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Author
Elser, V.

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V. Elser

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Veit Elser

Lawrence Berkeley Laboratory

and

Department of Physics

University of California

Berkeley, California 94720

ABSTRACT

A constrained SOS model is used to describe the edge of a simple-cubic crystal. Low and high temperature results are derived as well as the detailed behavior near the crystal facet.

1. Introduction

It is well known that the large scale equilibrium shape of crystal surfaces is best characterized by facets. A realistic facet, however, is never infinite in extent and must meet other facets at finite intersection angles to form edges. Consequently, edges are a generic feature of the crystal surface the properties of which we would like to know.

For the simple-cubic crystal structure, a statistical mechanical model of the edge is provided by the partition function

$$Z_N(n, m; \beta) = \sum_{\{y_{xz}\}} \exp\left(-\beta \sum_{x,z} |y_{xz} - y_{xz+1}|\right) \qquad (1a)$$

where the sum is over all the $n \times N$ sets of integer variables $\{y_{xz}\}$ that satisfy the constraint:

$$0 \leq y_{1z} \leq y_{2z} \leq \cdots \leq y_{nz} \leq m \qquad z = 1, \ldots, N. \qquad (1b)$$

The Boltzmann factor of (1a) is precisely that of the usual SOS model for the special case that the height variables y_{xz} are monotonic in the x-direction as implied by (1b). Another way of describing the interface as it is cut by a plane of constant z is in terms of a lattice path taking n steps in the $+x$-direction and m steps in the $+y$-direction. Using this interpretation the Boltzmann weight of (1a) is just the sum of positive areas between consecutive lattice paths. Moreover, it obviously follows that $Z_N(n, m; \beta) = Z_N(m, n; \beta)$.

The free energy appropriate to (1) is given by ($L = n + m$):

$$\lim_{\substack{N \to \infty \\ L \to \infty}} (NL)^{-1} \log Z_N(\rho L, (1 - \rho)L; \beta) = -F(\rho, \beta). \qquad (2)$$

Here ρ is the density of steps in the $+x$-direction. As $\rho \to 0(1)$ we approach the facet having $x = \text{const}$ ($y = \text{const}$).

The equilibrium shape of the crystal edge is obtained by the Wulff construction[1] . In order to proceed we have to be able to count the number of atoms in the crystal phase. We do this separately for each layer of constant z and begin by choosing a completely filled quadrant of atoms as a reference configuration. As pointed out above, such an edge can be represented as a semi-infinite sequence of $+y$-steps followed by a semi-infinite sequence of $+x$-steps. For convenience, we consider each x-step as a particle and each y-step as the absence of a particle on a linear lattice. The reference configuration has all the sites to the right of the origin occupied and the remaining ones empty. Other configurations can be generated by moving a finite number of the already existing particles. The statement of particle conservation can be expressed as

$$0 = \sum_{\xi > 0} (n_\xi - 1) + \sum_{\xi \le 0} n_\xi \qquad (3)$$

where ξ is the coordinate along the linear lattice and n_ξ is the occupation number (0 or 1) of site ξ (see figure 1).

To understand the general situation it is enough to follow the consequences of moving a single particle by one lattice unit. One discovers that a motion in the positive(negative) ξ-direction corresponds to the creation(annihilation) of a crystal atom at the interface. The number of atoms removed from the filled quadrant can thus be written as

$$N = -\sum_{\xi > 0} \xi(n_\xi - 1) - \sum_{\xi \le 0} \xi n_\xi . \qquad (4)$$

When N is large and the configuration is more appropriately described by a density of particles $\rho(\xi)$, we use the continuum forms of (3) and (4):

$$0 = \int_0^\infty (\rho(\xi) - 1)d\xi + \int_{-\infty}^0 \rho(\xi)d\xi \qquad (3')$$

$$N = -\int_0^\infty \xi(\rho(\xi) - 1)d\xi - \int_{-\infty}^0 \xi\rho(\xi)d\xi . \qquad (4')$$

We can now apply the Wulff construction and obtain the functional

$$W[\rho] = \int_{-\infty}^\infty \left(\lambda(\xi - \xi_0)\rho(\xi) - F(\rho, \beta)\right)d\xi$$

where the Lagrange multipliers $\lambda\xi_0$ and λ apply to constraints (3') and (4') respectively. The equilibrium shape can now be found by maximizing $W[\rho]$ subject to the conditions:

$$0 \le \rho(\xi) \le 1$$

$$\lim_{\xi \to -\infty} \rho(\xi) = 0 \qquad \lim_{\xi \to \infty} \rho(\xi) = 1 .$$

The functional $W[\rho]$ is extremized for the choice

$$\frac{\partial}{\partial \rho} F(\rho, \beta) = \lambda(\xi - \xi_0) \equiv t$$

which can be inverted (locally) to yield ρ as a function of ξ. However, we will see in subsequent calculations that for $\beta > 0$

$$\frac{\partial}{\partial \rho} F(0, \beta) = -t_0 \qquad \frac{\partial}{\partial \rho} F(1, \beta) = t_0 \qquad (5)$$

$$-t_0 < \frac{\partial}{\partial \rho} F(\rho, \beta) < t_0 \qquad (0 < \rho < 1)$$

where $t_0 > 0$ is finite. This means that in general,

$$\rho(t) = \begin{cases} 0 & t < -t_0 \\ (\partial_\rho F)^{-1}(t) & -t_0 < t < t_0 \\ 1 & t_0 < t . \end{cases} \qquad (6)$$

The parameters ξ_0 and λ are related to the position and scale of the edge respectively; their values are determined by equations (3')

and (4′). The coordinate ξ has the geometrical interpretation of being measured along an axis rotated 45° with respect to the original x and y axes of the crystal (see figure 1). If in some range from ξ to $\xi + \Delta\xi$ the lattice path makes n steps in the $+x$-direction and m steps in the $+y$-direction, the change in position $\Delta\eta$, perpendicular to the ξ-axis is just $m - n$. Consequently,

$$\frac{\Delta\eta}{\Delta\xi} = \frac{m - n}{n + m} = 1 - 2\rho \ .$$

Finally, upon substituting the rescaled variables $t = \lambda\xi$ and $s = \lambda\eta$, the edge profile is given by the expression

$$s(t) = \int_0^t \left(1 - 2\rho(u)\right)du + \text{const} \ . \tag{7}$$

In the following sections the free energy (2) will be calculated in the limits $\beta \to \infty$, $\beta \to 0$, and $\rho \to 0$. These results can then be used to obtain the low and high temperature limits of the edge profile as well as the behavior in the region where the surface joins a facet.

2. Low Temperature Expansion

The partition function (1) can in principle be expressed in terms of a transfer matrix M as

$$Z_N(n, m; \beta) = \text{tr}M^N \ .$$

The elements of M are simple, however, only in the limit $\beta \to \infty$ when they can be expanded in powers of $e^{-\beta}$. If we let $L = n + m$ then the 'states' appropriate to M, as discussed in section 1, are the configurations of n particles on a linear lattice of L sites. The matrix element between two such states is unity when the states are the same and $e^{-\beta}$ if the states differ by the displacement of one particle by one unit. If we neglect the other matrix elements which are $O(e^{-2\beta})$, then M is naturally written in the form

$$M = 1 + e^{-\beta} \sum_{i=1}^{L-1} (a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1}) + O(e^{-2\beta}) \ . \tag{8}$$

The operators $a^\dagger$ and a are the usual bosonic creation and annihilation operators with the additional properties

$$(a_i^\dagger)^2 = (a_i)^2 = 0 \ .$$

This is necessary since we require that M acting on a state never produce a state with two particles occupying the same site.

When M is written as the exponential of a hamiltonian the free energy (2) can be expressed in terms of the lowest n-particle energy eigenvalue $E(L, n)$:

$$M = \exp\left(-H_1 + O(e^{-2\beta})\right)$$

$$H_1 = -e^{-\beta} \sum_{i=1}^{L-1} (a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1})$$

$$F(\rho, \beta) = \lim_{L \to \infty} L^{-1} E(L, \rho L) \ .$$

By use of the Jordan-Wigner transformation[2] the operators introduced above can be written in terms of fermionic operators with the result that the operators in H_1 are now interpreted as fermionic. Since we have effectively hard-wall boundary conditions, the hamiltonian is diagonalized

by the canonical transformation

$$a_i^{(\dagger)} = \sqrt{\tfrac{2}{L}} \sum_{k=1}^{L} \sin(\tfrac{\pi i k}{L+1}) \, b_k^{(\dagger)}$$

$$H_1 = -e^{-\beta} \sum_{k=1}^{L} \epsilon(k) b_k^\dagger b_k \qquad \epsilon(k) = 2\cos(\tfrac{\pi k}{L+1})$$

with ground state eigenvector and energy given by:

$$\Psi_0 = \prod_{k=1}^{n} b_k^\dagger |0\rangle$$

$$E(L,n) = -e^{-\beta} \sum_{k=1}^{n} \epsilon(k) + O(e^{-2\beta})$$

$$F(\rho,\beta) = -\frac{2}{\pi} \sin(\pi\rho) e^{-\beta} + O(e^{-2\beta}) \ .$$

We see that the form of the free energy as a function of ρ agrees with the claims made in section 1. Using equations (5) and (6) we have

$$t_0 = 2e^{-\beta}$$

$$\rho(t) = \frac{1}{\pi} \cos^{-1}\left(\frac{-t}{t_0}\right) \qquad (-t_0 < t < t_0) \qquad (9)$$

with the edge profile given by (7):

$$s(t) = \begin{cases} t & t < -t_0 \\ t - \frac{2}{\pi}\left(t\cos^{-1}\left(\frac{-t}{t_0}\right) + \sqrt{t_0^2 - t^2}\right) & -t_0 < t < t_0 \\ -t & t_0 < t \ . \end{cases}$$

It is apparent from (9) that the density $\rho(t)$ has square-root singularities at $t = \pm t_0$ (see figure 2). Since $s(t)$ is essentially the integral

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of $\rho(t)$ this implies that the edge profile joins the facet with a $t^{3/2}$ behavior. The square-root singularities of ρ can be traced to the fact that the present form of the free energy satisfies

$$\frac{\partial^2}{\partial\rho^2} F(0,\beta) = 0 \qquad \frac{\partial^2}{\partial\rho^2} F(1,\beta) = 0 \ . \qquad (10)$$

As will be shown later, the above holds for all finite temperatures so that the $t^{3/2}$ behavior of the surface near the facet follows in general.

To illustrate the nature of the expansion we will also calculate the $O(e^{-2\beta})$ term of the free energy. It is first necessary to extend the transfer matrix (8) to include operators that generate two units of particle displacement. Most of these operators appear in the product $\frac{1}{2}H_1^2$ where H_1 is the $O(e^{-\beta})$ piece of the hamiltonian. Being the product of two 'hopping' operators $(a_{i\pm1}^\dagger a_i)(a_{j\pm1}^\dagger a_j)$, these terms are correct except possibly when their subscripts overlap. To correct for these possible mistakes, we subtract out all the overlapping products and add in the correct terms. The latter are

$$a_i^\dagger a_{i-1} a_{i+1}^\dagger a_i + \text{h.c.} \qquad (11)$$

$$a_{i+1}^\dagger a_i a_i^\dagger a_{i-1} + \text{h.c.} \qquad (12)$$

where (11) moves two particles each by one unit while (12) moves a single particle through two units. Following the above strategy, the transfer matrix can by written as

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$$M = 1 - H_1 + \frac{1}{2}H_1^2$$

$$- e^{-2\beta}\left\{ \frac{1}{2}\sum_{i=2}^{L-1}[(a_i^\dagger a_{i-1})(a_{i+1}^\dagger a_i) + (a_{i+1}^\dagger a_i)(a_i^\dagger a_{i-1}) + \text{h.c.}] \right.$$

$$\left. + \frac{1}{2}\sum_{i=1}^{L-1}[(a_{i+1}^\dagger a_i)(a_i^\dagger a_{i+1}) + (a_i^\dagger a_{i+1})(a_{i+1}^\dagger a_i)] \right\}$$

$$+ e^{-2\beta}\sum_{i=2}^{L-1}[a_i^\dagger a_{i-1}a_{i+1}^\dagger a_i + a_{i+1}^\dagger a_i a_i^\dagger a_{i-1} + \text{h.c.}]$$

$$+ O(e^{-3\beta}) .$$

The Jordan-Wigner transformation replaces the pairs $a_{i\pm1}^\dagger a_i$ by corresponding fermionic operators so that once again we may interpret all the operators as fermionic. Taking the logarithm of M we obtain the hamiltonian

$$H = H_1 + H_2 + O(e^{-3\beta})$$

$$H_2 = e^{-2\beta}\left\{ \sum_{i=2}^{L-1}[a_{i+1}^\dagger(a_i^\dagger a_i - \tfrac{1}{2})a_{i-1} + \text{h.c.}] \right.$$

$$\left. \sum_{i=1}^{L-1} a_{i+1}^\dagger a_i^\dagger a_{i+1} a_i \quad + n \right\}.$$

In one of the simplifications the number operator was replaced by n, the number of particles. It is now a straightforward problem to evaluate the correction to the ground state energy by taking the expectation value of H_2 in the zeroth order ground state. This part of the calculation is relatively unenlightening so we merely give the final result:

$$F(\rho,\beta) = -\frac{2}{\pi}\sin(\pi\rho)e^{-\beta}$$

$$+ \left[\rho(1-\rho) + \frac{2\rho-1}{2\pi}\sin(2\pi\rho) - \frac{1}{\pi^2}\sin^2(\pi\rho)\right]e^{-2\beta}$$

$$+ O(e^{-3\beta}) . \tag{13}$$

As a simple check we note that the correction is symmetric about $\rho = \frac{1}{2}$. It can also be verified that this term satisfies equation (10).

3. High Temperature Limit

We will concentrate again on the ξ and η coordinate system introduced earlier. The set of lattice paths or cross-sections of the interface may be thought of as random walks $\eta_1(\xi),\ldots,\eta_N(\xi)$ with ξ as a common 'time' parameter. For each step in time the particle positions $\eta_i(\xi)$ change by ±1 with the Boltzmann weight acting as an attractive force between consecutive particles. In the limit $\beta \to 0$ the particles can drift very far apart so that over short periods of time the fluctuations in the positive area between two consecutive paths are unimportant. In other words, for periods of time that are in some sense small compared to the separation between consecutive particles, the random walks are free.

We have to be careful however, to remember the global constraint that during a time $\Delta\xi$ the random walk makes on the average exactly $\rho\Delta\xi$ steps in the $+x$-direction. This is evident from the boundary conditions (1a) of the partition function. However, for our present purposes it will be more convenient to let the boundaries be free while introducing activities ρ and $1 - \rho$ respectively for motion in the $+x$ and $+y$ directions. To

recover the original partition function (1) we must then divide by

$$[\rho^n(1-\rho)^m]^N$$

which merely adds the constant

$$\rho\log\rho + (1-\rho)\log(1-\rho) \tag{14}$$

to the free energy.

Now suppose that the particle positions are $\eta_1, \ldots, \eta_N$ at some initial time ξ_0 and $\eta'_1, \ldots, \eta'_N$ at some later time $\xi_0 + \Delta\xi$. For $\Delta\xi \gg 1$ but fixed as $\beta \to 0$ we will be able to sum over the configurations at intermediate times and thereby obtain a transfer matrix. In this limit it will almost always be true that

$$|\eta_i - \eta'_i| \ll |\eta_i - \eta_{i\pm1}| \simeq |\eta'_i - \eta'_{i\pm1}|$$

so that the Boltzmann factor is relatively constant and can be taken outside the summation. In terms of the ξ and η coordinates we see from figure 1 that this factor is given by

$$\exp\left\{-\frac{1}{2}\beta\Delta\xi\sum_{i=1}^{N-1}|\eta_i - \eta_{i+1}|\right\}. \tag{15}$$

What remains is just the sum over N independent random walks having specified endpoints and the activity factors discussed above ($\Delta\eta_i = \eta'_i - \eta_i$):

$$\prod_{i=1}^{N}\binom{\Delta\xi}{\frac{1}{2}(\Delta\xi - \Delta\eta_i)}\rho^{\frac{1}{2}(\Delta\xi - \Delta\eta_i)}(1-\rho)^{\frac{1}{2}(\Delta\xi + \Delta\eta_i)}. \tag{16}$$

Since $\Delta\xi \gg 1$, it can be shown that each term in the product is strongly peaked at $\Delta\eta_i = (1 - 2\rho)\Delta\xi$. If we change from the η-coordinates to the

new set $z_i = \eta_i - (1 - 2\rho)\xi$, then (16) takes the asymptotic form:

$$\prod_{i=1}^{N}\frac{1}{\sqrt{8\pi\rho(1-\rho)\Delta\xi}}\exp\left\{-\frac{(z'_i - z_i)^2}{8\rho(1-\rho)\Delta\xi}\right\}. \tag{17}$$

From the Gaussian factor in (17) it is clear that the z_i are effectively continuum variables. Changing to the z_i variables in (15) and taking the product with (17) we end up with the transfer matrix:

$$K(z, z'; \Delta\xi) = \left(\frac{1}{8\pi\rho(1-\rho)\Delta\xi}\right)^{N/2}\exp\left\{-\sum_{i=1}^{N}\frac{(z'_i - z_i)^2}{8\rho(1-\rho)\Delta\xi}\right.$$
$$\left.-\frac{1}{2}\beta\Delta\xi\sum_{i=1}^{N-1}|z_i - z_{i+1}|\right\}.$$

This result is indistinguishable from the short-time kernel

$$K(z, z'; t) = \lim_{t\to0}\langle z'|\exp(-tH_N)|z\rangle$$

with continuum hamiltonian

$$H_N = 2\rho(1-\rho)\sum_{i=1}^{N}p_i^2 + \frac{1}{2}\beta\sum_{i=1}^{N-1}|z_i - z_{i+1}|$$

where $t = \Delta\xi$.

The validity of this derivation depended on having the mean separation between consecutive particles be large. This is a statement about the ground state wavefunction that we can now test. Suppose the mean separation is of order l, then p_i^2 is of order l^{-2}. Since the kinetic and potential parts of the hamiltonian have the same order of magnitude in the ground state we have that

$$\frac{\rho(1-\rho)}{l^2} \sim \beta l$$

or

$$l \sim \left(\frac{\rho(1-\rho)}{\beta}\right)^{1/3} \gg 1 \, .$$

Since this breaks down for $\rho \to 0$ and $\rho \to 1$, the present approximation cannot give the behavior of the surface near the crystal facets.

Recalling that the free energy (2) was defined per unit of ξ, we see that this is just E_N/N where E_N is the ground state energy of H_N. The β and ρ dependence of E_N can be made explicit by the rescaling

$$z = 2\left(\frac{\rho(1-\rho)}{\beta}\right)^{1/3} x$$

$$H_N = \left(\rho(1-\rho)\beta^2\right)^{1/3} \overline{H}_N$$

$$\overline{H}_N = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N-1} |x_i - x_{i+1}| \, .$$

If the ground state energy of $\overline{H}_N$ is $\overline{E}_N$ and

$$e_0 = \lim_{N \to \infty} N^{-1}\overline{E}_N \, ,$$

then, remembering to include (14), our final result is:

$$F(\rho,\beta) = \rho\log\rho + (1-\rho)\log(1-\rho)$$
$$+ e_0\left(\rho(1-\rho)\beta^2\right)^{1/3} \qquad \beta \ll \rho(1-\rho) \, .$$

The exact value of e_0 is not known but it is easy to obtain the variational bound

$$e_0 < 1.0188$$

using the trial wavefunction

$$\Psi_0 = \prod_{i=1}^{N-1} \Phi(x_i - x_{i+1}) \, .$$

4. Low Density Expansion

We will consider once again the transfer matrix M introduced in section 2. However, rather than derive an approximate hamiltonian as was done for the low temperature expansion, we will try to compute the largest eigenvalue of M directly. In terms of the original y_{xz} variables, the eigenvalue equation takes the form

$$\Lambda_{nm}\Psi(y_1,\ldots,y_n) = \sum_{y'\in\mathcal{R}} \exp\left(-\beta\sum_{i=1}^n |y_i - y'_i|\right)\Psi(y'_1,\ldots,y'_n) \quad (18)$$

where by $y' \in \mathcal{R}$ we mean that the sum is over the region

$$\mathcal{R}: \quad 0 \le y'_1 \le \cdots \le y'_n \le m \, .$$

The free energy is now given by

$$\lim_{L\to\infty} L^{-1}\log\Lambda_{\rho L\ (1-\rho)L} = -F(\rho,\beta) \, . \qquad (19)$$

We can view (18) as a kernel for n particles moving on a linear lattice of $m + 1$ sites. At low particle density the separations $|y_i - y'_i|$ are of the order β^{-1} so that there is little interaction among the particles when $\beta^{-1} \ll m/n$ or $\rho \ll \beta$. In this limit (18) approaches the diffusion kernel for n particles that are prevented from moving through each other.

The eigenvalue equation (18) defines the eigenfunction $\Psi(y)$ also when the point $y = (y_1, \ldots, y_n)$ lies outside the region $\mathcal{R}$. It is therefore valid to write equations for $\Psi(y)$ that sample points outside this region. One such equation involves the second order difference operator

$$\nabla f(x) \equiv \cosh\beta\, f(x) - \tfrac{1}{2}[f(x+1) + f(x-1)]$$

with the property:

$$\nabla \exp(-\beta|x - x'|) = \sinh\beta\, \delta_{x\,x'}\,.$$

If we apply this operator n times on (18) we obtain the equation

$$\Lambda_{nm} \nabla_1 \cdots \nabla_n \Psi(y) = (\sinh\beta)^n \theta(y)\Psi(y) \qquad (20)$$

where

$$\theta(y) = \begin{cases} 1 & y \in \mathcal{R} \\ 0 & \text{otherwise}\,. \end{cases}$$

A different sort of equation using the first order difference operator

$$\partial f(x) \equiv f(x+1) - f(x)$$

follows from the identity:

$$\left.(\partial_1 + 1 - e^{-\beta})(\partial_2 + 1 - e^{\beta})\exp(-\beta|x_1 - x_1'| - \beta|x_2 - x_2'|)\right|_{x_1 = x_2}$$

$$= 0 \qquad \text{for} \quad x_1' \le x_2'\,.$$

Since the above inequality is satisfied by each pair of consecutive variables $y_i' \le y_{i+1}'$ in the summation region $\mathcal{R}$, we can derive from (18) the boundary conditions ($i = 1, \ldots, n-1$):

$$\left.(\partial_i + 1 - e^{-\beta})(\partial_{i+1} + 1 - e^{\beta})\Psi(y)\right|_{y_i = y_{i+1}} = 0 \qquad (21)$$

Equation (20) together with the set of boundary conditions (21) are reminiscent of some one-dimensional many-body problems that can be solved exactly using the Bethe-*ansatz* method[3]. In particular, if we take the limit $\beta \to 0$ while still maintaining $\rho \ll \beta$, the product of the operators ∇ in (21) exponentiates to give

$$\exp\left(-\beta^{-2} \sum_{i=1}^{n} \frac{\partial^2}{\partial y_i^2}\right)\Psi(y) = \frac{1}{\Lambda_{nm}}\left(\frac{2}{\beta}\right)^n \theta(y)\Psi(y)$$

since the momentum components of $\Psi(y)$ are of the order $\rho \ll \beta$. In the same limit the boundary conditions (21) become

$$\left.\left(\frac{\partial}{\partial y_{i+1}} - \frac{\partial}{\partial y_i} - \beta\right)\Psi(y)\right|_{y_i = y_{i+1}} = 0 \qquad i = 1, \ldots, n-1$$

giving us the full set of equations that define the problem of the 'delta-function gas'[4].

The exact equations (20) and (21) can in fact also be solved using the Bethe-*ansatz*. Unfortunately, however, this solution does not satisfy the original eigenvalue equation (18) except in the limit of vanishing density. In order to understand this rather remarkable failure it is perhaps instructive to consider in detail the two-body problem first.

When the two particles are free to move on an infinite line of lattice sites we have to solve the equation

$$\Lambda\Psi(y_1, y_2) = \sum_{y_1' \le y_2'} \exp(-\beta|y_1 - y_1'| - \beta|y_2 - y_2'|)\Psi(y_1', y_2')\,.$$

The center of mass motion can be eliminated using

$$\Psi(y_1, y_2) = \exp(iky_1)R(y_2 - y_1)$$

where now, in terms of the relative coordinate $r = y_2 - y_1 \ge 0$, the eigenvalue equation becomes:

$$\Lambda R(r) = \sum_{r'=0}^{\infty} K(r - r')R(r') \qquad (22)$$

$$K(u) = K(-u)^* = \sum_{v=-\infty}^{\infty} \exp(-\beta|v| - \beta|u+v| - ikv) .$$

Equation (22) is of the kind that can be solved using the Wiener-Hopf method. Since this method is explained at length elsewhere (see for example ref. 5) we will only give the final answer. Although the form of our wavefunction is exact, the constants that appear have been approximated for the case that Λ is in the vicinity of the maximum eigenvalue. These wavefunctions are best characterized in terms of two small momentum values p_1 and p_2:

$$\Psi(y_1, y_2) = \exp(ip_1 y_1 + ip_2 y_2) - \exp(i\phi)\exp(ip_2 y_1 + ip_1 y_2)$$
$$+ A \exp\left(i\tfrac{1}{2}(p_1 + p_2)(y_1 + y_2) - b(y_2 - y_1)\right) \quad (23)$$

where,

$$\phi = c(p_1 - p_2) + O(p^2) \quad (24)$$

$$A = i\frac{(e^{-b} - e^{-\beta})^2}{(1 - e^{-b})(1 - e^{-\beta})^2}(p_1 - p_2) + O(p^2)$$

and,

$$b = -\log\left(1 - 4v(\sqrt{1 + \tfrac{1}{2v}} - 1)\right) + O(p)$$

$$c = 1 + \sqrt{1 + \tfrac{1}{v}} - \tfrac{1}{4v}(\sqrt{1 + \tfrac{1}{2v}} - 1)^{-1}$$

$$v = (\sinh\tfrac{\beta}{2})^2 .$$

We see that the first two terms of the wavefunction (23) have exactly the Bethe-*ansatz* form with the phase shift given by ϕ. However, there is also an exponentially decaying term that describes a 'bound-state'

piece of the wavefunction. It is this term that spoils the Bethe-*ansatz*. One would also expect analogues of this term to arise in the general n-body problem. We can nevertheless make some progress by taking advantage of the fact that relative to the plane-wave terms, the bound-state amplitude is small:

$$A \sim O(p) \sim O(\rho) .$$

The first term in a low density expansion would thus proceed along the Bethe-*ansatz* lines while pretending $A = 0$. The question is then the following: to what order in momentum may we keep terms in the phase shift ϕ ? We conjecture that it is valid to retain the terms up to $O(p)$ but cannot provide a simple proof of this claim. Some evidence in favor will appear at the end of this section.

The boundary conditions implicit in (18) due to the endpoints of the lattice are not ideally suited to the present discussion. We therefore modify the original problem by wrapping the lattice into a circle of m points. This should not affect the thermodynamic limit and allows us to impose the periodic boundary conditions

$$\Psi(y_1, \ldots, y_n) = \Psi(y_2, \ldots, y_n, m + y_1) . \quad (25)$$

One of the terms appearing in the wavefunction Ψ is the product of n plane waves:

$$\exp(ip_1 y_1 + \cdots + ip_n y_n) . \quad (26)$$

By suitably normalizing Ψ the coefficient of this term can be set equal to unity. Other terms in Ψ obtained from (26) by permuting the momenta will have coefficients given by appropriate phases. For the permutation that shifts the momenta in an n-cycle the phase can be deduced trivially since by (25) the term (26) becomes

$$\exp(ip_n m)\exp(ip_n y_1 + ip_1 y_2 + \cdots + ip_{n-1} y_n) . \quad (27)$$

In the usual Bethe-*ansatz* problem one generates the same permutation by the sequence of transpositions

$$T_2 \cdots T_{n-1} T_n$$

$$T_i: \quad \exp(ip_{i-1}y_{i-1} + ip_n y_i) \to$$

$$- \exp\big(i\phi(p_{i-1}, p_n)\big) \exp(ip_n y_{i-1} + ip_{i-1} y_i) \qquad (28)$$

where the phase shifts ϕ are obtained directly from an equation of the type (21). In the present situation, however, we use the result (24) of the two-body problem. Equating the phase in (27) with the accumulated phase from (28) we end up with the set of equations (N_i = integer, n = odd):

$$p_i m = \sum_{j \neq i} \phi(p_j, p_i) + 2\pi N_i$$

$$= -cnp_i + c \sum_j p_j + 2\pi N_i . \qquad (29)$$

A nontrivial ground state wavefunction is found by choosing a distinct set of momenta that satisfy (29) and maximize the eigenvalue Λ_{nm}. Recalling the action of the difference operator

$$\nabla \exp(ipy) = (\cosh\beta - \cos p) \exp(ipy) ,$$

the eigenvalue, according to (20), is just

$$\Lambda_{nm} = \prod_{i=1}^{n} \left(\frac{\sinh\beta}{\cosh\beta - \cos p_i} \right) .$$

From (29) we see that (to this approximation) the momenta are equally spaced. The maximum eigenvalue results when these are chosen symmetrically about $p = 0$:

$$p_i = \frac{2\pi N_i}{m} \left(1 - c\frac{n}{m} + O(\rho^2) \right)$$

$$-\tfrac{1}{2}(n-1) \leq N_i \leq \tfrac{1}{2}(n-1) .$$

Using (19) we arrive at our final result:

$$F(\rho, \beta) = -\rho \log\left(\frac{\sinh\beta}{\cosh\beta - 1} \right) + \frac{\pi^2}{6} \left(\frac{1}{\cosh\beta - 1} \right)(\rho^3 + 2(1 - c)\rho^4)$$

$$+ O(\rho^5) . \qquad (30)$$

The first term above is simply related to the free energy of a single particle on an infinite lattice, while the $O(\rho^3)$ term reflects the impenetrability of the two adjacent particles. These terms are insensitive to the precise nature of the interaction among the particles except that these are short range and hard-core. The $O(p)$ dependence of the phase shift first appears in the $O(\rho^4)$ term of (30) and required the solution of the two-body problem. Presumably the $O(\rho^5)$ term will involve the inclusion of three-body effects.

A useful check on our result (in particular the $O(\rho^4)$ term) follows from the observation that (30) and the low temperature result (13) have a common region of validity. Indeed, it can be verified that an expansion of the coefficients of (30) in powers of $e^{-\beta}$ agrees with the expansion of (13) in powers of ρ.

Finally, we observe that the $O(\rho^2)$ term vanishes for all values of the temperature, thus confirming (10) and our claims about the behavior of the surface near a facet.

After the completion of this work it was pointed out to the author that the $t^{3/2}$ behavior near the crystal facet has been discussed previously[6].

Acknowledgments

References

(1) see, *e.g.*, L. D. Landau and E. M. Lifshitz "Statistical Physics" (Addison-Wesley, Reading, Mass., 1969) *sec. 143*

(2) see, *e.g.*, E. H. Lieb, T. D. Schultz, and D. C. Mattis *Ann. Phys.* **16** *407* (1961)

(3) see, *e.g.*, E. H. Lieb and D. C. Mattis "Mathematical Physics in One Dimension" (Academic Press, New York, 1966) *ch. 6*

(4) E. H. Lieb and W. Liniger *Phys. Rev.* **130** *1605* (1963)

(5) J. Mathews and R. L. Walker "Mathematical Methods of Physics" (W. A. Benjamin Inc., New York, 1970) *p. 312*

(6) C. Jayaprakash *et. al. Phys. Rev. Lett.* **50** *2017* (1983)

Figure Captions

Fig. 1: Two lattice paths and their particle representations.

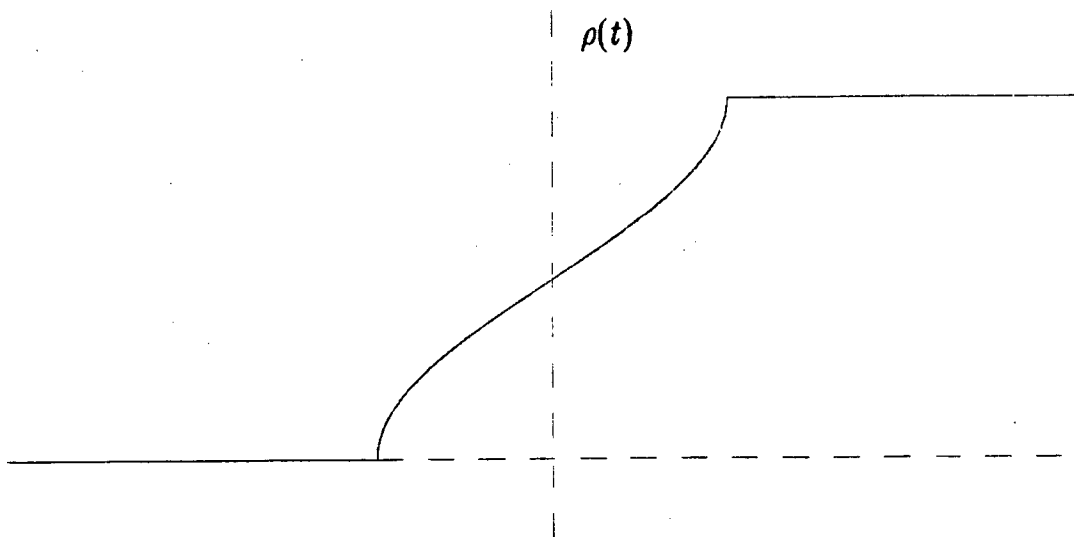Fig. 2: The particle density in the low temperature limit.

Figure 1

Figure 2