Surface Critical Phenomena of a Free Bose Gas with Enhanced Hopping at the Surface

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Abstract We study the Bose–Einstein condensation in the tight-binding model with the hopping rate enhanced only on a surface. We show that this model exhibits two different critical phenomena depending on whether the hopping rate on the surface $J_s$ exceeds the critical value $5J/4$, where $J$ is the hopping rate in the bulk. For $J_s/J < 5/4$, normal Bose–Einstein condensation occurs, while the Bose–Einstein condensation for $J_s/J \geq 5/4$ is characterized by the spatial localization of the macroscopic number of particles at the surface. By exactly calculating the surface free energy, we find that the singularity type of the surface free energy is different from that of the bulk free energy for $J_s/J > 5/4$.

Keywords Bose–Einstein condensation · Surface critical phenomena · Surface phase transition

1 Introduction

Surfaces are rarely the focus of thermodynamics research and yet specific and interesting behaviors may be observed on a surface. Typical examples are wetting of the liquid on a solid wall [1–3] and surface melting [4]. In particular, some phenomena related to surfaces can be understood in the context of critical phenomena. These phenomena have been understood employing theory and methods developed to investigate standard critical phenomena; e.g., mean field theory, scaling theory, the renormalization group method and Monte Carlo simulation [5–8]. The surface long-range order was discovered in this development. The surface long-range order is a long-range order occurring only on the surface in a regime where the bulk remains disordered. The surface long-range

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order was found in the analysis of semi-infinite Ising ferromagnets [9–12], and it has been confirmed experimentally to the present [13–15].

There is a limitation to the long-range order of pure two-dimensional systems, referred to as the Mermin–Wagner theorem [16,17]. This theorem claims that a two-dimensional system with a continuous symmetry does not exhibit long-range order owing to its symmetry breaking at finite temperatures. We ask whether this limitation applies also to the surface long-range order. The simplest model with which to consider this question is the semi-infinite Heisenberg ferromagnet [18–20]. Whether or not this model exhibits surface long-range order was intensively investigated using, for example, high-temperature expansion [21], scaling theory [22], real-space renormalization group theory [23] and Monte Carlo simulation [24,25]. These studies did not give any evidence of the existence of the surface long-range order. It is currently thought that there is no surface long-range order of Heisenberg ferromagnets, although we do not have any theorem that denies the existence of surface long-range order for a wide class of two-dimensional surfaces like the Mermin–Wagner theorem does for a pure two-dimensional system [21,23].

We focus on the possibility of the surface long-range order of systems for a continuous symmetry. Our interest and motivation arise from the following argument. We consider the effective two-dimensional system involving only the degree of freedom in the surface layer. In general, this effective system can be obtained by taking the trace over all the interior degrees of freedom. The effective system characterizes the surface critical phenomena. For the effective system to exhibit long-range order, it is necessary that the interaction through the bulk is a long-range interaction. The question we should ask is then "Can the coupling term of surface degrees of freedom interacting through the bulk be a long-range interaction?". We propose that the conservation law of the whole system is an important factor in considering this question. For example, we consider the case that the number of particles is conserved. At this time, we may employ the canonical ensemble with conservation of the particle number or the grand canonical ensemble. In particular, when we employ the grand canonical ensemble, the effective system includes a coupling term for the chemical potential, which is a physical quantity associated with the particle number of the total system. This term may make a nontrivial contribution to the statistical mechanics of the surface because it is a connection to a region far from the surface through particle conservation.

In this paper, in order to consider the role of the conserved quantity in the surface long-range order, we shall analyze an ideal Bose gas as an example. Specifically, we study a tight-binding Bose gas with a hopping rate enhanced only on the surface. In this model, a new type of Bose–Einstein condensation occurs under the effect of the surface; i.e., the two-dimensional bound state appears near the surface and $O(L^3)$ particles occupy the bound state when the hopping rate of the surface exceeds a certain critical value. From this point of view, this Bose–Einstein condensation is a bulk critical phenomenon in which there is "singular behavior" on the surface. Meanwhile, this phenomenon can be analyzed from the standpoint of the surface critical phenomenon at the
critical point, the surface has critical behaviors different from those of the bulk region, through coupling of the enhanced hopping effect of the surface with the bulk critical behavior. This Bose–Einstein condensation includes the surface critical phenomenon strongly affected by the bulk. In this model, the bulk and surface strongly affect each other and change the critical behavior of each other.

As a related study, Robinson reported an ideal Bose gas with an attractive boundary condition from the standpoint of the bulk critical phenomenon [26]. This model exhibits essentially the same Bose–Einstein condensation as our model. In this study, the boundary-condition dependence of physical properties was investigated [27] and pathological behavior involving the order of the limit operation was reported [28]. The attractive boundary condition was introduced under a mathematical motivation and it is not clear how this boundary condition can be realized. By contrast, we introduce our model while considering a more realistic experimental system. Furthermore, our analysis is performed in terms of both the bulk critical phenomenon and the surface critical phenomenon.

The remainder of this paper is organized as follows. Section 2 explains the setup of our model. We derive the quantum mechanical nature of our model in Section 3. We find that our model exhibits Bose–Einstein condensation regardless of the enhanced strength on the surface in Section 4. We then demonstrate that the particle number at the surface becomes of macroscopic order when the hopping rate at the surface exceeds a critical value. The singularity type of the bulk free energy and that of the surface free energy are respectively studied in Sections 5 and 6. The final section is devoted to a brief summary and concluding remarks.

2 Model

2.1 Quantum mechanical setup and formulation

We study a free Bose gas confined in a cubic box by considering a tight-binding model on a cubic lattice. We express the cubic lattice by

\[ A = \{(i_1, i_2, j) \in \mathbb{Z}^3 \mid 1 \leq i_1 \leq L, 1 \leq i_2 \leq L, 1 \leq j \leq L\}. \]

The index \( j \) denotes the vertical position and \( \mathbf{i} = (i_1, i_2) \) represents the lattice position in the horizontal layer. We assume periodic boundary conditions in the horizontal directions and free surface boundary conditions in the vertical direction. The Hamiltonian of this system is written as

\[
\hat{H} = - \sum_{j=1}^{L} J^\parallel \sum_{\langle \mathbf{i}, \mathbf{i}' \rangle} \left( \hat{a}_{\mathbf{i}, j}^\dagger \hat{a}_{\mathbf{i}', j} + \hat{a}_{\mathbf{i}', j}^\dagger \hat{a}_{\mathbf{i}, j} \right) \\
- \sum_{j=1}^{L-1} J_j^\perp \sum_{\mathbf{i}} \left( \hat{a}_{\mathbf{i}, j}^\dagger \hat{a}_{\mathbf{i}, j+1} + \hat{a}_{\mathbf{i}, j+1}^\dagger \hat{a}_{\mathbf{i}, j} \right),
\]

(2)
where \((i, i')\) represents a nearest-neighbor pair in a horizontal layer. \(\hat{a}_{i,j}\) and \(\hat{\alpha}_{i,j}^\dagger\) are respectively the bosonic annihilation and creation operators, which obey the bosonic commutation relations

\[
\left[\hat{a}_{i,j}, \hat{a}_{i',j'}^\dagger\right] = \delta_{ii'} \delta_{jj'}, \tag{3}
\]

\[
\left[\hat{a}_{i,j}^\dagger, \hat{a}_{i',j'}\right] = [\hat{a}_{i,j}, \hat{a}_{i',j'}^\dagger] = 0. \tag{4}
\]

We concentrate on the case

\[
J_{j} \parallel j = \begin{cases} J_s \equiv J(1 + \Delta) & \text{for } j = 1, \\ J & \text{otherwise}, \end{cases} \tag{5}
\]

\[
J_{j} \perp j = J \quad \text{for } j = 1, 2, \ldots, L - 1, \tag{6}
\]

where \(\Delta \geq 0\) represents the enhanced hopping strength at the surface layer.

Owing to translational invariance in layer \(j\), the Fourier momentum representation in the horizontal direction allows us to diagonalize the Hamiltonian. The transformation from the coordinate representation is expressed by

\[
a_{i,j}^\dagger = \frac{1}{L} \sum_k \hat{a}_{k,j}^\dagger e^{-ik_i}, \tag{7}
\]

\[
a_{i,j} = \frac{1}{L} \sum_k \hat{a}_{k,j} e^{ik_i}, \tag{8}
\]

\[
a_{k,j}^\dagger = \frac{1}{L} \sum_i \hat{a}_{i,j}^\dagger e^{ik_i}, \tag{9}
\]

\[
a_{k,j} = \frac{1}{L} \sum_i \hat{a}_{i,j} e^{-ik_i}. \tag{10}
\]

Here \(k\) is defined as

\[
k_d \equiv \frac{2\pi}{L} n_d, \tag{11}
\]

with

\[
n_d = \begin{cases} \frac{L-2}{2}, \cdots, -2, -1, 0, 1, 2, \cdots, \frac{L-2}{2}, \frac{L}{2} & \text{for } L : \text{even}, \\ \frac{L-1}{2}, \cdots, -2, -1, 0, 1, 2, \cdots, \frac{L-3}{2}, \frac{L-1}{2} & \text{for } L : \text{odd}, \end{cases} \tag{12}
\]

where \(d = 1, 2\). The Hamiltonian can then be written in the form

\[
\hat{H} = \sum_{j=1}^{L} \sum_{j'=1}^{L} \sum_k \hat{a}^\dagger_{k,j} A_{jj'}(k) \hat{a}_{k,j'}. \tag{13}
\]
The $L \times L$ matrix $A(k)$ is given by

$$A(k) = \begin{pmatrix} (1 + \Delta)\omega(k) & -J & 0 \\ -J & \omega(k) & -J \\ 0 & -J & \omega(k) \\ \vdots \\ 0 & \omega(k) & -J \\ -J & \omega(k) \end{pmatrix},$$

(14)

where $\omega(k)$ is defined as

$$\omega(k) = -2J \sum_{d=1}^{2} \cos k_d.$$  

(15)

Note that $\omega(k)$ is the single-particle energy eigenvalue of the system cutting out only one layer with hopping constant $J$.

Let $n_{k,j}$ be the number of particles occupying the single-particle state $(k,j)$. A complete set of bases for the Fock space $\mathcal{F}$ is represented by

$$|n\rangle \equiv \prod_{k,j} \left( \hat{a}_{k,j}^{\dagger} \right)^{n_{k,j}} \sqrt{n_{k,j}!} |0\rangle,$$

(16)

where $n = (n_{k,j})_{k,j}$.

2.2 thermodynamic setup and formulation

We focus on thermodynamic properties of the system that consists of $N$ Bose particles. In this paper, all calculations are carried out in the grand canonical ensemble with inverse temperature $\beta$ and chemical potential $\mu$. The ensemble average of an operator $\hat{Q}$ that is a function of $(\hat{a}_i, \hat{a}_i^{\dagger})$ (or $(\hat{a}_i, \hat{a}_k^{\dagger})$) is expressed as

$$\langle \hat{Q} \rangle_{\beta,\mu} \equiv e^{\beta J(\beta,\mu)} \text{Tr}(\hat{Q} e^{-\beta(\hat{H} - \mu \hat{N})}) = e^{\beta J(\beta,\mu)} \sum_{n} \langle n | \hat{Q} e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle,$$

(17)

where $\hat{N}$ is the total-particle-number operator

$$\hat{N} \equiv \sum_{i} \sum_{k} \hat{a}_{i,k}^{\dagger} \hat{a}_{i,k},$$

(18)

and $J(\beta,\mu)$ is the grand canonical free energy

$$J(\beta,\mu) \equiv -\frac{1}{\beta} \log \text{Tr}(e^{-\beta(\hat{H} - \mu \hat{N})}).$$

(19)
3 Quantum mechanical nature

This section summarizes the quantum mechanical nature. Let \( \epsilon_n(k) \) and |\( \lambda_n(k) \rangle \) be the single-particle energy eigenvalue and single-particle energy eigenstate of the Hamiltonian \( \hat{H} \), respectively. These satisfy the single-particle eigenvalue equation

\[
\hat{H}|\lambda_n(k)\rangle = \epsilon_n(k)|\lambda_n(k)\rangle,
\]

where we label the quantum states by (\( n, k \)). \( k \) corresponds to the Fourier momentum. The index \( n \) is used following the rule \( \epsilon_1(k) \leq \epsilon_2(k) \leq \epsilon_3(k) \leq \cdots \leq \epsilon_L(k) \).

Equation (20) is equivalent to

\[
A(k)u_n(k) = \epsilon_n(k)u_n(k),
\]

where \( u_n(k) = (u^1_n(k), u^2_n(k), \cdots, u^L_n(k)) \) is the \( L \)-component vector. Using \( u_n(k) \), we express |\( \lambda_n(k) \rangle \) as

\[
|\lambda_n(k)\rangle = \sum_{j=1}^{L} u^j_n(k)\hat{a}^\dagger_{k,j}|0\rangle.
\]

For convenience, we restrict ourselves to wave numbers satisfying \( \omega(k) < 0 \) in this section. See Appendix A for the other wave numbers \( \omega(k) \geq 0 \).

3.1 Unenhanced case

We study the case \( \Delta = 0 \). Equation (22) is rewritten as

\[
B(k)u^0_n(k) = \epsilon^0_n(k)u^0_n(k)
\]

with the \( L \times L \) matrix \( B(k) \)

\[
B(k) = \begin{pmatrix}
\omega(k) & -J & 0 \\
-J & \omega(k) & -J \\
0 & -J & \omega(k) \\
& \ddots & \ddots \\
0 & \omega(k) & -J \\
-J & \omega(k)
\end{pmatrix}.
\]

The superscript 0 represents quantities for the unenhanced case \( \Delta = 0 \). The equation can be solved using the translational invariance. The result is

\[
\epsilon^0_n(k) = \omega(k) - 2J \cos\left(\frac{n\pi}{L+1}\right),
\]

\[
u^0_{n,j}(k) = C \sin\left(\frac{jn\pi}{L+1}\right),
\]

where \( n = 1, 2, 3, \cdots, L \). \( C \) is the normalization constant.
3.2 Relation between $\epsilon_{n}^{0}(k)$ and $\epsilon_{n}(k)$

$\epsilon_{n}(k)$ is given by a solution $z$ for the characteristic equation

$$\det [A(k) - zE_L] = 0, \quad (28)$$

where $E_L$ is the $L \times L$ unit matrix. To estimate $\epsilon_{n}(k)$, we define $f(z; k)$ as

$$f(z; k) \equiv \det [A(k) - zE_L]. \quad (29)$$

Using the cofactor expansion, we express $f(z; k)$ as

$$f(z; k) = \left(-z + (1 + \Delta)\omega(k)\right)\det [B_{L-1}(k) - zE_{L-1}]$$

$$- J^2 \det [B_{L-2}(k) - zE_{L-2}]$$

$$= \det [B_{L}(k) - zE_L] + \Delta\omega(k) \det [B_{L-1}(k) - zE_{L-1}], \quad (30)$$

where the size of matrix $B(k)$ is explicitly written as the subscript. Here $f(z; k)$ is an $L$-th polynomial of $z$ because

$$\det [B_{L}(k) - zE_L] = \prod_{n=1}^{L} \left(-z + \omega(k) - 2J\cos\left(\frac{n\pi}{L+1}\right)\right), \quad (31)$$

where we have used (26).

We associate $\epsilon_{n}(k)$ with $\epsilon_{n}^{0}(k)$ for given $(n, k)$. From (30) and (31), we obtain

$$f(-\infty; k) > 0 \quad (32)$$

and

$$f(\epsilon_{1}^{0}(k); k) = \Delta\omega(k) \prod_{n=1}^{L-1} \left(2J\cos\left(\frac{n\pi}{L+1}\right) - 2J\cos\left(\frac{n\pi}{L}\right)\right) < 0. \quad (33)$$

From (32) and (33), we obtain

$$-\infty < \epsilon_{1}(k) < \epsilon_{1}^{0}(k). \quad (34)$$

Similarly, because

$$f(\epsilon_{2}^{0}(k); k) = \Delta\omega(k) \prod_{n=1}^{L-1} \left(2J\cos\left(\frac{2n\pi}{L+1}\right) - 2J\cos\left(\frac{n\pi}{L}\right)\right) > 0, \quad (35)$$

we find

$$\epsilon_{1}(k) < \epsilon_{2}(k) < \epsilon_{2}^{0}(k). \quad (36)$$
Repeating similar procedures, we derive
\[ \epsilon_{n-1}^0(k) < \epsilon_n(k) < \epsilon_n^0(k) \]  
(37)
for \(3 \leq n \leq L\). Because these relations hold for any \(L\), the energy eigenvalue \(\epsilon_n(k)\) with \(n \geq 2\) cannot finitely deviate from \(\epsilon_n^0(k)\) in the large system size limit, while there is no such restriction for the energy eigenvalue \(\epsilon_1(k)\) as shown in (34).

3.3 \(\epsilon_1(k)\) in the large system size limit

We derive a condition for \(\epsilon_1(k)\) stronger than the relation (37) in the large system size limit. We first rewrite (31) as
\[
\det \left[ B_L(k) - zE_L \right] = \exp \left\{ L \sum_{n=1}^{L} \log \left( -z + \omega(k) - 2J \cos \left( \frac{n\pi}{L+1} \right) \right) \right\} \\
\simeq \exp \left\{ L \int_0^1 dy \log \left( -z + \omega(k) - 2J \cos (\pi y) \right) \right\}. 
\]  
(38)
This integral converges when \(-z + \omega(k) - 2J > 0\) and is calculated as
\[
\det \left[ B_L(k) - zE_L \right] \simeq \frac{1}{2\pi} \exp \left\{ L \log \left( \sqrt{(z - \omega(k))^2 - 4J^2} - z + \omega(k) \right) \right\}. 
\]  
(39)
Recalling (30), we then express the characteristic equation (28) as
\[
\exp \left[ (L - 2) \log \left( \sqrt{(z - \omega(k))^2 - 4J^2} - z + \omega(k) \right) \right] \left[ \frac{1}{2} \left( -z + (1 + \Delta) \omega(k) \right) \right]
\times \left( \sqrt{(z - \omega(k))^2 - 4J^2} - z + \omega(k) \right) - J^2 = 0 
\]  
(40)
for \(z < \omega(k) - 2J\). Because
\[
\exp \left[ (L - 2) \log \left( \sqrt{(z - \omega(k))^2 - 4J^2} - z + \omega(k) \right) \right] > 0, \quad (41)
\]
(40) is equivalent to
\[
\frac{1}{2} \left( -z + (1 + \Delta) \omega(k) \right) \left( \sqrt{(z - \omega(k))^2 - 4J^2} - z + \omega(k) \right) - J^2 = 0. \quad (42)
\]
For wave numbers satisfying
\[
\Delta \omega(k) < -J, \quad (43)
\]
we find the solution to (42) with \( z < \omega(k) - 2J \) as
\[
    z = \frac{J^2 + \Delta^2 \omega(k)^2}{\Delta \omega(k)} + \omega(k). \tag{44}
\]

Meanwhile, for wave numbers satisfying
\[
    \Delta \omega(k) \geq -J, \tag{45}
\]
there is no solution to the characteristic equation (28) for \( z < \omega(k) - 2J \). See Appendix B for the derivation.

Recalling that the energy eigenvalue satisfying \( \epsilon_n(k) < \omega(k) - 2J \) corresponds to \( \epsilon_1(k) \), we obtain
\[
    \epsilon_1(k) \rightarrow \frac{J^2 + \Delta^2 \omega(k)^2}{\Delta \omega(k)} + \omega(k) \tag{46}
\]
for \( L \to \infty \), where \( k \) satisfies (43). Meanwhile, for wave numbers satisfying (45), there is no energy eigenvalue in the range \( \epsilon_n(k) < \omega(k) - 2J \). Recalling (34), we obtain a condition for \( \epsilon_1(k) \) as
\[
    \omega(k) - 2J < \epsilon_1(k) < \epsilon_0^1(k). \tag{47}
\]
Note that \( \epsilon_1(k) \) converges to \( \epsilon_0^1(k) \) in the large system size limit.

### 3.3.1 ground state

Recalling (15), we find that the existence condition of the wave numbers satisfying (43) is
\[
    \Delta > \frac{1}{4}. \tag{48}
\]
Note that the wave number \( k = 0 \) satisfies condition (43) for any \( \Delta > 1/4 \). Therefore, with regard to the ground-state energy eigenvalue, (46) and (47) are written as
\[
    \lim_{L \to \infty} \epsilon_1(0) = \begin{cases} 
        -6J & \text{for } \Delta \leq \frac{1}{4}, \\
        -4J - 2J \frac{1 + \Delta^2}{4} & \text{for } \Delta > \frac{1}{4}.
    \end{cases} \tag{49}
\]

### 3.4 Expression of \( \mathbf{u}_n(k) \)

Let \( \theta_n(k) \) be the \( n \)-th solution of the equation for \( \theta \):
\[
    -J \sin((L + 1)\theta) - \Delta \omega(k) \sin(L\theta) = 0. \tag{50}
\]
Using \( \theta_n(k) \), we derive \( \epsilon_n(k) \) and \( \mathbf{u}_n(k) \) as
\[
    \epsilon_n(k) = \omega(k) - 2J \cos \theta_n(k), \tag{51}
\]
\[ u_n^j(k) = \frac{u_n^1(k)}{\sin \theta_n(k)} \left( \sin(j \theta_n(k)) - \Delta \omega(k) \sin((j - 1) \theta_n(k)) \right), \]

with \( j = 1, 2, \cdots, L \) [29]. Substituting (52) into the normalization condition

\[ \sum_{j=1}^{L} |u_n^j(k)|^2 = 1, \]

we obtain

\[ |u_n^1(k)|^2 = \frac{\sin^2 \theta_n(k)}{\sum_{j=1}^{L} \left[ \sin(j \theta_n(k)) - \Delta \omega(k) \sin((j - 1) \theta_n(k)) \right]^2}. \] (54)

3.4.1 \( \Delta \leq \frac{1}{4} \)

From (15), (36), (37) and (47), we find

\[ -6J < \epsilon_n(k) < 6J \] (55)

for all \( n \) and \( k \). From (15), (51) and (55), we obtain

\[ -1 < \cos \theta_n(k) < 1. \] (56)

Because all \( \theta_n(k) \) are real numbers, the denominator of (54) is evaluated as

\[
\sum_{j=1}^{L} \left[ \sin(j \theta_n(k)) - \Delta \omega(k) \sin((j - 1) \theta_n(k)) \right]^2 \\
= L \int_0^1 dx \left[ \sin(Lx \theta_n(k)) - \Delta \omega(k) \sin((Lx - 1) \theta_n(k)) \right]^2 + O(L^0) \\
= \frac{L}{2} \left( 1 + \Delta^2 \omega(k)^2 - 2 \Delta \omega(k) \cos \theta_n(k) \right) + O(L^0). \] (57)

Substituting this result into (54), we obtain

\[ |u_n^1(k)|^2 \approx \frac{2 \sin^2 \theta_n(k)}{L \left( 1 + \Delta^2 \omega(k)^2 - 2 \Delta \omega(k) \cos \theta_n(k) \right)} \] (58)

in the large system size limit. Using (52) and (58), we express all \( u_n(k) \) in terms of \( \theta_n(k) \).
3.4.2 $\Delta > \frac{1}{4}$

From (15), (36), (37) and (46), we find

$$
\begin{cases}
\epsilon_n(k) < -6J \text{ for } n = 1 \text{ and } \Delta\omega(k) < -J, \\
-6J < \epsilon_n(k) < 6J \text{ otherwise}.
\end{cases}
$$

From (15), (51) and (59), we find that $\theta_1(k)$ satisfies

$$
\cos \theta_1(k) > 1,
$$

where $k$ satisfies $\Delta\omega(k) < -J$. This means that $\theta_1(k)$ is a complex number. For the other wave numbers, we find that $\theta_1(k)$ is a real number. Note that the complex solution to (50), $\theta_1(k)$, corresponds to the energy eigenvalue expressed by (46).

When $\theta_1(k)$ is a complex number, (58) does not hold. Instead we can calculate $|u_n^1(k)|^2$ using the path integral expression. As shown in Appendix C.2, we obtain

$$
|u_n^1(k)|^2 = \lim_{z \to \epsilon_n(k)} \left\{ (-z + \epsilon_n(k)) \frac{\det(B_{L-1}(k) - zE_{L-1})}{\det(A(k) - zE_L)} \right\}.
$$

(61)

Substituting (30), (39) and (46) into (61), we obtain

$$
|u_1^1(k)|^2 = \frac{1}{4\Delta\omega(k)} \left\{ \sqrt{\frac{(1 + 4\Delta^2\omega(k))^2}{(4\Delta\omega(k))^2} - 1} - \frac{1 + 4\Delta^2\omega(k)^2}{4\Delta\omega(k)} + 2\Delta\omega(k) \right\}
$$

(62)

in the large size limit, where $k$ satisfies (43). Using (52) and (62), we express $u_1^1(k)$ in terms of $\theta_1(k)$. When $\theta_1(k)$ is a real number, the previous result (58) holds. From (15), (51) and (59), we find that $\theta_n(k)$ is a real number and the previous result (58) holds for $n \geq 2$. We then express all $u_n(k)$ in terms of $\theta_n(k)$.

4 Bose–Einstein condensation

This section demonstrates that the model exhibits Bose–Einstein condensation. More precisely, above a critical density or below a critical temperature, the occupation number of the single-particle basis state is found to be of order $L^3$ regardless of $\Delta$.

Let $\hat{n}_n(k)$ be the operator of the occupation number of the single-particle state $(n, k)$ corresponding to the energy eigenvalue $\epsilon_n(k)$. The grand canonical average of this quantity is given as

$$
< \hat{n}_n(k) >_{\beta, \mu} = \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1}.
$$

(63)
The chemical potential satisfies the condition
\[ \mu < \epsilon_1(0), \]  
so that the mean occupation number \( \langle \hat{n}_n(k) \rangle \) is not negative for any \( \epsilon_n(k) \).

The total number of particles \( N \) is obtained by the summation of the occupation number over all states:
\[ N = \sum_{n=1}^{\infty} \sum_{k} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1}. \]  

In particular, the particle number density \( \rho \) is given as
\[ \rho = \frac{1}{L^3} \sum_{n=1}^{\infty} \sum_{k} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1}. \]  

Solving this equation in \( \mu \), we obtain the chemical potential \( \mu = \mu(\beta, \rho) \) as a function of \((\beta, \rho)\). In the thermodynamic limit, \( 66 \) is expressed as
\[ \rho = \frac{1}{L^3} \frac{1}{e^{\beta(\epsilon_1(0) - \mu)} - 1} + G(\beta, \mu) \]  
with
\[ G(\beta, z) = \int \frac{d^3 \rho}{(2\pi)^3} \frac{1}{e^{\beta(-2J \sum_{d=1}^{3} \cos \rho_d - z)} - 1}, \]
where \( z \) satisfies \(-\infty < z \leq -6J \). See Appendix D for the derivation. The first term on the right-hand side of \( 67 \) is the particle number density occupying the ground state and the second term represents the contribution of all excited states.

### 4.1 Derivation of Bose–Einstein condensation

For \( 67 \), we must consider that possible values of \( \mu \) are restricted by condition \( 64 \). Recalling \( 49 \), we find that this restriction can be classified into two cases depending on \( \Delta \).

#### 4.1.1 \( \Delta < \frac{1}{4} \)

From \( 36 \), \( 37 \) and \( 47 \), we find that no single-particle energy eigenvalue \( \epsilon_n(k) \) finitely changes from the case \( \Delta = 0 \) in the large system size limit. Because neither \( 67 \) nor condition \( 64 \) changes from that for \( \Delta = 0 \), we observe the same critical behavior as for \( \Delta = 0 \). To demonstrate this behavior, we consider the setting where \( \rho \) is controlled by varying \( \mu \), while \( \beta \) is fixed.

We consider \( G(\beta, \mu) \) as the function of \( \mu \) with \( \beta \) fixed. \( G(\beta, \mu) \) is the monotonically increasing function of \( \mu \) for any \( \beta \). Then, \( G(\beta, \mu) \leq G(\beta, -6J) \) because \( \mu \leq -6J \). Figure 1 shows \( G(\beta, \mu) \) as a function of \( \mu \) at some fixed \( \beta \).
For $\rho < G(\beta, -6J)$, we find a one-to-one correspondence between $\mu$ and $\rho$ through (69). This pair $(\mu, \rho)$ also satisfies (67) in the thermodynamic limit because

$$\lim_{L \to \infty} \frac{1}{L^3} e^{\beta(\epsilon_1(0) - \mu)} - 1 = 0$$

holds. We therefore obtain $\mu$ satisfying (67) as a function of $\rho$, which is expressed as

$$\mu = G^{-1}(\beta, \rho)$$

for $\rho < G(\beta, -6J)$, where $G^{-1}(\beta, \rho)$ is the inverse function of $G(\beta, \mu)$ as a function of $\mu$ with $\beta$ fixed.

Meanwhile, for $\rho \geq G(\beta, -6J)$, there is no $\mu$ satisfying (69) (See Figure 1). However, we find a one-to-one correspondence between $\mu$ and $\rho$ employing equation (67) because the first term on the right-hand side of (67) diverges when $\mu \to -6J$. We thus consider (67) under the condition

$$\beta(\epsilon_1(0) - \mu) \ll 1.$$  

We then estimate the right-hand side of (67) in this region as

$$\rho = \frac{1}{L^3} \frac{1}{\beta(\epsilon_1(0) - \mu)} + G(\beta, -6J) + o\left(\frac{1}{L^3}\right).$$

As a result, we obtain $\mu$ satisfying (67) as a function of $\rho$:

$$\mu = \epsilon_1(0) - \frac{1}{L^3} \frac{1}{\beta(\epsilon_1(0) - \mu) - G(\beta, -6J)} + o\left(\frac{1}{L^3}\right).$$
for $\rho \geq G(\beta, -6J)$. Note that, in the thermodynamic limit, because

$$\mu = -6J,$$

(75)

$\mu$ does not determine $\rho$ uniquely in this $\rho$ region.

Recalling that the first term on the right-hand side of (67) is the particle number density occupying the ground state, we obtain

$$\frac{<\hat{n}_1(0)>_{\beta,\rho}}{L^3} = \rho - G(\beta, -6J)$$

(76)

for $\rho \geq G(\beta, -6J)$, where $<\hat{n}_1(0)>_{\beta,\rho}$ is not the canonical average but is defined as

$$<\hat{n}_1(0)>_{\beta,\rho} \equiv <\hat{n}_1(0)>_{\beta,\mu(\beta,\rho)}.$$  

(77)

When $<\hat{n}_1(0)>_{\beta,\rho} / L^3$ is finite, Bose–Einstein condensation is identified. In this sense, we define the critical density $\rho_c$ as

$$\rho_c = G(\beta, -6J).$$

(78)

One may also consider the Bose–Einstein condensation for the setting where $\beta$ is controlled with $\rho$ fixed. In this setting, we define the critical inverse temperature $\beta_c$ as

$$\rho = G(\beta_c, -6J).$$

(79)

We then observe Bose–Einstein condensation in the low-temperature regime $\beta \geq \beta_c$.

4.1.2 $\Delta \geq 1/4$

As shown in (49), the ground-state energy finitely changes from that for $\Delta = 0$ in the large system size limit. This change leads to a different type of critical phenomenon. We consider the setting that $\rho$ is controlled through $\mu$, while $\beta$ is fixed. From (49) and (64), we find that possible values of $\mu$ are restricted to

$$\mu < \mu_*,$$

(80)

where we have introduced

$$\mu_* = -4J - \frac{1 + 16\Delta^2}{4\Delta}.$$  

(81)

In this range, we consider (67).

We first consider (69) for $\rho < G(\beta, \mu_*)$. This equation is identical to that for $\Delta < 1/4$ because $\rho < G(\beta, \mu_*)$ implies $\rho < G(\beta, -6J)$ (See Figure 2). Therefore, repeating the same argument for $\Delta < 1/4$, we obtain $\mu$ satisfying

$$\mu = G^{-1}(\beta, \rho)$$

(82)

for $\rho < G(\beta, \mu_*)$. 
For any positive \( \rho < G(\beta, \mu_*) \), there exists a unique \( \mu \) satisfying \( \rho = G(\beta, \mu) \). Because we consider the restricted \( \mu \) region, we find that there is no \( \mu \) for \( \rho \geq G(\beta, \mu_*) \).

We next consider (69) for \( \rho \geq G(\beta, \mu_*) \). There is no \( \mu \) satisfying (69) in the range (80) (See Figure 2). However, we find a one-to-one correspondence between \( \mu \) and \( \rho \) through (67) because the first term of (67) makes a finite contribution. Considering (67) under the condition \( \beta (\epsilon_1(0) - \mu) \ll 1 \),

we obtain \( \mu \) satisfying (67) as a function of \( \rho \):

\[
\mu = \epsilon_1(0) - \frac{1}{L^3} \frac{1}{\beta (\rho - G(\beta, \mu_*) )} + o \left( \frac{1}{L^3} \right)
\]

for \( \rho \geq G(\beta, \mu_*) \). In the thermodynamic limit, we obtain

\[
\mu = \mu_*.
\]

The particle number density occupying the ground state is given as

\[
< \hat{n}_1(0) >_{\beta, \rho} = \rho - G(\beta, \mu_*)
\]

for \( \rho \geq G(\beta, \mu_*) \). The occupation density of the ground state is finite so that Bose–Einstein condensation occurs even for the case \( \Delta > 1/4 \). We obtain the critical density \( \rho_c \) as

\[
\rho_c = G(\beta, \mu_*).
\]

The Bose–Einstein condensation for \( \Delta \geq 1/4 \) has unusual behavior such that the critical density \( \rho_c \) depends on the value of \( \Delta \) defined only at the boundary. Keeping this strong surface effect in mind, we refer to the behavior for \( \Delta \geq 1/4 \) as the Bose–Einstein condensation affected by the surface.

Similarly, when \( \beta \) is controlled with \( \rho \) fixed, we obtain the critical inverse temperature \( \beta_c \) as

\[
\beta = G(\beta, \mu_*).
\]

In the low-temperature regime \( \beta \geq \beta_c \), we observe the Bose–Einstein condensation state affected by the surface.
4.2 Particle number near the surface

The grand canonical average of the particle number in the $j$th layer $N_j$ is given by

$$N_j = \langle \sum_k \hat{a}_{j,k}^\dagger \hat{a}_{j,k} \rangle >_{\beta,\mu}.$$  \hspace{1cm} (89)

Using (63), we express $N_j$ in terms of the single-particle energy eigenvector $u_n(k)$ as

$$N_j = \sum_k \sum_{n=1}^L |u_n^j(k)|^2 \frac{1}{e^{\beta \epsilon_n(k) - \mu} - 1}.$$  \hspace{1cm} (90)

Below, we estimate $N_j$ for cases $\Delta < 1/4$ and $\Delta \geq 1/4$ by calculating $|u_n^j(k)|^2$.

4.2.1 $\Delta < 1/4$

From (52) and (58), we obtain

$$|u_n^j(k)|^2 \simeq \frac{1}{L} \frac{\left( \sin(j \theta_n(k)) - \Delta \omega(k) \sin((j-1) \theta_n(k)) \right)^2}{1 + \Delta^2 \omega(k)^2 - 2 \Delta \omega(k) \cos \theta_n(k)}.$$  \hspace{1cm} (91)

Because $|u_n^j(k)|^2$ is $O(L^{-1})$, $N_j$ is $O(L^2)$. Such dependence on $L$ is the same as that for $\Delta = 0$.

4.2.2 $\Delta \geq 1/4$

We focus on the particle number in the first layer $N_1$. For $k$ satisfying (43), $|u_1^1(k)|^2$ is given by (62), which is $O(1)$. For the other $k$, $|u_1^1(k)|^2$ is given by (91), which is $O(L^{-1})$. For the Bose–Einstein condensate, the contribution of the ground state to $N_1$ is

$$L^3 \frac{1}{4 \Delta \omega(0)} \left\{ \sqrt{\frac{(1 + 4 \Delta^2 \omega(0)^2)^2}{(4 \Delta \omega(0))^2} - 1 - \frac{1 + 4 \Delta^2 \omega(0)^2}{4 \Delta \omega(0)} + 2 \Delta \omega(0)} \right\} \times (\rho - G(\beta, \mu_*)),$$  \hspace{1cm} (92)

which is $O(L^3)$. $N_1$ is therefore also $O(L^3)$. This $L$-dependence of $N_1$ is different from that for $\Delta < 1/4$. This result implies that the Bose–Einstein condensate for $\Delta \geq 1/4$ is a spatially localized state in the first layer.
5 Bulk free energy density

This section investigates the free energy density for the two types of Bose–Einstein condensation focusing on the nonanalyticity of the free energy density. Here, the bulk free energy density of the grand canonical ensemble is defined by

\[ j(\beta, \mu; \Delta) \equiv \lim_{L \to \infty} \frac{1}{L^3} J(\beta, \mu; \Delta), \quad (93) \]

where \( J(\beta, \mu; \Delta) \) is given by (19). We first consider the \( \Delta \)-dependence of \( j(\beta, \mu; \Delta) \). By straightforward calculation, the total free energy is expressed in terms of energy eigenvalues as

\[ J(\beta, \mu; \Delta) = \frac{1}{\beta} \sum_{k} \sum_{n=1}^{L} \log(1 - e^{-\beta(\epsilon_n(k) - \mu)}). \quad (94) \]

Taking the thermodynamic limit, we obtain

\[ \beta j(\beta, \mu; \Delta) = \beta j(\beta, \mu; \Delta) = \lim_{L \to \infty} \frac{1}{L^3} \log(1 - e^{-\beta(\epsilon_{1}(0) - \mu)}) + H(\beta, \mu) \quad (95) \]

with

\[ H(\beta, \mu) \equiv \int \frac{d^3 \rho}{(2\pi)^2} \log(1 - e^{-\beta(-2J \sum_{d=1}^{3} \cos \rho_d - \mu)}). \quad (96) \]

Because \( H(\beta, \mu) \) is independent of \( \Delta \), \( j(\beta, \mu; \Delta) \) depends on \( \Delta \) only through the first term, which represents the contribution of the ground state. We consider the setting where \( \rho \) is controlled through \( \mu \) while \( \beta \) is fixed.

First, we consider the case \( \Delta < 1/4 \). Recalling (70), we neglect the first term of (95) for \( \rho < G(\beta, -6J) \). We therefore obtain

\[ \beta j(\beta, \mu; \Delta < \frac{1}{4}) = H(\beta, \mu). \quad (97) \]

where \( \mu < -6J \). For \( \rho \geq G(\beta, -6J) \), \( \mu \) is given by (74). Substituting (74) into (95), we calculate the first term of (95) as

\[ \lim_{L \to \infty} \frac{1}{L^3} \log(1 - e^{-\beta(\epsilon_{1}(0) - \mu)}) = \lim_{L \to \infty} \frac{1}{L^3} \log(1 - e^{-\frac{\rho}{L^3} \sum_{d=1}^{3} \cos \rho_d - \mu}) \]

\[ = 0. \quad (98) \]

We therefore obtain

\[ \beta j(\beta, \mu; \Delta < \frac{1}{4}) = H(\beta, -6J) \quad (99) \]

in the thermodynamic limit. We thus conclude that the bulk free energy density is independent of \( \Delta \).
Second, we consider the case $\Delta \geq 1/4$. Through a similar calculation, for the case that $\rho$ is controlled with $\beta$ fixed, we obtain

$$\beta_{j}(\beta, \mu; \Delta \geq 1/4) = \begin{cases} H(\beta, \mu) & \text{for } \rho < G(\beta, \mu_{\ast}), \\ H(\beta, \mu_{\ast}) & \text{for } \rho \geq G(\beta, \mu_{\ast}). \end{cases}$$

(100)

In the Bose–Einstein condensate, the free energy density explicitly depends on $\Delta$ because the condensation is localized at the surface layer with the enhanced coupling constant $J(1 + \Delta)$.

5.1 Non-analytic behavior

We study the non-analyticity of the bulk free energy. In this section, we calculate the chemical potential $\mu$ as a function of $(\rho, \beta)$ by solving (67) in $\mu$. In particular, we focus on the non-analytic behavior in $\beta$ near the critical point with $\rho$ fixed.

5.1.1 $\Delta < 1/4$

In the low-temperature region $\beta > \beta_{c}$, we obtained $\mu$ as a function of $(\rho, \beta)$ as shown in (74) and (75). In the high-temperature region $\beta < \beta_{c}$, we expand $G(\beta, \mu)$ in $\mu$ around $\mu = -6J$. We define the new variable $m$ according to

$$4Jm^{2} \equiv \{(−6J) − \mu\}.$$

(101)

We then rewrite $G(\beta, \mu)$ in terms of $m$ as

$$G(\beta, \mu) = \int \frac{d^{3}\rho}{(2\pi)^{2}\pi} \frac{1}{e^{4\beta J(m^{2} + \sum_{d=1}^{3}\sin^{2} x_{d})} - 1}.$$

(102)

When $m$ is small, the dominant contribution to this integral arises from long-wavelength components. We explain this by considering the function

$$\frac{\partial G(\beta, \mu)}{\partial \mu} = \int \frac{d^{3}\rho}{(2\pi)^{2}\pi} \frac{\beta e^{4\beta J(m^{2} + \sum_{d=1}^{3}\sin^{2} x_{d})}}{\{e^{4\beta J(m^{2} + \sum_{d=1}^{3}\sin^{2} x_{d})} - 1\}^{2}}.$$

(103)

We may rewrite this integral using the new variable $\rho = mx$ and focus on the contribution from small $m$. The integral is evaluated as

$$\frac{\partial G(\beta, \mu)}{\partial \mu} \simeq m^{-1} \int d^{3}x \frac{1}{(1 + |x|^{2})^{2}}.$$

(104)

This means that this function diverges as $m \to 0$. Integrating this function in $\mu$, we obtain

$$G(\beta, \mu) \simeq G(\beta, -6J) + A(\beta)((−6J) − \mu)^{1/2},$$

(105)
where $A(\beta)$ is a positive function depending on $\beta$. This expansion is valid when $\mu$ is near $-6J$. Substituting (105) into (67), we obtain

$$\rho \simeq G(\beta, -6J) + A(\beta)((-6J) - \mu)^\frac{1}{2},$$

(106)

which leads to

$$\mu = (-6J) \simeq -\frac{1}{A(\beta)^2} \left( \rho - G(\beta, -6J) \right)^2.$$

(107)

Because $A(\beta)$ and $G(\beta, -6J)$ do not exhibit any singularity, we expand the right-hand side of (107) around $\beta = \beta_c$ as

$$\mu = (-6J) \simeq -C \left( \beta - \beta_c \right)^2,$$

(108)

with

$$C \equiv \left( \frac{1}{A(\beta_c)} \frac{\partial G(\beta, -6J)}{\partial \beta} \bigg|_{\beta = \beta_c} \right)^2,$$

(109)

for $\beta < \beta_c$, where we have used (79).

From (75) and (108), we find that $\mu$ vanishes quadratically as $\beta \to \beta_c - 0$ so that $\mu = \mu(\beta, \rho)$ has a discontinuous second derivative at $\beta_c$. This result is the same as that for $\Delta = 0$. Recalling that the chemical potential $\mu$ is related to the Helmholtz free energy density through

$$\mu = \left( \frac{\partial f}{\partial \rho} \right)_\beta,$$

(110)

we conclude that this Bose–Einstein condensation is the bulk critical phenomenon related to the non-analyticity of the bulk free energy density.

5.1.2 $\Delta \geq \frac{1}{4}$

In the low-temperature region $\beta > \beta_c$, $\mu$ is given by (85). In the high-temperature region $\beta < \beta_c$, we expand $G(\beta, \mu)$ in $\mu$ around $\mu = \mu_*$. Unlike the case $\Delta < 1/4$, the dominant contribution to the integral of $G(\beta, \mu)$ does not arise from the long-wavelength component and the derivative of $G(\beta, \mu)$ in $\mu$ does not diverge at $\mu = \mu_*$. We therefore have the expansion

$$G(\beta, \mu) \simeq G(\beta, \mu_*) + \left. \frac{\partial G(\beta, \mu)}{\partial \mu} \right|_{\mu = \mu_*} (\mu_* - \mu).$$

(111)

Substituting (111) into (67), we derive $\mu - \mu_*$ as

$$\mu - \mu_* \simeq -\frac{1}{\left. \frac{\partial G(\beta, \mu)}{\partial \rho} \right|_{\mu = \mu_*}} \left( \rho - G(\beta, \mu_*) \right).$$

(112)
Using (88), we obtain

\[ \mu - \mu_* \simeq -C'(\beta_c - \beta) \quad (113) \]

with

\[ C' \equiv \frac{\partial G(\beta, \mu_*)}{\partial \mu} \bigg|_{\beta = \beta_c} > 0, \quad (114) \]

where \( \beta < \beta_c \). The result implies that \( \mu \) vanishes linearly as \( \beta \to \beta_c - 0 \) so that \( \mu = \mu(\beta, \rho) \) has a discontinuous first derivative at \( \beta_c \). Because \( f(\beta, \rho) \) has non-analyticity, we conclude that this Bose–Einstein condensation is described as the bulk phase transition. However the singularity type is different from that for \( \Delta < 1/4 \). It is noted that this singularity type is the same as that of the Bose–Einstein condensation in higher dimensions \( d \geq 4 \).

### 5.2 Non-analytic behavior of the specific heat

We study the constant-volume specific heat. The internal energy \( U(\beta, \rho) \) and internal energy density \( u(\beta, \rho) \) are defined by

\[ U(\beta, \rho) \equiv \sum_{n=1}^{\infty} \sum_{\mathbf{k}} \frac{\epsilon_n(\mathbf{k})}{e^{\beta(\epsilon_n(\mathbf{k}) - \mu)} - 1} \bigg|_{\mu = \mu(\beta, \rho)} \quad (115) \]

and

\[ u(\beta, \rho) \equiv \lim_{L \to \infty} \frac{1}{L^3} U(\beta, \rho). \quad (116) \]

The internal energy density is rewritten as

\[ u(\beta, \rho) = \rho \epsilon_1(\mathbf{0}) + I(\beta, \mu(\beta, \rho)), \quad (117) \]

where \( I(\beta, \mu) \) is defined by

\[ I(\beta, \mu) = \int \frac{d^3 \rho}{(2\pi)^3} e^{\beta(-2J \sum_{d=1}^{\beta} \cos \rho_d - \epsilon_1(\mathbf{0}) - 1)} \quad (118) \]

\( I(\beta, \mu) \) is expanded in \( \mu \) around \( \mu = \epsilon_1(\mathbf{0}) \) as

\[ I(\beta, \mu) \simeq I(\beta, \epsilon_1(\mathbf{0})) + \frac{\partial I(\beta, \mu)}{\partial \mu} \bigg|_{\mu = \epsilon_1(\mathbf{0})} (\mu - \epsilon_1(\mathbf{0})) \quad (119) \]

for \( \mu \leq \epsilon_1(\mathbf{0}) \). Substituting (119) into (117), we obtain

\[ u(\beta, \rho) \simeq \begin{cases} 
\epsilon_1(\mathbf{0}) \rho + I(\beta, \epsilon_1(\mathbf{0})) + \frac{\partial I(\beta, \mu)}{\partial \mu} \bigg|_{\mu = \epsilon_1(\mathbf{0})} (\mu(\beta, \rho) - \epsilon_1(\mathbf{0})) & \text{for } \beta < \beta_c, \\
\epsilon_1(\mathbf{0}) \rho + I(\beta, \epsilon_1(\mathbf{0})) & \text{for } \beta \geq \beta_c. \end{cases} \quad (120) \]
Note that (120) holds regardless of $\Delta$. The constant-volume specific heat is given by the derivative of $u(\beta, \rho)$ in the temperature $1/\beta$. Clearly, the non-analyticity of the constant-volume specific heat originates from the term $\mu(\beta, \rho) - \epsilon_1(0)$. As shown in (108) and (113), the behavior of $\mu(\beta, \rho) - \epsilon_1(0)$ changes at $\Delta = 1/4$. Therefore, the behavior of the constant-volume specific heat also changes at $\Delta = 1/4$. When $\Delta \leq 1/4$, as is well known in the case $\Delta = 0$, the constant-volume specific heat exhibits a cusp singularity at $\beta = \beta_c$.

When $\Delta > 1/4$, the constant-volume specific heat has the discontinuous gap at $\beta = \beta_c$. The gap width depends on $\Delta$.

6 Surface free energy per unit area

We define an effective two-dimensional system by taking the partial trace over the degrees of freedom in the bulk. For convenience, we refer to this two-dimensional system as the effective surface system. This section studies the relation between the critical phenomenon in the effective surface system and the Bose–Einstein condensation in the bulk.

In this section, we consider the tight-binding Bose gas model on a cubic lattice

$$A' = \{(i_1, i_2, j) \in \mathbb{Z}^3 \mid 1 \leq i_1 \leq M, 1 \leq i_2 \leq M, 1 \leq j \leq L\}, \quad (121)$$

instead of (1). We explicitly express the $L$ dependence of each physical quantity by writing $L$ as the subscript. For example, the total free energy of the system is written as $J_L(\beta, \mu; \Delta)$.

6.1 Surface free energy per unit area

Let $J^0_L(\beta, \mu)$ denote the total free energy of the system with $\Delta = 0$; i.e.,

$$J^0_L(\beta, \mu) \equiv J_L(\beta, \mu; \Delta = 0). \quad (122)$$

We define $J^1_L(\beta, \mu; \Delta)$ as

$$J^1_L(\beta, \mu; \Delta) \equiv J_L(\beta, \mu; \Delta) - J^0_L(\beta, \mu). \quad (123)$$

We express $J^1_L(\beta, \mu)$ as

$$e^{-\beta J^1_L(\beta, \mu)} = \int_{-\infty}^{\infty} \mathcal{D}[\bar{\psi}_1, \psi_1] e^{-S^s_L[\bar{\psi}_1, \psi_1]}, \quad (124)$$

where

$$S^s_L[\bar{\psi}_1, \psi_1] \equiv \sum_{k,m} \bar{\psi}_{1,k,m} \mathcal{G}_L(k; \omega_m; \mu) \psi_{1,k,m}, \quad (125)$$
with
\[
G_L(k, \omega_m; \mu) \equiv (A_{11}(k) - (\mu + i\omega_m)) - J^2 (B_{L-1}(k) - (\mu + i\omega_m)E_{L-1})^{-1}_{11}.
\]
(126)

See Appendix C.3 for the derivation. \(J^s_L(\beta, \mu)\) corresponds to the free energy of the effective surface system and \(S^s_L[\bar{\psi}_1, \psi_1]\) corresponds to the action associated with the effective surface system. We define \(f^s(\beta, \rho)\) as
\[
f^s(\beta, \rho) = j^s(\beta, \mu(\beta, \rho)),
\]
(127)

where \(j^s(\beta, \mu)\) is given by
\[
j^s(\beta, \mu) \equiv \lim_{M \to \infty} \frac{J^s_L(\beta, \mu)}{M^2}.
\]
(128)

We hereafter refer to \(f^s(\beta, \rho)\) as the surface free energy per unit area. In the remainder of this section, we consider the non-analytic behavior of \(f^s(\beta, \rho)\) near the critical point. Focusing on the setting that \(\beta\) is controlled with \(\rho\) fixed, we study the non-analyticity of \(f^s(\beta, \rho)\) as a function of \(\beta\).

Calculating the integral (124), we obtain
\[
\beta J^s_L(\beta, \mu(\beta, \rho)) = \sum_{m=-\infty}^{\infty} \sum_{k} \log G_L(k, \omega_m; \mu(\beta, \rho))
\]
\[
= \sum_{m(\neq 0)} \sum_{k} \log G_L(k, \omega_m; \mu(\beta, \rho))
\]
\[
+ \sum_{k} \log \left( (1 + 2\Delta)\omega(k) - \mu(\beta, \rho) + \sqrt{(\omega(k) - \mu(\beta, \rho))^2 - (2J)^2} \right),
\]
(129)

where we have used (C.37). We assume that the contribution of the component of \(m \neq 0\) can be neglected as long as we focus on the non-analytic behavior of \(f^s(\beta, \rho)\) near the critical point. We note that the validity of this assumption is confirmed for \(\Delta \geq 1/4\) by straightforwardly computing the sum over Matsubara frequencies. From this assumption, we find that the non-analytic behavior of \(f^s(\beta, \rho)\) originates from the last term of (129). We then define
\[
\beta F^s_{0L}(\beta, \rho) \equiv \sum_{|k| < \Lambda} \log \left( (1 + 2\Delta)\omega(k) - \mu(\beta, \rho) + \sqrt{(\omega(k) - \mu(\beta, \rho))^2 - (2J)^2} \right),
\]
(130)

where we have introduced the cutoff wavenumber \(\Lambda\) because the contribution of the long-wavelength component is dominant in the non-analytic behavior of
Let $A$ be a sufficiently small but finite wave number. We then expand (130) around $k = 0$ as

$$
\beta F_{sL}(\beta, \rho) \simeq \sum_{|k| < A} \log \left( \{-4J(1 + 2\Delta) - \mu(\beta, \rho)\} + J(1 + 2\Delta)k^2 \right.
\left. + \sqrt{(4J + \mu(\beta, \rho))^2 - (2J(4J + \mu(\beta, \rho))k^2)} \right),
$$

(131)

where we have used (15). We define $f_{s0}(\beta, \rho)$ as

$$
f_{s0}(\beta, \rho) \equiv \lim_{L \to \infty} \frac{F_{sL}(\beta, \rho)}{M^2}.
$$

(132)

As long as we focus on the non-analyticity, we have only to study $f_{s0}(\beta, \rho)$ instead of $f_{s}(\beta, \rho)$.

We define the constant-volume specific heat $c_{s}^v$ of the effective surface system as

$$
c_{s}^v = -\frac{T}{k_B} \left( \frac{\partial^2 f_{s}(\beta, \rho)}{\partial T^2} \right)_{\rho}.
$$

(133)

To study the non-analytic behavior of $f^{*}(\beta, \rho)$, we calculate the non-analytic behavior of $c_{s}^v$ in $\beta$ near the critical point with $\rho$ fixed.

6.2 Singularity type for the case $\Delta < \frac{1}{4}$

Near the critical point $\beta = \beta_c, \mu(\beta, \rho)$ is given by (75) and (108). Substituting (75) and (108) into (131), we express $F_{sL}(\beta, \rho)$ as

$$
\beta F_{sL}(\beta, \rho) \simeq \sum_{|k| < A} \log \left( \{2J(1 + 4\Delta) + C(\beta - \beta_c)^2\} + J(1 + 2\Delta)k^2 \right.
\left. + \sqrt{4JC(\beta - \beta_c)^2 + C^2(\beta - \beta_c)^4 - 2J(4J - C(\beta - \beta_c)^2)k^2} \right)
$$

(134)

for $\beta < \beta_c$, and

$$
\beta F_{sL}(\beta, \rho) \simeq \sum_{|k| < A} \log \left( 2J(1 + 4\Delta) + J(1 + 2\Delta)k^2 + \sqrt{4J^2k^2} \right)
$$

(135)

for $\beta \geq \beta_c$. We then note that the argument of the logarithm contains a term proportional to $|k|$ at the limit $|k| \to 0$. Such a term does not exist when $\beta < \beta_c$. The origin of this term is the long-range interaction through the ordered bulk. Such long-range interaction leads to the non-analyticity of $f^{*}(\beta, \rho)$ and introduces a new phase.

We define $u_{s0}(\beta, \rho)$ as

$$
u_{s0}(\beta, \rho) \equiv -\left( \frac{\partial}{\partial \beta} \beta f_{s0}(\beta, \rho) \right)_{\rho}.
$$

(136)
We calculate the leading term in $u^s_0(\beta, \rho)$ as $|\beta - \beta_c| \to 0$. We first consider the case $\beta < \beta_c$. Substituting (134) into (136), we obtain

$$u^s_0(\beta, \rho) = -(\beta - \beta_c) \frac{1}{M^2} \sum_{|k| < \Lambda} \frac{B(\beta - \beta_c, k^2)}{\sqrt{(\beta - \beta_c)^2(4JC + 2JCk^2) + 4J^2k^2}}.$$  

(137)

where

$$B(x, k^2) = \frac{2C \sqrt{x^2(4JC + 2JCk^2) + 4J^2k^2} + 8JC + 4J^2Ck^2}{2J(1 + 4\Delta) + Cx^2 + J(1 + 2\Delta)k^2 + \sqrt{x^2(4JC + 2JCk^2) + 4J^2k^2}}.$$  

(138)

As $x \to 0$ and $k \to 0$, $B(x, k^2)$ converges to a non-zero value $B(0, 0)$. The leading term of the $\beta - \beta_c$-dependence of $u^s_0(\beta, \rho)$ is kept even when replacing $B(\beta - \beta_c, k^2)$ by $B(0, 0)$ in (137). Then, taking the limit $M \to \infty$, we replace the sum in $k$ by the integral as

$$u^s_0(\beta, \rho) \approx -(\beta - \beta_c) \int_{0}^{\Lambda} d^2k \frac{B(0, 0)}{\sqrt{4JC(\beta - \beta_c)^2 + 2JC(\beta - \beta_c)k^2 + 4J^2k^2}}.$$  

(139)

Extracting the $\beta - \beta_c$-dependence from this integral, we obtain

$$u^s_0(\beta, \rho) \sim (\beta - \beta_c)^2.$$  

(140)

We next consider the case $\beta \geq \beta_c$. Substituting (135) into (136), we obtain

$$u^s_0(\beta, \rho) = 0.$$  

(141)

The singular behavior of the constant-volume specific heat originates from the derivative of $u^s_0(\beta, \rho)$ in the temperature $1/\beta$. From (140) and (141), we find that the constant-volume specific heat of the effective surface system has the cusp singularity at $\beta = \beta_c$. The singularity type of this quantity is the same as that of the constant-volume specific heat of the bulk. We thus conclude that the singularity type of $f^s(\beta, \rho)$ is also the same as that of $f(\beta, \rho)$. This result means that the critical phenomena of the effective surface system are induced by the ordered bulk.

6.3 Singularity type for the case $\Delta \geq \frac{1}{4}$

Near the critical point $\beta = \beta_c$, the behavior of $\mu(\beta, \rho)$ is given by (85) and (113). Using these results, we express $F^s_{0L}(\beta, \rho)$ as

$$\beta F^s_{0L}(\beta, \rho) \approx \sum_{k < \Lambda} \log \left(A_1(\beta - \beta_c) + A_2(\beta - \beta_c)k^2\right)$$  

(142)
for $\beta < \beta_c$ and

$$\beta F^*_{0L}(\beta, \rho) \simeq \sum_{k<\Lambda} \log \left( A_2(0) k^2 \right)$$

(143)

for $\beta \geq \beta_c$, with

$$A_1(x) = \frac{16Ax}{\{c - 8\Delta\} - \frac{C'}{J}x - \sqrt{c^2 - 4 - 2cC'x + (\frac{C'}{J})^2x^2}}$$

(144)

$$A_2(x) = J(1 + 2\Delta) + \frac{Jc}{\sqrt{c^2 - 2cC'x + (\frac{C'}{J})^2x^2 - 4}}$$

(145)

$$c \equiv \frac{1 + 16\Delta^2}{4\Delta}.$$  (146)

We immediately confirm $A_1(0) = 0$ and $A_2(0) \neq 0$. Calculating the sum of (143) in the limit $M \to \infty$, we find that $F^*_{0L}$ is $O(M^2 \log M)$. The surface free energy per unit area defined by (128) therefore exhibits logarithmic divergence in the limit $M \to \infty$. It is noted that the $x$-dependence of $A_1(x)$ is

$$A_1(x) \sim x \text{ for } x \to 0.$$  (147)

From (142), (143) and (147), we find that $F^*(\beta, \rho)$ is the same as that of the two-dimensional Gauss model. We therefore obtain the behavior of the constant-volume specific heat as

$$c^v \sim \frac{1}{|\beta_c - \beta|}$$

(148)

for $\beta < \beta_c$. The singularity type of the constant-volume specific heat of the effective surface system is different from that defined from the bulk free energy. This means that the type of non-analyticity of $f^*(\beta, \rho)$ is different from that of $f(\beta, \rho)$. We confirm that the critical phenomena in the effective surface system are induced by connecting the ordered bulk and the surface.

7 Conclusion and discussion

In this paper, we investigated the Bose–Einstein condensation in the tight-binding model with the hopping rate enhanced only on a surface. Regardless of the strength of the enhanced hopping rate $J_s$, this model exhibits Bose–Einstein condensation. However, we found that two different critical behaviors occur depending on the case $J_s < 5/4$ or $J_s \geq 5/4$. We analyzed the critical behaviors as the bulk critical phenomenon and the surface critical phenomenon.

In the case $J_s/J < 5/4$, our model exhibits the same critical behavior as in the unenhanced case $J_s = J$. At the criticality of the bulk, the second derivative of the surface free energy $\partial^2 f^*(\beta, \rho)/\partial \beta^2$ has a cusp singularity, which is
the same as that of the bulk. The origin of the surface critical phenomenon is the long-range interaction through the ordered bulk. Such long-range interaction leads to a coincidence between the singularity type of the bulk free energy and that of the surface free energy.

In the case $J_s/J \geq 5/4$, unique and pathological Bose–Einstein condensation occurs. The singularity type of the bulk free energy is the same as that of the Bose–Einstein condensation with $J_s = J$ in higher dimensions $d \geq 4$. Meanwhile, the singularity type of the surface free energy is the same as that of the two-dimensional Gauss model. In the Bose–Einstein condensate, $O(L^3)$ particles are spatially localized in the surface layer. As a result, the bulk free energy density explicitly depends on $J_s$ defined only at the boundary. Furthermore, the surface free energy per unit area exhibits logarithmic divergence in the thermodynamic limit. The chemical potential $\mu$ also explicitly depends on $J_s$ for the Bose–Einstein condensate. Noting that the chemical potential is associated with the particle number of the total system, we find that the bulk and the surface strongly affect each other through the chemical potential. This effect leads to a change in the bulk and surface critical phenomena.

We note that the two-dimensional localization of $O(L^3)$ particles is possible because our model is a collection of free bosons. If we take a repulsive interaction between the bosons into account, such spatial localization can never occur. The chemical potential no longer depends on the surface parameter. We then conjecture that the singular type of the bulk free energy density is not affected by the surface and is determined by the bulk properties. However, the singular type of the surface free energy remains subtle. In fact, for the XY model and the Heisenberg model, it was reported that a special transition occurs at one point when a surface parameter is controlled at the bulk critical point [25,30]. Additionally, at this special point in the XY model, it is believed that the surface free energy exhibits a singularity type different from that of the bulk free energy [25]. We expect that our model with a repulsive interaction exhibits a similar special transition.

Let us return to the definition of the surface free energy per unit area (127). The physical meaning of $f_s(\beta, \rho)$ remains to be elucidated. If the equivalence of ensembles holds even on the level of the $O(L^{-1})$ correction term of the free energy, $f_s(\beta, \rho)$ corresponds to the $O(L^{-1})$ correction term of the Helmholtz free energy density. Otherwise, it seems that $f_s(\beta, \rho)$ has no physical meaning. In general, the expectation of the local quantity depends on the choice of the ensemble. In the Bose–Einstein condensate, for example, the second cumulant of the particle number occupying the ground state depends on the choice of ensemble, although the fraction of the ground state atoms is independent of the choice of ensemble [31–33]. One should take care that the choice of ensemble may change the singularity type of the free energy.

We finally remark on the possibility of the surface long-range order in the nonequilibrium steady states of systems with conservative dynamics. In particular, it is interesting to consider the case that these systems are subjected to an external forcing parallel to the surface. It is known that the spatial correlations of fluctuations of conserved quantities generally decay via a power
law [34, 35]. We expect that this spatially long-range correlation gives a long-range nature to the interaction between surface degrees of freedom. Such long-range correlation may then induce the surface long-range order.

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Appendix A: energy eigenvalues for the case $\omega(k) \geq 0$

First, we consider the energy eigenvalues for the case $\omega(k) = 0$. Substituting $\omega(k) = 0$ into (30), we obtain

$$f(z; k) = \det \left[ B_L(k) - zE_L \right].$$ (A.1)

This result immediately leads to

$$\epsilon_n(k) = \epsilon_0^n(k).$$ (A.2)

Second, we consider the energy eigenvalues for the case $\omega(k) > 0$. We define $k'$ as

$$\omega(k') = -\omega(k).$$ (A.3)

Noting

$$\det \left[ B_L(k') - zE_L \right] = \prod_{n=1}^{L} \left( -z - \omega(k) - 2J \cos \left( \frac{n\pi}{L + 1} \right) \right)$$

$$= (-1)^L \prod_{n=1}^{L} \left( -z + \omega(k) - 2J \cos \left( \frac{n\pi}{L + 1} \right) \right)$$

$$= (-1)^L \det \left[ B_L(k) - (-z)E_L \right],$$ (A.4)

we obtain

$$f(-z; k') = (-1)^L f(z; k).$$ (A.5)

Therefore we associate $\epsilon_n(k)$ with $\omega(k) < 0$ to $\epsilon_n(k')$ with $\omega(k') = -\omega(k) > 0$ as

$$\epsilon_n(k) = -\epsilon_{L-(n-1)}(k').$$ (A.6)
Appendix B: Solution of (42)

We derive the solution $z$ of (42). In particular, because we have considered only the range $z < \omega(k) - 2J$ to transform the characteristic equation (28) into (42), we focus on the solution $z$ within $z < \omega(k) - 2J$.

We define the function

$$g(x) \equiv \frac{1}{2} \left( x + \Delta \omega(k) \right) \left( \sqrt{x^2 - 4J^2} + x \right) - J^2. \quad (B.7)$$

Using this function $g(x)$, we rewrite (42) as

$$g(-z + \omega(k)) = 0. \quad (B.8)$$

Because $g(x)$ is the monotonically increasing function of $x$ for $x > 2J$, (B.8) has a solution for $z < \omega(k) - 2J$ when

$$g(2J) = J \left( 2J + \Delta \omega(k) \right) - J^2 < 0. \quad (B.9)$$

Simplifying this condition, we obtain

$$\Delta \omega(k) < -J. \quad (B.10)$$

Therefore (42) has the solution for wave numbers satisfying (B.10). Solving (42), we obtain the solution

$$z = \frac{J^2 + \Delta^2 \omega(k)^2}{\Delta \omega(k)} + \omega(k). \quad (B.11)$$

Meanwhile for wave numbers

$$\Delta \omega(k) \geq -J, \quad (B.12)$$

(42) does not have the solution for $z < \omega(k) - 2J$.

Appendix C: Derivation of some formulae by using path integral expression

We use the path integral method to derive some formulae in this paper. We shall summarize details of the calculation.
C.1 Preliminary

Introducing the path integral expression, the partition function of the grand canonical ensemble is written as

$$e^{-\beta J(\beta, \mu)} = \sum_n <n| \sum_k e^{-\beta (\hat{H} - \mu \hat{N})}|n> = \int_{-\infty}^{\infty} \mathcal{D}(\bar{\psi}, \psi) e^{-S[\bar{\psi}, \psi]}$$  \hspace{1cm} (C.13)

with

$$S[\bar{\psi}, \psi] \equiv \sum_m^{\infty} \sum_{j, j'} \sum_k \bar{\psi}_{k, j, m}(A_{jj'}(k) - (\mu + i\omega_m)\delta_{jj'})\psi_{k, j', m},$$ \hspace{1cm} (C.14)

and

$$\int_{-\infty}^{\infty} \mathcal{D}(\bar{\psi}, \psi) \equiv \int_{-\infty}^{\infty} \left( \prod_k L \prod_j \prod_m^{\infty} \frac{d\bar{\psi}_{k, j, m} d\psi_{k, j, m}}{\beta \pi} \right),$$ \hspace{1cm} (C.15)

where $\omega_m$ is the Matsubara frequency in Boson systems

$$\omega_m \equiv \frac{2m\pi}{\beta}. $$ \hspace{1cm} (C.16)

Because the integral in (C.13) is Gaussian, the convergence condition of this integral is that all eigenvalues of the $L \times L$ matrix $A(k) - (\mu + i\omega_m)E_L$ have a positive real part. This condition is the same as (64).

When the condition (64) is satisfied, we can calculate the integral in (C.13) as

$$e^{-\beta J(\beta, \mu)} = \prod_m^{\infty} \prod_k \frac{\beta^{-L}}{\det \left( A(k) - (\mu + i\omega_m)E_L \right)},$$ \hspace{1cm} (C.17)

which leads to

$$\beta J(\beta, \mu) = \sum_m^{\infty} \sum_k \log \left[ \beta^L \det \left( A(k) - (\mu + i\omega_m)E_L \right) \right].$$ \hspace{1cm} (C.18)

Computing the sum over the Matsubara frequencies, we obtain (94).
C.2 Derivation of (61)

To derive (61), we start with the path integral expression of $< \sum_k \hat{a}^{\dagger}_{k,j} \hat{a}_{k,j'} >_{\beta,\mu}$:

$$< \sum_k \hat{a}^{\dagger}_{k,j} \hat{a}_{k,j'} >_{\beta,\mu} = e^{\beta J(\beta,\mu)} \sum_n < \sum_k \hat{a}^{\dagger}_{k,j} \hat{a}_{k,j'} e^{-\beta(\hat{H} - \mu \hat{N})} >$$

$$= e^{\beta J(\beta,\mu)} \frac{1}{\beta} \sum_k \sum_{m,m'} \int_{-\infty}^{\infty} \mathcal{D}(\tilde{\psi}, \psi) \tilde{\psi}_{k,j}^m \psi_{k,j'}^{m'} e^{-S[\tilde{\psi}, \psi]}$$  \hspace{1cm} (C.19)

When the condition (64) is satisfied, we can calculate the integral in (C.19) as

$$\int_{-\infty}^{\infty} \mathcal{D}(\tilde{\psi}, \psi) \tilde{\psi}_{k,j}^m \psi_{k,j'}^{m'} e^{-S[\tilde{\psi}, \psi]} = e^{-\beta J(\beta,\mu)} (A(k) - (\mu + i\omega_m)E_L)^{-1}_{jj'} \delta_{m,m'}$$ \hspace{1cm} (C.20)

Substituting this result into (C.19), we obtain

$$< \sum_k \hat{a}^{\dagger}_{k,j} \hat{a}_{k,j'} >_{\beta,\mu} = \frac{1}{\beta} \sum_k \sum_{m=-\infty}^{\infty} (A(k) - (\mu + i\omega_m)E_L)^{-1}_{jj'} \cdot (C.21)$$

Here, we focus on the component $(j,j') = (1,1)$ and we rewrite the inverse of the matrix $A(k) - (\mu + i\omega_m)E_L$ as

$$\left( A(k) - zE_L \right)^{-1}_{11} = \frac{\text{det} \left( B_{L-1}(k) - zE_{L-1} \right)}{\text{det} \left( A(k) - zE_L \right)}$$

$$= \frac{\text{det} \left( B_{L-1}(k) - zE_{L-1} \right)}{\Pi_{n=1}^{N_L} \left( -z + \epsilon_n(k) \right)}$$ \hspace{1cm} (C.22)

Using (C.22), we can formally compute the sum over the Matsubara frequencies of (C.21) as follows

$$\frac{1}{\beta} \sum_{m=-\infty}^{\infty} \left( A(k) - (\mu + i\omega_m)E_L \right)^{-1}_{11}$$

$$= \frac{1}{2\pi i} \oint_{\gamma} dz \left( A(k) - (\mu + z)E_L \right)^{-1}_{11} \frac{1}{e^{\beta z} - 1}$$

$$= \frac{1}{2\pi i} \oint_{\gamma} dz \frac{\text{det} \left( B_{L-1}(k) - (\mu + z)E_{L-1} \right)}{\Pi_{n=1}^{L} \left( -z - \mu + \epsilon_n(k) \right)} \frac{1}{e^{\beta z} - 1}$$

$$= -\sum_{n=1}^{L} \lim_{z \to -\mu + \epsilon_n(k)} \left\{ \frac{\text{det} \left( B_{L-1}(k) - (\mu + z)E_{L-1} \right)}{\Pi_{n=1}^{L} \left( -z - \mu + \epsilon_n(k) \right)} \frac{1}{e^{\beta z} - 1} \right\}$$

$$= \sum_{n=1}^{L} \frac{f_n(k)}{e^{\beta(z - \mu + \epsilon_n(k))} - 1}.$$ \hspace{1cm} (C.23)
where we choose the integration contour $\gamma$ so as to enclose the poles $\{i\omega_m\}_m$ in the clockwise direction and we introduce $f_n(k)$ as

$$f_n(k) \equiv \lim_{z \to \epsilon_n(k)} \left\{ \frac{\det (B_{L-1}(k) - zE_{L-1})}{\det (A(k) - zE_L)} \right\}. \quad (C.24)$$

Recalling (90), we obtain

$$\langle \sum_{k} \hat{a}^\dagger_{k,1} \hat{a}_{k,1} \rangle = \sum_{k} \sum_{n=1}^L \left| u_{n,k}(k) \right|^2 \frac{1}{\exp(\epsilon_n(k) - \mu) - 1}. \quad (C.25)$$

Therefore, we obtain

$$\left| u_{n,k}(k) \right|^2 = f_n(k). \quad (C.26)$$

C.3 Derivation of the effective surface system

We obtain the effective action associated with the surface system by integrating (C.13) over the degrees of freedom $(\psi_{k,n,m}, \bar{\psi}_{k,n,m})_{k,n \geq 2,m}$ except for the degrees of freedom $(\psi_{k,1,m}, \bar{\psi}_{k,1,m})_{k,m}$.

In order to compute this procedure, we pick up one component $(k, m)$ from $S[\bar{\psi}, \psi]$ and define as

$$S(\bar{\psi}_{k,m}, \psi_{k,m}) \equiv \sum_{j,j'} \bar{\psi}_{k,j,m} \left( A_{jj'}(k) - (\mu + i\omega_m)\delta_{jj'} \right) \psi_{k,j',m}. \quad (C.27)$$

By straightforward calculation, we obtain

$$\int_{-\infty}^{\infty} \left( \prod_{i=2}^{L} \frac{d\bar{\psi}_{k,i,m} d\psi_{k,i,m}}{\beta \pi} \right) e^{-S(\bar{\psi}_{k,m}, \psi_{k,m})}$$

$$= \frac{\beta^{-(L-1)}}{\det (B_{L-1}(k) - (\mu + i\omega_m)E_{L-1})} e^{-S_1(\bar{\psi}_{k,1,m}, \psi_{k,1,m}, k, m)}, \quad (C.28)$$

where

$$S_1(\bar{\psi}_{k,1,m}, \psi_{k,1,m}; k, m) \equiv \bar{\psi}_{k,1,m} \mathcal{G}(k, \omega_m; \mu) \psi_{k,1,m} \quad (C.29)$$

with

$$\mathcal{G}(k, \omega_m; \mu) \equiv A_{11}(k) - (\mu + i\omega_m) - J^2 \left( B_{L-1}(k) - (\mu + i\omega_m)E_{L-1} \right)_{11}^{-1}. \quad (C.30)$$

Using (C.28), we integrate (C.13) over the degrees of freedom $(\bar{\psi}_{k,n,m}, \bar{\psi}_{k,n,m})_{k,n \geq 2,m}$ as

$$e^{-\beta J(\beta, \mu)} = e^{-\beta J_{L-1}(\beta, \mu; \Delta=0)} \int_{-\infty}^{\infty} \mathcal{D}(\bar{\psi}_1, \psi_1) e^{-S_1(\bar{\psi}_1, \psi_1)} \quad (C.31)$$
with

$$S_1[\psi_1, \psi_1] \equiv \sum_{k,m} S_1(\psi_{k,1,m}, \psi_{k,1,m}; k, m), \quad (C.32)$$

$$\int_{-\infty}^{\infty} \mathcal{D}(\psi_1, \psi_1) \equiv \int_{-\infty}^{\infty} \left( \prod_k \prod_m d\psi_{k,1,m} d\psi_{k,1,m} \right), \quad (C.33)$$

and

$$e^{-\beta J_{L-1}(\beta, \mu; \Delta=0)} = \prod_{m=-\infty}^{\infty} \frac{\beta^{-(L-1)}}{\det \left( B_{L-1}(k) - (\mu + i\omega_m) E_{L-1} \right)}. \quad (C.34)$$

where we have used (C.17). Note that $J_{L-1}(\beta, \mu; \Delta=0)$ corresponds to the total free energy of the system consisting of $L-1$ layers with $\Delta = 0$.

As a special case, we focus on $G(k, 0; \mu)$. Recalling that the eigenvalues and eigenvectors of the $L \times L$ matrix $B(k)$ are given by (26) and (27) respectively, we can calculate

$$\left( B_{L-1}(k) - (\mu + i\omega_m) E_{L-1} \right)^{-1}_{11} = \frac{2}{L-2} \sum_{i=1}^{L-1} \frac{\sin^2 \left( \frac{i\pi}{L} \right)}{\omega(k) - (\mu + i\omega_m) - 2J \cos \left( \frac{i\pi}{L} \right)} \approx 2 \int_0^{\pi} d\theta \frac{\sin^2 \theta}{2\pi \omega(k) - (\mu + i\omega_m) - 2J \cos \theta} \quad (C.35)$$

for any $m$, where we have taken the large system size limit for the last equation. For the case $m = 0$, this integral is calculated as

$$\int_0^{\pi} d\theta \frac{\sin^2 \theta}{2\pi \omega(k) - \mu - 2J \cos \theta} = \frac{(\omega(k) - \mu) - \sqrt{(\omega(k) - \mu)^2 - (2J)^2}}{(2J)^2} \quad (C.36)$$

where $\mu < -6J$. Using this result, we obtain

$$\lim_{L \to \infty} G(k, 0; \mu) = \frac{(1 + 2\Delta) \omega(k) - \mu + \sqrt{(\omega(k) - \mu)^2 - (2J)^2}}{2}, \quad (C.37)$$

where $\mu < -6J$. 

Appendix D: Derivation of (67)

We derive (67) from (66) in the thermodynamic limit. Especially we focus on the singularity when $\mu$ approaches the value $\epsilon_1(0)$. In order to see it, we divide the right hand side of (66) into four terms as

$$
\rho = \frac{1}{L^3} e^{\beta(\epsilon_1(0)-\mu)} - 1 + \frac{1}{L^3} \sum_{k \neq 0} \frac{1}{\epsilon(\epsilon_1(k))-\mu} - 1
$$

$$
+ \frac{1}{L^3} \sum_{n=2}^{L} \sum_{k} \frac{1}{\epsilon_n(k)-\mu} - 1 + \frac{1}{L^3} \sum_{n=1}^{L} \sum_{k} \frac{1}{\epsilon_n(k)-\mu} - 1 \quad (D.38)
$$

It should be noted that $\epsilon_1(k)$ in $\Delta > \frac{1}{4}$ finitely deviates from that of $\Delta = 0$ in some $k$ regime.

D.1 Preliminary

As a preliminary, we estimate $\epsilon_1(k') - \epsilon_1(0)$ with $k' = (2\pi/L, 0)$ and $\epsilon_2(0) - \epsilon_1(0)$ in the large system size limit. First we consider the case of $\Delta < 1/4$. Substituting (15) into (50) and using addition formulas, we obtain

$$
\tan(L\theta) = -\frac{\sin \theta}{\cos \theta - 2\Delta \sum_{d=1}^{2} \cos k_d}
$$

$$
\simeq -\frac{\sin \theta}{\cos \theta - (4\Delta - \Delta|k|^2)}, \quad (D.39)
$$

where $k$ is sufficiently small in the second line. To estimate the solutions of

Fig. 3 Schematic graph of $y = \tan(L\theta)$ and $y = -\sin \theta/(\cos \theta - (4\Delta - \Delta|k|^2))$. Intersections of these graphs correspond to solutions of (D.39).
(D.39), we use Figure. 3. In Figure. 3, the points of intersection of two graphs correspond to the solutions of (D.39). Therefore we find

\[ \frac{\pi}{2L} < \theta_1(0) < \frac{\pi}{L}, \]  

(D.40)

and

\[ \frac{3\pi}{2L} < \theta_2(0) < \frac{2\pi}{L}. \]  

(D.41)

Furthermore, because

\[ \frac{-\sin \theta}{\cos \theta - 4\Delta} < \frac{-\sin \theta}{\cos \theta - (4\Delta - \Delta|k'|^2)} \]  

(D.42)

near \( \theta = 0 \), we find

\[ \frac{\pi}{2L} < \theta_1(0) < \theta_1(k') < \frac{\pi}{L}. \]  

(D.43)

From (51), (D.40), (D.41) and (D.43), we obtain

\[ \epsilon_2(0) - \epsilon_1(0) = O\left(\frac{1}{L^2}\right), \]  

(D.44)

and

\[ \epsilon_1(k') - \epsilon_1(0) = O\left(\frac{1}{L^2}\right). \]  

(D.45)

Next, we consider the case of \( \Delta \geq 1/4 \). Because (46) implies

\[ \epsilon_1(k') - \epsilon_1(0) \simeq |k'|^2, \]  

(D.46)

it is reasonable to conjecture

\[ \epsilon_1(k') - \epsilon_1(0) = O\left(\frac{1}{L^2}\right). \]  

(D.47)

From (36) and (47), we obtain

\[ (\omega(0) - 2J) - \epsilon_1(0) < \epsilon_2(0) - \epsilon_1(0), \]  

(D.48)

and from (15) and (46), we obtain

\[ \lim_{L \to \infty} \{ (\omega(0) - 2J) - \epsilon_1(0) \} = J \frac{1 + 16\Delta^2}{4\Delta} - 2J. \]  

(D.49)

From (D.48) and (D.49), we find that the difference between \( \epsilon_1(0) \) and \( \epsilon_2(0) \) is the finite. To summarize these results, the energy gap between the grand state and the first excited state is always \( O(L^{-2}) \) in the large system size limit.
D.2 Third term of (D.38) in the thermodynamic limit

Based on the preliminary results, we consider the third term of (D.38). From (36) and (37), we find that $\epsilon_n(k)$ does not finitely deviate from that for $\Delta = 0$ in any $\Delta$. As the result, the third term of (D.38) is the same as that of $\Delta = 0$ in the thermodynamic limit. We demonstrate this.

Using (36) and (37), we have

$$
\frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1} < \frac{1}{e^{\beta(\epsilon_0(k) - \mu)} - 1} < \frac{1}{e^{\beta(\epsilon_{n-1}(k) - \mu)} - 1}
$$

(D.50)

for $n = 2, 3, \cdots, L$, where $k$ satisfies $\omega(k) < 0$. (D.50) immediately leads to

$$
\frac{1}{L^3} \sum_{n=2}^{L} \sum_{k \langle \omega(k) < 0 \rangle} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1} < \frac{1}{L^3} \sum_{n=2}^{L} \sum_{k \langle \omega(k) < 0 \rangle} \frac{1}{e^{\beta(\epsilon_0(k) - \mu)} - 1}
$$

(D.51)

Using (64) we evaluate the last term in this inequality as

$$
\frac{1}{L^3} \frac{1}{e^{\beta(\epsilon_0(0) - \mu)} - 1} < \frac{1}{L^3} \frac{1}{e^{\beta(\epsilon_0(0) - \epsilon_1(0))} - 1} \sim O\left(\frac{1}{L}\right),
$$

(D.52)

where we have used (D.44) and (D.48). Using (D.51) and (D.52), we confirm

$$
\lim_{L \rightarrow \infty} \frac{1}{L^3} \sum_{n=2}^{L} \sum_{k \langle \omega(k) < 0 \rangle} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1} = \int_{\omega(k) < 0} \frac{d^3 \rho}{(2\pi)^2} \frac{1}{e^{\beta(-2J \sum_{d=1}^{3} \cos \rho_d - \mu)} - 1},
$$

(D.53)

where $\rho = (k_1, k_2, \rho_3)$.

D.3 Fourth term of (D.38) in the thermodynamic limit

Next, we consider the second term of (D.38). Using (36), (37) and (A.6) we have

$$
0 < \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} < \frac{1}{e^{\beta(\epsilon^0_n(k') - \mu)} - 1},
$$

(D.54)

and

$$
\frac{1}{e^{\beta(\epsilon^0_n(k') - \mu)} - 1} < \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} < \frac{1}{e^{\beta(\epsilon^0_n(k') - \mu)} - 1}
$$

(D.55)
for $n = 1, 2, \cdots, L - 1$, where $k'$ satisfies $\omega(k') > 0$. (D.54) and (D.55) lead to

$$
\frac{1}{L^3} \sum_{n=1}^{L-1} \sum_{k' : \omega(k') > 0} \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} < \frac{1}{L^3} \sum_{n=1}^{L} \sum_{k' : \omega(k') > 0} \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} < \frac{1}{L^3} \sum_{n=1}^{L} \sum_{k' : \omega(k') > 0} \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} - 1.
$$

(D.56)

From (A.2) and (D.56) we obtain

$$
\lim_{L \to \infty} \frac{1}{L^3} \sum_{n=1}^{L} \sum_{k' : \omega(k') \geq 0} \frac{1}{e^{\beta(\epsilon_n(k') - \mu)} - 1} = \int_{\omega(k') \geq 0} \frac{d^3 \rho}{(2\pi)^2} \frac{1}{e^{\beta(-2J \sum_{d=1}^{3} \cos \rho_d - \mu)} - 1}. \quad (D.57)
$$

Combining (D.53) and (D.57) we obtain

$$
\lim_{L \to \infty} \left[ \frac{1}{L^3} \sum_{n=1}^{L} \sum_{k : \omega(k) \geq 0} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1} + \frac{1}{L^3} \sum_{n=2}^{L} \sum_{k : \omega(k) < 0} \frac{1}{e^{\beta(\epsilon_n(k) - \mu)} - 1} \right] = \int \frac{d^3 \rho}{(2\pi)^2} \frac{1}{e^{\beta(-2J \sum_{d=1}^{3} \cos \rho_d - \mu)} - 1}. \quad (D.58)
$$

D.4 Second term of (D.38) in the thermodynamic limit

Finally, we consider the second term of (D.38). Using (64), we obtain

$$
\frac{1}{L^3} \sum_{k \neq 0} \frac{1}{e^{\beta(\epsilon_1(k) - \mu)} - 1} < \frac{1}{L^3} \sum_{k \neq 0} \frac{1}{e^{\beta(\epsilon_1(k) - \epsilon_1(0))} - 1} - 1. \quad (D.59)
$$

As $L \to \infty$, the summation in the right hand side of (D.59) can be replaced by the integral

$$
\lim_{L \to \infty} \frac{1}{L^3} \sum_{k \neq 0} \frac{1}{e^{\beta(\epsilon_1(k) - \epsilon_1(0))} - 1} = \lim_{L \to \infty} \frac{1}{L} \int_{\mathbb{R}^3} \frac{d^2 k}{(2\pi)^2} \frac{1}{e^{\beta(\epsilon_1(k) - \epsilon_1(0))} - 1}. \quad (D.60)
$$
where we have used (D.45). We divide this integral by introducing a small finite wavelength $\Lambda$ as

$$
\int \frac{d^2k}{2\pi/L} \frac{1}{e^{\beta(\epsilon_1(k)-\epsilon_1(0))} - 1} = \int_{2\pi/L}^{A} \frac{d^2k}{(2\pi)^2} \frac{1}{e^{\beta(\epsilon_1(k)-\epsilon_1(0))} - 1} + \int_{\Lambda} \frac{d^2k}{(2\pi)^2} \frac{1}{e^{\beta(\epsilon_1(k)-\epsilon_1(0))} - 1}.
$$

(D.61)

The second term converges, while the first term diverges because we estimate

$$
\int_{\Lambda} \frac{d^2k}{(2\pi)^2} \frac{1}{e^{\beta(\epsilon_1(k)-\epsilon_1(0))} - 1} \sim \int_{\Lambda} \frac{d^2k}{(2\pi)^2} \frac{1}{e^{\beta k^2} - 1} \sim O(log L).
$$

(D.62)

Because this divergence is at most $O(log L)$, (D.60) becomes

$$
\lim_{L \to \infty} \frac{1}{L^3} \sum_{k(\neq 0)} \frac{1}{e^{\beta(\epsilon_1(k)-\mu)} - 1} = 0.
$$

(D.63)

As the result, the second term of (D.38) can be neglected. By combining (D.58) and (D.63), we obtain (67).
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