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Bose–Einstein Condensation in an Exactly Soluble System of Interacting Particles

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The model investigated recently by Tóth, a lattice gas of bosons with hard-core repulsion on a complete graph, is studied here by diagonalizing the Hamiltonian. The thermodynamic free energy per site is shown to be f, where

$$\beta f = \beta \rho^2 + \min_{0 \leqslant x \leqslant \mathrm{Min}(\rho, 1-\rho)} \{\beta x(1-x) + x \log x + (1-x)\log(1-x)\}$$

where β is the inverse temperature and $\rho \in [0, 1]$ is the number of particles per site. This formula is equivalent to the one obtained by Tóth. There is a phase transition at $\beta = \beta^*(\rho) = (1-2\rho)^{-1} \log[(1-\rho)/\rho]$. If $\beta \geqslant \beta^*(\rho)$, Bose–Einstein condensation is shown to be present, the condensate density (number of condensed particles per site) in the thermodynamic limit being $[\rho - x^*][1-\rho-x^*]$, where x^* is the minimizing value of x, satisfying $\beta^*(x^*) = \beta$.

KEY WORDS: Bose–Einstein condensation; quantum lattice gas; XY model; mean-field theories.

1. INTRODUCTION

A recent paper by Tóth$^{(15)}$ shows that the thermodynamic functions for a lattice gas of bosons on a complete graph, the only interaction being an "on-site" hard-core repulsion, can be calculated exactly. His method uses results from large-deviation theory applied to the random walk representation of the partition function. (This representation is the discrete analogue of the Feynman–Kac formula.) From a statistical mechanics points of view, his most interesting result is that the Bose system shows a phase transition, whereas the corresponding Fermi system does not. It is natural to interpret

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This paper is dedicated to Joel L. Lebowitz on the occasion of this 60th birthday.

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this phase transition as the analogue of the condensation, first noted by Einstein,(3) which is exhibited by an ideal Bose gas in a continuous space of three or more dimensions.

Bose–Einstein condensation in an interacting system is of interest to the physicist because of its importance in the theory of liquid helium-4. Experiment shows(13) that liquid helium-4 has a Bose condensate—that is,(12) a finite fraction of the particles all in the same one-particle quantum state—and the hypothesis that such a condensate is present provides the microscopic basis for our current theoretical understanding of superfluidity in bulk liquid helium-4. One is therefore naturally led to ask whether the system studied by Tóth has such a condensate. The purpose of the present paper is to show that it does and, moreover, to give an explicit formula for the condensate density. At the same time, we also exhibit a new method for studying this system; instead of Tóth's random walk representation, we calculate the eigenvalues and eigenfunctions of the Hamiltonian operator. This leads to a simpler formula for the thermodynamic functions, which turn out to be almost identical with those of the Bragg–Williams theory.

The main results of this paper can be summarized in the following theorems.

Theorem 1. The thermodynamic free energy per site f at inverse temperature β is given (in units where the energy levels of the one-particle system are 0 and 1) by

$$\beta f = \beta\rho^2 + \operatorname*{Min}_{0 \leqslant x \leqslant \operatorname{Min}(\rho, 1-\rho)} \{\beta x(1-x) + x\log x + (1-x)\log(1-x)\} \tag{1}$$

$$= \begin{cases} \beta\rho + \rho\log\rho + (1-\rho)\log(1-\rho) & \text{if } \beta \leqslant \beta^*(\rho) \quad (2) \\ \beta\rho^2 + \beta\rho^*(1-\rho^*) + \rho^*\log\rho^* + (1-\rho^*)\log(1-\rho^*) & \text{if } \beta \geqslant \beta^*(\rho) \quad (3) \end{cases}$$

where ρ is the number of particles per site, and $\beta^*(\rho)$ is defined by

$$\beta^*(\rho) = \frac{1}{1-2\rho}\log\frac{1-\rho}{\rho} = \frac{2\operatorname{arctanh}(1-2\rho)}{1-2\rho} \quad \text{if} \quad \rho \neq \frac{1}{2} \quad (0<\rho<1) \tag{4}$$

and by continuity if $\rho = 1/2$ [i.e., $\beta^*(1/2) = 2$] (see Fig. 1), and where in the case $\beta > \beta^*(\rho)$ we denote by $\rho^*(\beta)$ the minimizing value of x, which is the smaller of the two values of ρ^* satisfying

$$\beta^*(\rho^*) = \beta \tag{5}$$

The proof of this theorem is given in Section 7.

Corollary. There is a phase transition when $\beta = \beta^*(\rho)$.

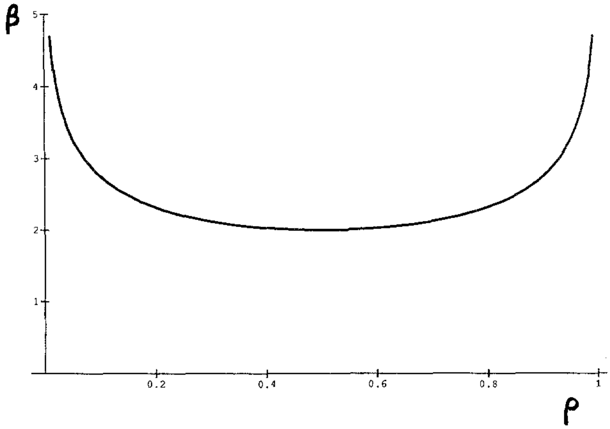

Fig. 1. Phase diagram of the system considered. Bose–Einstein condensation is present for points above the phase transition curve, but not for those below it. The equation of the curve is $\beta = \beta^*(\rho)$, i.e., $\beta = 2[\operatorname{arctanh}(1-2\rho)]/(1-2\rho)$. The left-hand half of the curve can also be interpreted as a graph of the equation $\rho = \rho^*(\beta)$, turned on its side.

Theorem 2. The condensate density ρ_c (number of condensed particles per site) is given in the thermodynamic limit by

$$\rho_c = \begin{cases} 0 & \text{if } \beta \leqslant \beta^*(\rho) \\ [\rho - \rho^*(\beta)][1-\rho-\rho^*(\beta)] & \text{if } \beta \geqslant \beta^*(\rho) \end{cases} \tag{6}$$

The proof of this theorem is given in Section 9.

Corollary. Bose–Einstein condensation, that is, a nonvanishing value of ρ_c, is present if and only if $\beta > \beta^*(\rho)$. The critical exponent for ρ_c is 1, i.e., $\rho_c \propto (\beta - 2)[1 + o(1)]$ as $\beta \searrow 2$ at $\rho = 1/2$.

Proof of Corollary. An expansion of Eq. (4) gives $\beta^*(\rho) = 2 + \frac{2}{3}(1-2\rho)^2 + \cdots$ and hence, by (5), $1 - 2\rho^* = [\frac{3}{2}(\beta - 2)]^{1/2} + \cdots$. Substituting in (6) and setting $\rho = 1/2$, we obtain (for $\beta \geqslant 2$) $\rho_c = \frac{3}{8}(\beta - 2) + O(\beta - 2)^2$, as required.

2. DEFINITION OF THE SYSTEM

For a general quantum lattice gas on a lattice Λ the Hamiltonian H is defined by

$$\begin{aligned} H\psi(x_1,\ldots,x_N) &= -\sum_{i=1}^{N}\sum_{y\in\Lambda} c(x_i,y)[\psi(x_1,\ldots,x_{i-1},y,x_{i+1},\ldots,x_N)-\psi(x_1,\ldots,x_n)] \\ &\quad + U(x_1,\ldots,x_N)\,\psi(x_1,\ldots,x_N) \end{aligned} \tag{7}$$

where $x_1,\ldots,x_N$ are lattice sites, $c(x, y)$ is minus the matrix element of the one-particle kinetic energy operator between sites x and y, and U is the potential energy function.

For a periodic lattice such as the simple cubic, $c(x, y)$ would be chosen so as to make the kinetic energy contribution to H for a one-particle system equal to the finite-difference approximation to the continuous-space kinetic energy operator, giving

$$c(x,y)=\begin{cases} \hbar^2/2ma^2 & \text{if } x, y \text{ are joined by a bond in } \Lambda \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

where $2\pi\hbar$ is Planck's constant, m is the mass of a particle, and a is the lattice spacing. Here, however, our lattice is a complete graph, on which every pair of sites is joined by a bond. We therefore take $c(x, y)$ to be a constant, independent of x and y. An appropriate value for this constant would be the average of (8) over all sites. This average is of the form const $\cdot\, V^{-1}$, where V is the number of lattice sites. For simplicity we shall (following Tóth(15)) take the constant to be 1, so that $c(x, y) = V^{-1}$ for all x, y; this amounts to taking the unit of energy to be the energy of the [$(V-1)$-fold degenerate] excited state of the one-particle system.

For the hard-core exclusion interaction we are considering here, the potential energy $U(x_1,\ldots,x_N)$ is 0 if all of $x_1,\ldots,x_N$ are different and otherwise is $+\infty$. Therefore, by (7), we have $\psi(x_1,\ldots,x_N)=0$ if $x_1,\ldots,x_N$ are not all different, and so we may restrict our attention to those states where at most one particle occupies each vertex; moreover, because of the Bose symmetry, it is not necessary to specify which particle is where, only which sites are occupied and which are not. The allowed quantum states of the system therefore lie in the vector space $\mathscr{H}_N$ spanned by a basis set of state vectors for each of which the N particles occupy a different N-vertex subset of the graph, the remaining $V-N$ vertices being unoccupied. Such a basis vector will be denoted by $|X\rangle$, where X denotes the set of occupied vertices. For a given N, there are $V!/N!\,(V-N)!$ such states and hence the dimension of $\mathscr{H}_N$ is $V!/N!\,(V-N)!$.

It will also be useful to consider a larger space $\mathscr{H}$, which is the direct sum of all the $\mathscr{H}_N$ for $N=0, 1,\ldots, V$. In this space, the number of particles is an operator rather than a fixed number; we shall denote this operator by $\hat{N}$. The dimension of the space $\mathscr{H}$ is

$$\sum_{N=0}^{V} V!/[N!\,(V-N)!]=2^V \tag{9}$$

Any state $|\psi\rangle$ can be written as a linear combination of the basis vectors. The coefficient of $|X\rangle$ in this linear combination could be denoted by $\psi(X)$, but Dirac's$^{(2)}$ notation $\langle X|\psi\rangle$ is very convenient for our purposes; thus we have

$$|\psi\rangle=\sum_X |X\rangle\langle X|\psi\rangle \tag{10}$$

where in general the sum goes over all subsets of the graph Γ, but may be restricted to the N-vertex subsets of Γ if $|\psi\rangle$ lies in $\mathscr{H}_N$. In particular, we find, on choosing $|\psi\rangle=|Y\rangle$, where Y is any subset of Γ, that

$$\langle X|Y\rangle=\begin{cases}1 & \text{if}\quad X=Y\\ 0 & \text{otherwise}\end{cases} \tag{11}$$

In this notation, the definition (7) of the Hamiltonian, with $c(x,y)=V^{-1}$ for all x, y, reads

$$\langle X|\,H\,|\psi\rangle=V^{-1}\left\{N(V-1)\langle X|\psi\rangle-\sum_{x\in X}\ \sum_{y\in\Gamma-X}\langle (X-x)\cup y\,|\psi\rangle\right\} \tag{12}$$

where $X-x$ means $X\backslash\{x\}$. Setting $|\psi\rangle=|Y\rangle$, where Y is an arbitrary subset of Γ, we obtain

$$\langle X|\,H\,|Y\rangle=\begin{cases}(1-V^{-1})\;\#(X) & \text{if}\quad X=Y\\ -V^{-1} & \text{if}\quad \#(X)=\#(Y)\text{ and }\#(X\triangle Y)=2\\ 0 & \text{otherwise}\end{cases} \tag{13}$$

where $\#(X)$ denotes the number of elements in the set X and $X\triangle Y$ denotes the set of vertices that are in just one of X and Y.

3. A FACTORIZATION OF THE HAMILTONIAN

The basis of our method is a factorization technique. We define an operator A whose matrix elements are

$$\langle X|\,A\,|Y\rangle=\begin{cases}V^{-1/2} & \text{if}\quad X=Y-x\text{ for some site }x\text{ in }Y\\ 0 & \text{if not}\end{cases} \tag{14}$$

As we shall see in more detail in Section 9, this operator can be thought of as destroying one particle in the single-particle state of lowest energy. Its adjoint A^+ has matrix elements

$$\langle Y|\, A^+\, |X\rangle = \begin{cases} V^{-1/2} & \text{if } \quad X = Y - x \text{ for some site } x \text{ in } Y \\ 0 & \text{if not} \end{cases} \tag{15}$$

The matrix elements of A^+A are given by

$$\begin{aligned} \langle X|\, A^+A\, |Y\rangle &= \frac{1}{V} \sum_{x \in X} \sum_{y \in Y} \langle X - x \,|\, Y - y\rangle \\ &= \begin{cases} \#(X)/V & \text{if } \quad X = Y \\ 1/V & \text{if } \quad \#(X) = \#(Y) \text{ and } \#(X \triangle Y) = 2 \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{16}$$

Combining this formula with (13), we see that

$$A^+A + H = \hat{N} \tag{17}$$

where $\hat{N}$ is the number operator, defined by

$$\langle X|\, \hat{N}\, |Y\rangle = \langle X|\, Y\rangle\ \#(X) \tag{18}$$

In this way we have expressed an operator closely related to the Hamiltonian, namely $\hat{N} - H$, as the product of two adjoint factors A and A^+. Moreover, we shall see later (Section 9) that the expectation of A^+A is the expected number of condensed particles, and so (17) shows that the expectation of H is precisely equal to the expected number of noncondensed particles. This is plausible because the eigenvalues of the one-particle Hamiltonian are 0 and 1, and the noncondensed particles are the ones with eigenvalue 1.

4. SOME COMMUTATION RELATIONS

The formula for AA^+ analogous to (16) is

$$\begin{aligned} \langle X|\, AA^+\, |Y\rangle &= \frac{1}{V} \sum_{x \in \Gamma - X} \sum_{y \in \Gamma - Y} \langle X \cup x \,|\, Y \cup y\rangle \\ &= \begin{cases} [V - \#(X)]/V & \text{if } X = Y \\ 1/V & \text{if } \#(X) = \#(Y) \text{ and } \#(X \triangle Y) = 2 \\ 0 & \text{otherwise} \end{cases} \end{aligned} \tag{19}$$

From (16), (18), and (19) we deduce the commutation relation

$$AA^{+} - A^{+}A = 1 - 2V^{-1}\hat{N} \tag{20}$$

In order to find the eigenvalues and eigenspaces of the Hamiltonian, we shall need some more commutation relations. From (15) and (18) we have

$$\hat{N}A^{+} - A^{+}\hat{N} = A^{+} \tag{21}$$

which has the interpretation that A^{+} increases the number of particles by 1. We also have, starting from (17),

$$\begin{aligned} HA^{+} - A^{+}H &= (\hat{N} - A^{+}A)A^{+} - A^{+}(\hat{N} - AA^{+}) \\ &= (\hat{N}A^{+} - A^{+}\hat{N}) - A^{+}(AA^{+} - AA^{+}) \\ &= A^{+} - A^{+}(1 - 2V^{-1}\hat{N}) \qquad [\text{by (21) and (20)}] \\ &= 2V^{-1}A^{+}\hat{N} \end{aligned} \tag{22}$$

Further, if we define the operator L by

$$L = H - V^{-1}(\hat{N}^{2} - \hat{N}) = \hat{N} - V^{-1}(\hat{N}^{2} - \hat{N}) - A^{+}A \tag{23}$$

[using (17)], then it follows from (21) and (22) that

$$LA^{+} - A^{+}L = 0 \tag{24}$$

5. THE EIGENSPACES OF THE HAMILTONIAN

Let r be any integer satisfying

$$0 \leqslant r \leqslant \tfrac{1}{2}V \tag{25}$$

and consider the subspace of $\mathscr{H}$, call it $\mathscr{K}_r$, defined by

$$\mathscr{K}_r = \{|\phi\rangle : \hat{N}|\phi\rangle = r|\phi\rangle \text{ and } A|\phi\rangle = 0\} \tag{26}$$

From this definition together with (17) and (23) we see that every state $|\phi\rangle$ in $\mathscr{K}_r$ satisfies

$$\hat{N}|\phi\rangle = r|\phi\rangle, \qquad H|\phi\rangle = r|\phi\rangle, \qquad L|\phi\rangle = [r - V^{-1}(r^{2} - r)]\,|\phi\rangle \tag{27}$$

For each r satisfying (25), consider the further sequence of subspaces

$$\mathscr{K}_{r,m} = (A^{+})^{m-r}\mathscr{K}_r, \qquad m = r, r+1, \ldots, V - r \tag{28}$$

(so that $\mathscr{H}_{r,r}=\mathscr{H}_r$). It follows from (26) and (27), and the commutation relations (21) and (24), that every state $|\phi\rangle$ in $\mathscr{H}_{r,m}$ satisfies

$$\hat{N}\,|\phi\rangle = m\,|\phi\rangle \tag{29}$$

$$L\,|\phi\rangle = [r - V^{-1}(r^2-r)]\,|\phi\rangle \tag{30}$$

and hence, by (23),

$$H\,|\phi\rangle = [r - V^{-1}(r^2-r) + V^{-1}(m^2-m)]\,|\phi\rangle \tag{31}$$

The subspaces $\mathscr{H}_{r,m}$ are all orthogonal, since they correspond to different pairs of eigenvalues for $\hat{N}$ and L. Moreover, by (31), they are all eigenspaces of the Hamiltonian.

Now we determine the dimensions of these subspaces. The first step is to find a lower bound on dim $\mathscr{H}_r$. The definition (26) says that $\mathscr{H}_r$ consists of all $|\phi\rangle$ such that

$$|\phi\rangle = \sum_{X:\,\#(X)=r} |X\rangle\langle X|\phi\rangle \tag{32}$$

and

$$\langle X|A|\phi\rangle = 0 \qquad \text{for all} \quad X\subset\Gamma \tag{33}$$

By (14), the condition (33) is automatically satisfied if $r=0$ and may otherwise be written

$$\sum_{x\in\Gamma-X} \langle X\cup x|\phi\rangle = 0 \qquad \text{for all} \quad X \text{ with } \#(X)=r-1 \tag{34}$$

It follows from (32) and (34) that the dimension of $\mathscr{H}_r$ is at least equal to the number of distinct $X\subset\Gamma$ with $\#(X)=r$, which is $\binom{V}{r}$, less the number of independent linear relations implied by the $\binom{V}{r-1}$ equations (34). The number of such relations is at most $\binom{V}{r-1}$ for $r\geqslant 1$, and when $r=0$ there are no equations at all in (34). So we have

$$\dim\mathscr{H}_r \geqslant \binom{V}{r} - \binom{V}{r-1} = \binom{V}{r}\left[1-\frac{r}{V-r+1}\right] \tag{35}$$

where we make the interpretation

$$\binom{V}{-1} = 0 \tag{36}$$

Since we are requiring $r\leqslant\frac{1}{2}V$, Eq. (35) shows that the dimension of $\mathscr{H}_r$ is certainly positive. We shall find later that it is in fact equal to the right-hand side of (35).

Now we consider $\mathscr{K}_{r,m}$. By the definition (28) we have

$$\mathscr{K}_{r,m+1}=\{A^{+}\,|\phi\rangle\colon |\phi\rangle\in\mathscr{K}_{r,m}\} \tag{37}$$

so that

$$\dim\mathscr{K}_{r,m+1}\leqslant\dim\mathscr{K}_{r,m} \tag{38}$$

But we can also show (proof below) that

$$\mathscr{K}_{r,m}=\{A\,|\psi\rangle\colon |\psi\rangle\in\mathscr{K}_{r,m+1}\}\qquad (m=r,\ldots,V-r-1) \tag{39}$$

so that

$$\dim\mathscr{K}_{r,m}\leqslant\dim\mathscr{K}_{r,m+1}\qquad (m=r,\ldots,V-r-1) \tag{40}$$

Combining (38) and (40) gives

$$\dim\mathscr{K}_{r,m+1}=\dim\mathscr{K}_{r,m}\qquad (m=r,\ldots,V-r-1) \tag{41}$$

so that, by induction

$$\dim\mathscr{K}_{r,m}=\dim\mathscr{K}_{r,r}=\dim\mathscr{K}_{r}\qquad (m=r,\ldots,V-r) \tag{42}$$

To prove (39), we use first (37) and afterwards (20) and (17) to see that the right-hand side of (39) can be written

$$\begin{aligned}\{A\,|\psi\rangle\colon \psi\in\mathscr{K}_{r,m+1}\}&=\{AA^{+}\,|\phi\rangle\colon |\phi\rangle\in\mathscr{K}_{r,m}\}\\&=\{[1-2V^{-1}\hat{N}+\hat{N}-H]\,|\phi\rangle\colon |\phi\rangle\in\mathscr{K}_{r,m}\}\end{aligned} \tag{43}$$

The right-hand side of (43) is equal to $\mathscr{K}_{r,m}$ if the operator in square brackets does not annihilate $|\phi\rangle$, that is, by (29) and (31), if

$$1-2V^{-1}m+m-r+V^{-1}(r^2-r)-V^{-1}(m^2-m)\neq 0 \tag{44}$$

The left-hand side of (44) can be written

$$V^{-1}(1+m-r)(V-m-r) \tag{45}$$

and is therefore nonzero provided that

$$r-1\neq m\neq V-r \tag{46}$$

So (43) tells us that the right-hand side of (39) is equal to $\mathscr{K}_{r,m}$ for all m satisfying (46), and hence that (39) is a true statement.

The total dimension of all the orthogonal subspaces $\mathscr{H}_{r,m}$ is

$$\begin{aligned}
&\sum_{r \leqslant V/2} \sum_{m=r}^{V-r} \dim \mathscr{H}_{r,m} \\
&\quad = \sum_{m=0}^{V} \sum_{r=0}^{\min(m,\, V-m)} \dim \mathscr{H}_r && \text{[by (42)]} \\
&\quad \geqslant \sum_{m=0}^{V} \sum_{r=0}^{\min(m,\, V-m)} \left[\binom{V}{r} - \binom{V}{r-1}\right] && \text{[by (35)]} \\
&\quad = \sum_{m=0}^{V} \binom{V}{\min(m,\, V-m)} = \sum_{m=0}^{V} \binom{V}{m} = 2^V && (47)
\end{aligned}$$

However, since the dimension of the entire space $\mathscr{H}$ is 2^V, it follows that the direct sum of the subspaces $\mathscr{H}_{r,m}$ is the whole of $\mathscr{H}$ and hence that the two expressions related by $\geqslant$ are in fact equal, so that (35) and (42) give

$$\dim \mathscr{H}_{r,m} = \binom{V}{r} - \binom{V}{r-1} = \binom{V}{r}\left[1 - \frac{r}{V-r+1}\right] \tag{48}$$

Thus, we have split $\mathscr{H}$ into eigenspaces of H, with eigenvalues given by (31), and dimensions given by (48).

Using this information about the spectrum of the Hamiltonian, we can write an explicit formula for the partition function for an N-particle system as the sum of contributions from the subspaces $\mathscr{H}_{r,m}$ with $m = N$:

$$\begin{aligned}
Z(N, V) &= \operatorname{tr}(e^{-\beta H}) \\
&= \sum_{r=0}^{\min(N,\, V-N)} \exp\{-\beta[r - V^{-1}(r^2 - r) + V^{-1}(N^2 - N)]\} \\
&\quad \times \binom{V}{r}\left(1 - \frac{r}{V-r+1}\right) && (49)
\end{aligned}$$

where β is the inverse temperature, and we have taken the eigenvalues of H from (31), their multiplicities from (48), and the allowed values of r from (28). The next step is to calculate the thermodynamic free energy from (49); this will be done in Section 7, after proving a mathematical lemma.

6. REPLACING A SERIES BY ITS LARGEST TERM

Lemma. Let a, b be real numbers with $a < b$, and let ϕ and h be continuous functions from $[a, b]$ to $\mathbb{R}$, with ϕ having a unique maximum at x^*, say (so that $\phi(x) < \phi(x^*)$ for all $x \neq x^*$ in $[a, b]$). Define

$$K_V = \{r \in \mathbb{Z}: r/V \in [a, b]\} \tag{50}$$

and let $\{\phi_V\colon V\in\mathbb{Z}^+\}$ and $\{h_V\colon V\in\mathbb{Z}^+\}$ be two bounded sequences of functions from K_V to $\mathbb{R}$, converging uniformly to ϕ and h, respectively, in the sense that (in the case of ϕ)

$$\lim_{V\to\infty}\delta_V=0 \tag{51}$$

where, by definition,

$$\delta_V=\operatorname*{Max}_{r\in K_V}|\phi_V(r/V)-\phi(r/V)| \tag{52}$$

if K_V is nonempty, and $\delta_V=+\infty$ if K_V is empty. Define, for each $V\in\mathbb{Z}^+$,

$$Z(V)=\sum_{r\in K_V}\exp V\phi_V(r/V) \tag{53}$$

Then we have: (a)

$$\lim_{V\to\infty}\frac{1}{V}\log Z(V)=\sup_x\phi(x) \tag{54}$$

and (b)

$$\lim_{V\to\infty}\frac{1}{Z(V)}\sum_{r\in K_V}h_V\left(\frac{r}{V}\right)\exp V\phi_V\left(\frac{r}{V}\right)=h(x^*) \tag{55}$$

Proof of the Lemma. Proof of Part (a). The sum in (53) is bounded above by the number of terms times the largest term, so that

$$\begin{aligned}Z(V)&\leqslant[V(b-a)+1]\operatorname*{Max}_{r\in K_V}\exp V\phi_V(r/V)\\&\leqslant[V(b-a)+1]\operatorname*{Max}_{r\in K_V}\exp V[\phi(r/V)+\delta_V]\qquad[\text{by (52)}]\end{aligned} \tag{56}$$

Using (50), (51), and the definition of x^*, we find that

$$\limsup_{V\to\infty}\frac{1}{V}\log Z(V)\leqslant\phi(x^*) \tag{57}$$

For a lower bound, let ε be any small positive number and define

$$J_\varepsilon=\{x\in[a,b]\colon|x-x^*|\leqslant\varepsilon\} \tag{58}$$

Provided $V>1/2\varepsilon$, the sum in (53) has at least one term for which $r/V\in J_\varepsilon$, and by (52) the value of this term is at least $\operatorname{Min}_{x\in J_\varepsilon}\exp V[\phi(x)-\delta_V]$. Since all the other terms in the sum are nonnegative we have, using (51),

$$\liminf_{V\to\infty}\frac{1}{V}\log Z(V)\geqslant\operatorname*{Min}_{x\in J_\varepsilon}\phi(x) \tag{59}$$

This is true for any positive ε, and so we can take the limit $\varepsilon \to 0$, obtaining (since ϕ is continuous)

$$\liminf_{V\to\infty} \frac{1}{V} \log Z(V) \geqslant \phi(x^*) \tag{60}$$

Combining (57) and (60) completes the proof of part (a).

Proof of Part (b). We want to prove that $\lim_{V\to\infty} \eta_V = 0$, where

$$\eta_V = \frac{1}{Z(V)} \sum_{r\in K_V} \left[h_V\left(\frac{r}{V}\right) - h(x^*) \right] \exp V\phi_V\left(\frac{r}{V}\right) \tag{61}$$

Let ξ be any positive number. Then by the continuity of h and the uniform convergence of $\{h_V\}$ we can find numbers ε and V_0 such that

$$|h_V(r/V) - h(x^*)| < \xi$$

whenever $V > V_0$ and $|r/V - x^*| < \varepsilon$. For an upper bound on $|\eta_V|$ we then have

$$|\eta_V| \leqslant \frac{A_1 + B_1}{A_0 + B_0} \tag{62}$$

where, for $k = 0$ and $k = 1$, we define

$$A_k = \sum_{r:\, r/V \in J_\varepsilon} |h_V(r/V) - h(x^*)|^k \exp V\phi_V(r/V) \tag{63}$$

$$B_k = \sum_{r:\, r/V \in K_V \setminus J_\varepsilon} |h_V(r/V) - h(x^*)|^k \exp V\phi_V(r/V) \tag{64}$$

These definitions imply, for $V > V_0$, the following estimates:

$$0 \leqslant A_1 \leqslant \xi A_0 \tag{65}$$

$$0 \leqslant B_1 \leqslant 2MB_0 \tag{66}$$

where M is the upper bound on the bounded sequence of functions $\{|h_V|\}$, and

$$0 \leqslant B_0 \leqslant [V(b-a)+1] \exp V[\sup_{x\in[a,b]\setminus J_\varepsilon} \phi(x) + \delta_V] \tag{67}$$

[which follows from (52) and the fact that there are at most $V(b-a)+1$ terms in the series for B_0].

We also need an estimate of the ratio B_0/A_0. Consider the interval $J_{1/V}$ defined as in (58). At least one element r of the set K_V is such that r/V lies in this interval. Provided $V > 1/\varepsilon$, we have $J_{1/V} \in J_\varepsilon$, so that this value of r corresponds to a term of the sum defining A_0; and A_0 is bounded below by this term, so that [using (52) again]

$$A_0 \geqslant \exp V[\inf_{x \in J_{1/V}} \phi(x) - \delta_V] \qquad \text{if} \quad V > 1/\varepsilon \tag{68}$$

Combining (67) and (68) gives, for $V > 1/\varepsilon$,

$$B_0/A_0 \leqslant [V(b-a)+1] \exp V\{2\delta_V + \sup_{x \in [a,b] \backslash J_\varepsilon} \phi(x) - \inf_{x \in J_{1/V}} \phi(x)\}$$

For sufficiently large V the expression in braces is bounded above by a negative constant, because of (51) and the fact that (by the continuity of ϕ and the definitions of x^*, $J_{1/V}$, and J_ε)

$$\lim_{V \to \infty} [\inf_{x \in J_{1|V}} \phi(x)] = \phi(x^*) > \sup_{x \in [a,b] \backslash J_\varepsilon} \phi(x)$$

Thus we obtain

$$\lim_{V \to \infty} B_0/A_0 = 0 \tag{69}$$

Using these estimates in (62), we find that

$$\begin{aligned} \lim_{V \to \infty} |\eta_V| &\leqslant \lim_{V \to \infty} \frac{(A_1/A_0) + (B_1/B_0)(B_0/A_0)}{1 + B_0/A_0} \\ &\leqslant \lim_{V \to \infty} [\xi + 2M(B_0/A_0)] \qquad [\text{by (65) and (66)}] \\ &= \xi \qquad\qquad\qquad\qquad\qquad\quad [\text{by (69)}] \end{aligned} \tag{70}$$

Since this is true for any positive ξ, we must have

$$\lim_{V \to \infty} |\eta_V| = 0$$

which, combined with (61), completes the proof of part (b).

7. THE THERMODYNAMIC FREE ENERGY

In this section we prove Theorem 1. The thermodynamic free energy per site at particle concentration ρ and inverse temperature β is defined in the usual way as $f(\rho, \beta)$, where

$$\beta f(\rho, \beta) = - \lim_{\substack{N, V \to \infty \\ N/V \to \rho}} V^{-1} \log_e Z(N, V) \tag{71}$$

with $Z(N, V)$ given by (49). We can apply the lemma, with $a=0$, $b=1/2$,

$$\phi_V\left(\frac{r}{V}\right)=V^{-1}\left\{-\beta[r-V^{-1}(r^2-r)+V^{-1}(N^2-N)]+\log\binom{V}{r}\right.$$
$$\left.+\log\left(1-\frac{r}{V-r+1}\right)\right\} \tag{72}$$

and

$$\begin{aligned}\phi(x)&=\lim_{V\to\infty}\phi_V(x)\\ &=-\{\beta\rho^2+\beta x(1-x)+x\log x+(1-x)\log(1-x)\}\end{aligned} \tag{73}$$

provided we can show that (51) holds. For then the main result (1) follows at once from (53) and (54). The rest of the theorem then follows by standard calculus, the minimizing value of x in (1) being ρ^* for $\beta>\beta^*(\rho)$ and $\mathrm{Min}(\rho, 1-\rho)$ for $\beta\leqslant\beta^*(\rho)$.

To show that (51) holds, we first do the case $r=0$. In this case we have

$$\phi_V(0)-\phi(0)=\beta[\rho^2-(N^2-N)/V^2] \tag{74}$$

which tends to 0 as $V\to\infty$ with $N/V\to\rho$. To do the case $1\leqslant r\leqslant\frac{1}{2}V$, define $\theta(n)$ by

$$n!=(n+\tfrac{1}{2})\log n-n+\theta(n) \qquad (n\geqslant 1) \tag{75}$$

It is shown by Feller$^{(5)}$ that

$$0\leqslant\theta(n)\leqslant 1 \qquad (n\geqslant 1) \tag{76}$$

Putting (75) into (72) and (73), we obtain, for $1\leqslant r\leqslant V-1$,

$$\phi_V\left(\frac{r}{V}\right)-\phi\left(\frac{r}{V}\right)=\beta\left(\rho^2-\frac{N^2-N}{V^2}\right)-\frac{\beta r}{V^2}+\frac{1}{2V}\log\left[\frac{V}{r(V-r)}\right]$$
$$+\frac{1}{V}\log\left(1-\frac{r}{V-r+1}\right)+\frac{1}{V}[\theta(V)-\theta(r)-\theta(V-r)] \tag{77}$$

The first term on the right is independent of r and tends to 0 as $V\to\infty$; the second is bounded above by 0 and below by $-\beta/V$; the third is bounded above by 0 and below by its value for $r=V/2$, which is $-(1/2V)\log(V/4)$; the fourth is bounded above by 0 and below (since $r\leqslant V/2$) by its value for $r=V/2$, which is $-(1/V)\log(1+V/2)$; and the fifth is, because of (76), bounded above by $1/V$ and below by $-2/V$. So the whole expression has upper and lower bounds independent of r which tend to 0 as $V \to \infty$, and (51) is proved.

8. COMPARISON WITH TÓTH'S FREE ENERGY FORMULA

Tóth[15] gives a formula for the free energy density which in our notation reads as follows:

$$\beta f = \beta\rho + \rho\log\rho + (1-\rho)\log(1-\rho) \qquad \text{when} \quad \beta \leqslant \beta^*(\rho) \tag{78}$$

$$\begin{aligned}\beta f = \beta\rho + \rho\log\rho + (1-\rho)\log(1-\rho) + \tfrac{1}{2}(1-2\rho)^2[\beta - \beta^*(\rho)] \\ + \tfrac{1}{2}\log[1-E(\beta)] + \rho(1-\rho)\,\beta E(\beta) \qquad \text{when} \quad \beta > \beta^*(\rho)\end{aligned} \tag{79}$$

where $E(\beta)$ is the solution of

$$y = [(1-2\rho)^2 + 4\rho(1-\rho)E]^{1/2} \tag{80}$$

with y defined as the unique positive solution of

$$\frac{1}{y}\log\frac{1+y}{1-y} = \beta \tag{81}$$

The results (2), (3), (78), and (79) were obtained by completely different methods, but, as we now show, they are equivalent. Since the formulas (2) and (78) for the case $\beta \leqslant \beta^*(\rho)$ are identical, only the case $\beta > \beta^*(\rho)$ gives any trouble.

To facilitate comparison with (3), we subtract $\beta\rho^2$ from both sides of (79) and then express the right-hand side in terms of ρ and ρ^* only. We already have a formula for β^* in terms of ρ, Eq. (4). For β, we use (5) and (4), obtaining

$$\beta = \frac{1}{1-2\rho^*}\log\frac{1-\rho^*}{\rho^*} \tag{82}$$

To express E in terms of ρ, we first compare (81) and (82), obtaining [since $\rho^* < 1/2$ and the solution of (81) for positive y is unique] $y = 1 - 2\rho^*$; hence, by solving (80) for E, we obtain

$$E = 1 - \frac{\rho^*(1-\rho^*)}{\rho(1-\rho)} \tag{83}$$

Now we substitute from (4), (82), and (83) into the expression for $\beta f - \beta\rho^2$ given by (79). The resulting formula eventually reduces to

$$\beta f - \beta\rho^2 = \frac{-\rho^{*2}\log\rho^* + (1-\rho^*)^2\log(1-\rho^*)}{1-2\rho^*} \tag{84}$$

For comparison, consider the expression for $\beta f - \beta p^2$ given by (3). Substituting for β from (82), we again obtain (84), verifying that (79) and (3) are equivalent and hence that the two methods give the same free energy density for all inverse temperatures β.

9. BOSE–EINSTEIN CONDENSATION

In this section we prove Theorem 2, which gives the condensate density, that is, the expectation of the operator giving the number of particles per site that are in the single-particle state for which the probability amplitude is the same at each site. This state, which we may call the zero state, is the state of lowest energy for the single-particle system.

A convenient way to find the number operator for the zero state is to use second quantization. Let $\mathscr{F}$ be the Fock space for bosons on the graph Γ, comprising states with any number of particles on each site, and let b_x: $\mathscr{F} \to \mathscr{F}$ be the boson annihilation operator in $\mathscr{F}$, annihilating one particle at the site x, and satisfying the usual commutation relation

$$b_x b_y^+ - b_y^+ b_x = \delta_{xy} \tag{85}$$

The operator annihilating one particle in the zero state is then

$$B = V^{-1/2} \sum_x b_x \tag{86}$$

It satisfies the commutation relation

$$BB^+ - B^+ B = 1 \tag{87}$$

The operator giving the number of particles in the zero state is

$$\hat{N}_0 = B^+ B \tag{88}$$

an operator whose eigenvalues are nonnegative integers.

For the system we are considering, all the quantum states lie in $\mathscr{H}$, the subspace of $\mathscr{F}$ for which there is at most one particle on each site. If b_x acts to the right on a state in $\mathscr{H}$, the resulting state is again in $\mathscr{H}$ (with one less particle). Let a_x be the restriction of b_x to $\mathscr{H}$; then the matrix elements of a_x are given by

$$\langle X | \, a_x \, | Y \rangle = \begin{cases} 1 & \text{if} \quad X = Y - x \\ 0 & \text{if} \quad \text{not} \end{cases} \tag{89}$$

The restriction of B to $\mathscr{H}$ is then

$$V^{-1/2}\sum_{x} a_x \tag{90}$$

an operator in $\mathscr{H}$ whose matrix elements [calculated from (89)] turn out to be the same as those of A given in (14); the restriction of B to $\mathscr{H}$ is therefore A.

In a similar way, we can show that the restriction of $B^{+}B$ to $\mathscr{H}$ is $A^{+}A$ and hence the expectation of $\hat{N}_0$ for any state in $\mathscr{H}$ is equal to the expectation of $A^{+}A$ is that state. It follows that the expectation of $\hat{N}_0$ in the canonical ensemble is given by

$$\langle \hat{N}_0 \rangle = \frac{\operatorname{tr}(A^{+}Ae^{-\beta H})}{\operatorname{tr}(e^{-\beta H})} \tag{91}$$

[On the other hand, it is not true that the restriction of BB^{+} to $\mathscr{H}$ is AA^{+}; this is because B^{+} acting on a state in $\mathscr{H}$ can produce a state which is not in $\mathscr{H}$, and is the reason why the commutation relations (20) and (87) have different right-hand sides.]

To calculate the right-hand side of (91), we use the decomposition of $\mathscr{H}$ into subspaces $\mathscr{H}_{r,m}$ explained in Section 5. Using first (17) and then (29) and (31), we see that $\mathscr{H}_{r,m}$ is an eigenspace of $A^{+}A$ with eigenvalue

$$m - [r - V^{-1}(r^2 - r) + V^{-1}(m^2 - m)]$$

The dimensions of these subspaces are given in (48). Using this information in (91), then dividing both sides by V and taking the thermodynamic limit, we obtain the condensate density ρ_c:

$$\begin{aligned}
\rho_c &= \lim_{\substack{N,V\to\infty\\ N/V\to\rho}} \frac{\langle \hat{N}_0\rangle}{V}\\
&= \lim \Bigg(\Bigg\{ \sum_{r=0}^{\min(N,V-N)} \frac{(N-r)(V-N-r+1)}{V^2}\\
&\qquad \times \exp\{-\beta[r - V^{-1}(r^2-r) + V^{-1}(N^2-N)]\} \binom{V}{r}\left[1-\frac{r}{V-r+1}\right]\Bigg\}\\
&\qquad \times \Bigg\{ \sum_{r=0}^{\min(N,V-N)} \exp\{-\beta[r - V^{-1}(r^2-r) + V^{-1}(N^2-N)]\}\\
&\qquad \times \binom{V}{r}\left[1-\frac{r}{V-r+1}\right]\Bigg\}^{-1}\Bigg)
\end{aligned}$$

To evaluate this formula, we apply part (b) of the Lemma, with

$$h_V(r/V) = (N/V - r/V)(1 - N/V - r/V + 1/V)$$
$$h(x) = \lim_{V \to \infty} h_V(x) = (\rho - x)(1 - \rho - x)$$

The result is

$$\rho_c = (\rho - x^*)(1 - \rho - x^*) \tag{92}$$

When $\beta < \beta^*(\rho)$, we have $x^* = \rho$, and so $\rho_c = 0$; but when $\beta \geqslant \beta^*(\rho)$, we have $x^* = \rho^*(\beta)$, and so $\rho_c = (\rho - \rho^*)(1 - \rho - \rho^*)$. QED

10. THE ONE-BODY REDUCED DENSITY MATRIX

Instead of characterizing Einstein condensation in terms of the occupation of the zero state, we can[10,12] use the one-body reduced density matrix, which may be defined as

$$D_1(x, x') = Z^{-1} \operatorname{tr}(b_{x'}^+ b_x) e^{-\beta H} \tag{93}$$

To compute this, we note first that (since all sites are equivalent) $D_1(x, x')$ takes only two different values, one for the diagonal elements $D_1(x, x)$ and another for the off-diagonal elements $D_1(x, x')_{x \neq x'}$. For the diagonal elements we have

$$\begin{aligned} D_1(x, x) &= (\text{probability of finding a particle at vertex } x) \\ &= N/V \end{aligned} \tag{94}$$

For the off-diagonal elements we use (88), (86), and (93) to obtain

$$\begin{aligned} \langle \hat{N}_0 \rangle &= \langle B^+ B \rangle = V^{-1} \sum_x \sum_{x'} D_1(x, x') \\ &= V^{-1}[V D_1(x, x) + V(V-1)\, D_1(x, x')_{x \neq x'}] \end{aligned} \tag{95}$$

Solving for $D_1(x, x')_{x \neq x'}$, using (94), and taking the thermodynamic limit, we find that in this limit the off-diagonal reduced density matrix elements are given by

$$\lim_{N, V \to \infty} D_1(x, x')_{x \neq x'} = \lim_{N, V \to \infty} \frac{1}{V-1} \left(\langle \hat{N}_0 \rangle - \frac{N}{V} \right) = \rho_c \tag{96}$$

At low temperatures ρ_c is nonzero and so "off-diagonal long-range order" as defined by Yang[17] is present.

11. DISCUSSION

It has been known for some time (see, for example, ref. 14) that mean-field theory is exact, in the appropriate limit, for the Curie-Weiss model, which is equivalent to a classical lattice gas on a complete graph. The present work extends this result to the quantum hard-core lattice gas. Indeed, apart from notation the free energy formula (1) is identical with the free energy in the Bragg-Williams mean-field theory of alloys. It is therefore only to be expected that the critical exponents of our model, in particular, the specific heat exponent, are the same as for mean-field theory. In the Bragg-Williams theory, the analogue of the quantity denoted here by $\rho^*(\beta)$ is the density of one of two phases in equilibrium with one another below the critical temperature, but in our model $\rho^*(\beta)$ does not have such a transparent physical interpretation. Indeed, for us the physically important density at low temperatures is not $\rho^*(\beta)$, but the condensate density ρ_c. As shown in the corollary to Theorem 2, this quantity has the critical exponent 1, which is the generally accepted mean-field value.(6,7)

The corresponding exponent for liquid helium-4 has not been measured directly, but according to Josephson,(8) this exponent, which he denotes by 2β, is related to the exponent for the superfluid density by

$$\rho_s \propto (T_c - T)^{2\beta - \eta\nu'} \tag{97}$$

where ρ_s is the superfluid density, T is the temperature, T_c is the critical temperature, and η, ν' are defined by

$$C(r) \propto r^{-1-\eta} \qquad \text{when} \quad T = T_c \tag{98}$$

$$(\text{correlation length}) \propto (T_c - T)^{-\nu'} \tag{99}$$

where $C(r)$ is the two-point correlation function of the order parameter (local condensate density). Experiment(1) shows that the exponent in (97) is about 2/3, and so, provided that η is small (the corresponding exponent for the three-dimensional Ising model is about 0.04), the exponent 2β for helium-4 should also be not far from 2/3.

There is an alternative method for proving Theorems I and II, based on the results of Fannes *et al.*(4) The alternative method also shows explicitly how the symmetry of the high-temperature state is broken at low temperatures: in the extremal states of the infinite system the various lattice sites are independent and the state of any one of these lattice sites corresponds to a density matrix

$$\begin{bmatrix} \rho & \rho_c^{1/2} e^{i\phi} \\ \rho_c^{1/2} e^{-i\phi} & 1-\rho \end{bmatrix}$$

where the first row or column refers to the site's being occupied and the second to its being unoccupied. At low temperatures, for which $\rho_c \neq 0$, the symmetry is broken because each value for the phase factor $e^{i\phi}$ gives a distinct state.

The Bose gas with hard-core repulsion on any lattice or graph is equivalent(9) to an XY model and so our model is equivalent to an XY model on a complete graph. The mean-field theory of the XY model was worked out by Matsubara and Matsuda,(9) who give a formula for the critical temperature equivalent to our (4), and by Zilsel,(18) who gives a free energy formula equivalent to (1) and a $\rho - T$ diagram essentially the same as our Fig. 1.

When the temperature is zero ($\beta = \infty$), Eq. (92) gives $\rho(1-\rho)$ as the value of the condensate density. For any other temperature the condensate density is less than this value. Tóth(16) has pointed out that $\rho(1-\rho)$ is also an upper bound on the condensate density for a quantum lattice gas at any temperature on any graph and with any interaction whatever, provided that the interaction has a hard core and that all the sites have the same ground-state occupation probability; this fact is proved by the same method as the corresponding zero-temperature result(11) for hard-core systems in continuous space.

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