1}{32t\pi}\int_{-\pi}^{\pi} dk_y \int_0^{\pi} dk_x \left[\tilde{\zeta} + i\epsilon + \frac{1}{2}(\cos\frac{K_x}{2}\cos k_x + \cos\frac{K_y}{2}\cos k_y)\right]^{-1}$$
$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_z \mathcal{R}_2(\tilde{\zeta},K_x,K_y), \tag{6.7}$$

where

$$8t(\tilde{\zeta}+1) = 12t(\zeta+1) - 4t\left(1-\cos\frac{K_z}{2}\cos k_z\right). \tag{6.8}$$

Using the analytic expression found for $\mathcal{R}_2$, $\mathcal{R}_3$ can be calculated by numerical integration of (6.7).

The next step is to obtain $F(\zeta)$ as given in (4.13) by integrating over $\mathbf{K}$. This is done numerically using Monte Carlo integration. The result is a function $F(\zeta)$ that is equal to $-\pi$ for $\zeta < -1$, where $\mathcal{R}_d$ is real and negative, equal to 0 for $\zeta > 1$, where $\mathcal{R}_d$ is real and positive, and that is in between these two values for $\zeta \in [-1,1]$, where $\mathcal{R}_d$ is complex. It follows from the symmetry of $\mathcal{R}_d$ that

$$F(-\zeta) = -\pi - F(\zeta). \tag{6.9}$$

Using $F(\zeta)$, $b_2^{\rm int}$ can be found from Eq. (4.12). Partial integration gives

$$b_2^{\rm int} = -e^{-4d\beta t}\left\{1 - \frac{8d\beta t}{\pi}\int_0^1 d\zeta F(\zeta)\sinh 4d\beta t\zeta\right\}. \tag{6.10}$$

To find $b_2^{\rm int}$, this equation can be numerically integrated for various values of βt.

As before, we compare this with the result for the ideal lattice gas (3.9)

$$b_2^0 = \frac{1}{2}b_1(2\beta) = \frac{1}{2}e^{-4d\beta t}[I_0(4\beta t)]^d. \tag{6.11}$$

The ratio $b_2^{\rm int}/b_2^0$ is given by

$$b_2^{\rm int}/b_2^0 = \frac{-2}{[I_0(4\beta t)]^d}\left\{1 - \frac{8d\beta t}{\pi}\int_0^1 d\zeta F(\zeta)\sinh 4d\beta t\zeta\right\}. \tag{6.12}$$

For $\beta t \to 0$, this ratio goes to -2. The second virial coefficient $b_2 = b_2^0 + b_2^{\rm int}$ thus approaches $-b_2^0$ for high temperatures. This is indicative of fermionic behavior, which is indeed what one would expect: At high temperatures, the only important contribution to the free energy of the system is the entropy involved in distributing a certain number of hard-core particles over the lattice. This is the same as for fermions. For $\beta t \to \infty$ the behavior of (6.12) depends on the behavior of $F(\zeta)$ for $\zeta \to 1$. In two dimensions, $F(\zeta) \propto (1-\zeta)/\ln(1-\zeta)$, which leads to $b_2^{\rm int}/b_2^0$ going to zero like $-1/\ln(\beta t)$ as $\beta t \to \infty$. The same low-temperature behavior is found for quantum hard disks.[5] In three dimensions, $F(\zeta) \propto (1-\zeta)^2$, which gives $b_2^{\rm int}/b_2^0 \propto -1/\sqrt{\beta t}$ for $\beta t \to \infty$, just as for quantum hard spheres.[6] So, in both cases, b_2 approaches

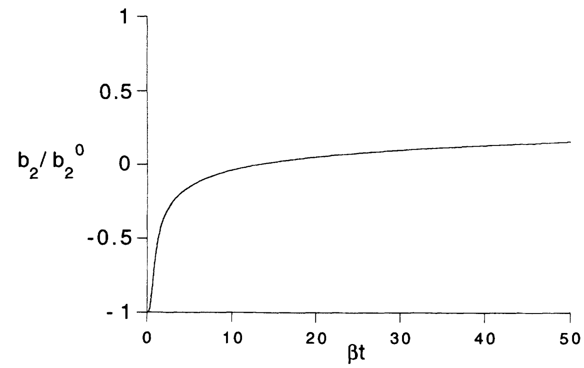

FIG. 3. The ratio b_2/b_2^0 as a function of βt for the square lattice. For high temperatures (small βt), $b_2 = -b_2^0$, which is the same value as for fermions. For lower temperatures its value crosses over to $b_2 = b_2^0$, the ideal boson value.

the value for the ideal Bose gas at low temperatures. This shows that when the thermal wavelength λ exceeds the lattice constant $a(=1)$, the effects of the Bose statistics starts to dominate. Plots of b_2/b_2^0 versus βt for two and three dimensions are given in Figs. 3 and 4.

VII. CONCLUSION

The pressure and density of a gas of quantum particles on a lattice can be expressed in fugacity expansions,

$$p = \frac{1}{\beta v_0} \sum_{\ell=1}^{\infty} b_\ell e^{-\ell\beta\Delta}, \tag{7.1}$$

$$n = \frac{1}{v_0} \sum_{\ell=1}^{\infty} \ell b_\ell e^{-\ell\beta\Delta}. \tag{7.2}$$

For bosons with a hard-core interaction, the first two coefficients, b_1 and b_2, can be calculated. It turns out that the effect of the hard-core interaction on b_2 depends strongly on temperature and on the transfer integral t. For small βt it is fermionic in character, as far as b_2 is concerned. For large βt the effect of the hard-core disappears, and only the Bose character remains.

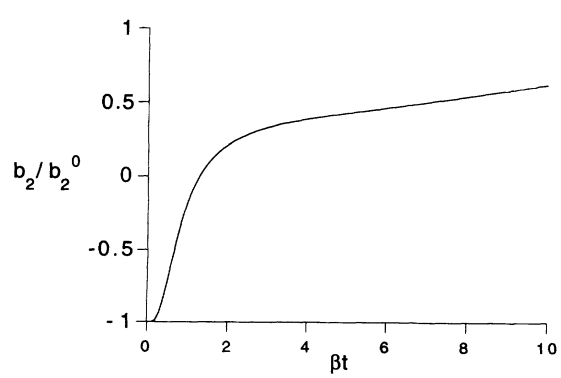

FIG. 4. The ratio b_2/b_2^0 as a function of βt for the cubic lattice. Note that the crossover to the ideal boson value is much faster than for the square lattice.

The system of vacancies that exists in solid ^{4}He should behave to a good approximation like this simple model: The vacancies move through the crystal lattice by a tunneling process, they are bosons, and they have a hard-core repulsion. The gas of vacancies has been experimentally studied by probing the attenuation and the velocity shift of sound in a ^{4}He crystal.[3] Very pure hcp helium was used, so that the effects of both the phonons and the delocalized, bosonic vacancies could be observed. Treating the vacancies as a gas of free particles, it was seen that they obey Bose statistics. For the expressions (7.1) and (7.2) this means that not only the first term, but at least also the second is experimentally observable. One can use the expressions (3.5) and (3.9) for a gas of free, ideal bosons to estimate the order of magnitude of the various terms in (7.1) and (7.2). One finds that $b_\ell^0 = v_0/\ell^{5/2}\lambda^3$, so that

$$p = \frac{1}{\beta\lambda^3} \sum_{\ell=1}^{\infty} \frac{e^{-\ell\beta\Delta}}{\ell^{5/2}}, \tag{7.3}$$

$$n = \frac{1}{\lambda^3} \sum_{\ell=1}^{\infty} \frac{e^{-\ell\beta\Delta}}{\ell^{3/2}}. \tag{7.4}$$

Using the value $\Delta/k_B = 0.71$ K found in Ref. 3, and the maximum temperature $T = 0.85$ K at which the experiments were performed, this shows that the ratio between the second and first terms in (7.4) is 0.15, and that between the third and first terms is 0.04.

If experiments can be done that detect the contribution of 15% of the second term in (7.4), it is also possible to detect the effects of the hard-core on the coefficient b_2 in (7.2). As can be seen from Fig. 4, it varies considerably with βt, and it can even change sign. However, it is difficult to extract this information from the attenuation experiment, since there it is not clear what exactly the relation between the measured quantities and the vacancy density is. It would be necessary to directly measure, say, the pressure due to the vacancies,[7] and then compare this with (7.1). In such an experiment it would be crucial to take the hard-core effects into account. Work is in progress to calculate the coefficient b_2 for the hcp lattice; however, the results are not expected to differ much from those given for the simpler cubic lattice here.

The results for the two-dimensional system might have relevance for low-density ^{4}He films on textured substrates.[8] There, the presence of adsorption sites localizes the helium particles on the points of a two-dimensional lattice, defined by the substrate. Thus the tight-binding approach used in this paper becomes applicable. The adsorption sites cannot hold more than one particle, so that the hard-core repulsion is also present.

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APPENDIX

The integral (6.4) can be expressed in terms of elliptic integrals as follows.[9,10] $\mathcal{R}_2$ is equal to

$$\mathcal{R}_2(\zeta,\mathbf{K}) = \frac{1}{16t\pi}\int_{A^2>B^2} dk_y \frac{\mathrm{sgn}(A)}{\sqrt{A^2-B^2}} - \frac{i}{16t\pi}\int_{A^2<B^2} dk_y \frac{1}{\sqrt{B^2-A^2}}, \tag{A1}$$

where $k_y \in [0,\pi]$. On making the substitution $p = \cos k_y$, and writing

$$A^2 - B^2 = \frac{\cos^2(K_y/2)}{4}(q_1-p)(q_2-p), \tag{A2}$$

where

$$q_1 = \frac{-2\zeta + \cos(K_x/2)}{\cos(K_y/2)}, \qquad q_2 = \frac{-2\zeta - \cos(K_x/2)}{\cos(K_y/2)}, \tag{A3}$$

we end up with integrals of the type

$$\int dp \frac{1}{\sqrt{|w|}}, \tag{A4}$$

where $w = (1-p)(1+p)(q_1-p)(q_2-p)$ and $p \in [-1,1]$. By defining

$$q_- = \min(q_1,q_2), \qquad q_+ = \max(q_1,q_2), \tag{A5}$$

we see that values of $p \in [q_-,q_+]$ give $A^2 < B^2$, and thus contribute to the imaginary part of $\mathcal{R}_2$. Values of p outside this interval give $A^2 > B^2$ and thus contribute to the real part, for $p < q_-$ with $\mathrm{sgn}(A) = -\mathrm{sgn}[\cos(K_y/2)]$, and for $p > q_+$ with $\mathrm{sgn}(A) = \mathrm{sgn}[\cos(K_y/2)]$. The result is a sum of integrals of the type (A4) between limits that are consecutive zeros of w. These integrals can all be expressed in terms of the complete elliptic integral of the first kind, $K(x)$,[11]

$$K(x) = \int_0^1 dp \frac{1}{\sqrt{(1-p^2)(1-x^2p^2)}} \qquad (x \in [0,1]). \tag{A6}$$

There are several cases to be considered:

(1a): $q_-, q_+ < -1$ and (1b): $q_-, q_+ > 1$

$$\mathcal{R}_2(\zeta,\mathbf{K}) = \frac{\epsilon}{4t\pi\cos(K_y/2)}\frac{K(r_1)}{\sqrt{(q_+-1)(q_-+1)}}, \tag{A7}$$

where $\epsilon = +$ for (1a) and $\epsilon = -$ for (1b).

(2): $q_- < -1, q_+ > 1$ or $q_-, q_+ \in [-1,1]$

$$\mathcal{R}_2(\zeta,\mathbf{K}) = \frac{-i}{4t\pi|\cos(K_y/2)|}\frac{K(r_2)}{\sqrt{(q_++1)(1-q_-)}}. \tag{A8}$$

(3a): $q_- < -1, q_+ \in [-1,1]$ and (3b): $q_- \in [-1,1], q_+ > 1$

$$\mathcal{R}_2(\zeta,\mathbf{K}) = \frac{\epsilon}{4t\pi\cos(K_y/2)}\frac{K(1/r_1)}{\sqrt{2(q_+-q_-)}} - \frac{i}{4t\pi|\cos(K_y/2)|}\frac{K(1/r_2)}{\sqrt{2(q_+-q_-)}}, \tag{A9}$$

where $\epsilon = +$ for (3a) and $\epsilon = -$ for (3b). In the above, r_1 and r_2 are given by

$$r_1 = \sqrt{\frac{2(q_+-q_-)}{(q_+-1)(q_-+1)}}, \qquad r_2 = \sqrt{\frac{2(q_+-q_-)}{(q_++1)(1-q_-)}}. \tag{A10}$$

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