I. INTRODUCTION

Phase separation in one-dimensional (1D) electron systems has attracted attention of condensed matter physicists, since it is observed that the superconducting correlation is enhanced near the phase-separated region. Many electron systems show phase separation, of which the $t$-$J$ model is the simplest. The Hamiltonian of the 1D $t$-$J$ model is written as

$$
\mathcal{H} = -J \sum_{i,\sigma} (c_i^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + J \sum_i (S_i \cdot S_{i+1} - n_i n_{i+1}/4),
$$

(1)
in the subspace without double occupancy. In general, unless some instability occurs, 1D electron systems belong to Tomonaga-Luttinger liquids (TLL), which is characterized by gapless charge and spin excitations and power-law decay of correlation functions. The charge part of the excitation is described by the $c = 1$ conformal field theory (CFT) with $U(1)$ symmetry, while the spin part is described by the $c = 1$ CFT with $SU(2)$ symmetry. The dominant correlations are determined by a single exponent $K_\rho$. In the phase diagram of the 1D $t$-$J$ model obtained by Ogata et al., the charge or the spin density fluctuations are dominant ($K_\rho < 1$) for the small $J/t$ region, while $J/t$ is increased, the superconducting fluctuations become dominant ($K_\rho > 1$). Finally, the compressibility diverges at $J/J_c = 2.5 - 3.5$ ($K_\rho \to \infty$) and the system goes into the phase-separated state for $J > J_c$.

As a typical instability of the $c = 1$ U(1) CFT, Berezinskii-Kosterlitz-Thouless (BKT) transition has been well known. In electron systems, the Mott transition belongs to this type. However, the asymptotic behavior of the $c = 1$ U(1) CFT with $K \to \infty$ has not been fully investigated. In 1D spin systems, this type of instability corresponds to the transition between the massless XY phase and the ferromagnetic phase. In this article, we argue the asymptotic behavior in the vicinity of the instability $K \to \infty$, relating it with the 1D spinless fermion system. Then we apply our speculation to the 1D $t$-$J$ model by analyzing the finite size effect from the result of the exact diagonalization.

Phase separation as an instability of the Tomonaga-Luttinger liquid

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Asymptotic behavior of the Tomonaga-Luttinger liquid in the vicinity of the phase-separated region is investigated in the one-dimensional $t$-$J$ model, to study the universal property of the $c = 1$ conformal field theory with $U(1)$ symmetry near the $K \to \infty$ instability. On the analogy of the spinless fermion, we discuss that the compressibility behaves as $\kappa \propto (J_c - J)^{-1}$, and that the Drude weight is constant and changes to zero discontinuously at the phase boundary. This speculation is confirmed by analyzing the finite size effect from the result of the exact diagonalization.

This paper is organized as follows. In section I, we discuss an instability of the $c = 1$ CFT with $U(1)$ symmetry, and review several physical examples. In section II, we numerically calculate physical quantities in the 1D $t$-$J$ model to examine the argument. Finally, a summary is given in section III.

II. PHASE SEPARATION AND THE $c = 1$ U(1) CFT

The $c = 1$ CFT with $U(1)$ symmetry is described by the Gaussian model

$$
\mathcal{H} = \frac{1}{2\pi} \int dx \left[ v K (\pi \Pi)^2 + \frac{v}{K} \left( \frac{\partial \phi}{\partial x} \right)^2 \right],
$$

(2)

where $\Pi$ is the momentum density conjugate to $\phi$, $[\phi(x), \Pi(x')] = i \delta(x - x')$, $K$ is the Gaussian coupling, and $v$ is the sound velocity. Its dual field $\theta$ is defined as $\partial_x \theta(x) = \pi \Pi(x)$. We make the identification $\phi \equiv \phi + 2\pi/\sqrt{2}, \theta \equiv \theta + 2\pi/\sqrt{2}$, which means the U(1) symmetry for the $\theta$ field. The scaling dimensions for the operators

$$
O_{n,m} = \exp(in\sqrt{2}\phi) \exp(im\sqrt{2}\theta)
$$

(3)

are

$$
x_{n,m} = \frac{1}{2} \left( n^2 K + \frac{m^2}{K} \right).
$$

(4)

Therefore, the scaling dimension $x_{n,m}$ decreases to 0 for $K \to \infty$, which implies phase separation in electron systems, or a ferromagnetic long-range order in spin systems.
For a finite $L$ size system with periodic boundary conditions, the excitation energies are related to the scaling dimension:

$$\Delta E_{n,m}(L) = \frac{2\pi v}{L} x_{n,m},$$

and the correction to the ground state energy is described by the conformal charge $E_0(L) = e_0 L - \frac{\pi v}{6L} c$, where $e_0$ is the bulk energy density.

### A. Spinless fermion systems

As the simplest physical model, we consider the spinless fermion with nearest neighbor interactions ($t$-$V$ model),

$$\mathcal{H} = -t \sum_i (c_i^\dagger c_{i+1}^\dagger c_i + c_{i+1}^\dagger c_i) - V \sum_i n_i n_{i+1}.$$  

For simplicity, we replace the parameters as $\Delta \equiv V/2t$. Then the metallic phase, which is described by the $\mathcal{C} = 1 U(1)$ CFT, becomes unstable and phase separation ($K \to \infty$) occurs for the region of $\Delta \geq 1$ at any fillings.

The quantum numbers in $\mathcal{H}$ correspond as $(n,m) = (\Delta D, \Delta N)$, where $\Delta D$ denotes the number of particles moved from the left Fermi point to the right one, and $\Delta N$ is the change of the total number of particles. The selection rule under periodic boundary conditions is

$$\Delta D = \frac{\Delta N}{2} \quad (\text{mod} 1).$$

Since the maximum values of $\Delta N$ and $\Delta D$ are of the order of the system size, and the excitation energies $\Delta E_{\Delta D,0}$ are limited by the band width ($\propto L$), so that $\sqrt{K}$ is expected to be constant near the critical point ($K \to \infty$).

It is thought that the transition between the metallic state and the phase-separated state is the first order, because the ground state of the phase-separated state (the state where the band is filled up or empty, i.e., $\Delta N = \pm L/2$ at half-filling), and the metallic state ($\Delta N = 0$) is thermodynamically different. Therefore, the excited energy corresponding to the phase-separated state from the metallic ground state should be

$$\Delta E_{0,\pm L/2} = \frac{\pi v}{L} \left( \frac{(L/2)^2}{K} \right) \propto (1 - \Delta)L, \quad \text{which means } v/K \propto 1 - \Delta.$$  

In fact, using the Jordan-Wigner transformation, the Hamiltonian $\mathcal{H}$ at half-filling is mapped onto the $S = 1/2$ $XXZ$ model with the anisotropy $D$. From the Bethe ansatz result, we obtain

$$1/K = \frac{1}{\pi} \arccos \Delta \approx \frac{1}{\pi} \sqrt{2(1-\Delta)},$$

and

$$v = \frac{\pi}{2} \frac{\sin(\arccos \Delta)}{\sqrt{2(1-\Delta)}},$$

Therefore, near $\Delta = 1$, the sound velocity behaves $v \propto 1/K$, as expected. Note that the phase-separated state has the excited energy near $\Delta = 1$

$$\Delta E_{0,\pm L/2} = \frac{L}{4}(1 - \Delta),$$

which is consistent with $\mathcal{H}$. Thus, near $\Delta = 1$, the asymptotic behaviors are $vK \sim \text{Const.}, v/K \propto 1 - \Delta$, as expected.

### B. Electron systems

In the case of 1D electron systems, generally, the charge and the spin degrees of freedoms are separated, and the charge part is described by the $\mathcal{C} = 1 U(1)$ CFT, while the spin part is described by the $\mathcal{S}(2)$ CFT:

$$\Delta E = \frac{2\pi v_c}{L} x_c + \frac{2\pi v_s}{L} x_s.$$  

Here the scaling dimensions are given by

$$x_c = \frac{1}{2} \left[ \frac{(\Delta N_c/2)^2}{K} + K(2\Delta D_c + \Delta D_s)^2 \right],$$

$$x_s = \frac{1}{2} \left( \Delta N_s - \frac{\Delta N_c}{2} \right)^2 + \frac{1}{2} \Delta D_s^2,$$  

where the subscripts $c,s$ denote the charge and the spin degrees of freedoms respectively, and $\Delta N_c$ means the change of the number of the down spins. These quantum numbers are restricted by the selection rule under periodic boundary condition:

$$\Delta D_c = \frac{\Delta N_c + \Delta N_s}{2} \quad (\text{mod} 1),$$

$$\Delta D_s = \frac{\Delta N_s}{2} \quad (\text{mod} 1).$$

Since both the spinless fermion ($S = 1/2$ $XXZ$ spin chain) and the charge part of the electron system, for example the 1D $t$-$J$ model, belong to the same universality class, we expect that the asymptotic behavior in the limit of $K \to \infty$ is the same for both cases. Therefore, the charge velocity and the exponent for the charge part are expected to behave as $v_c K \sim \text{Const.}$, $v_c/K \propto J_c - J$ respectively.

Next, we relate $v_c$ and $K$ to the compressibility and the Drude weight. From the universal relations of TLL, the compressibility is given by
\[
\frac{1}{n^2 \kappa} = \frac{\pi \varphi_c}{2 K_\rho},
\]
so that the compressibility is expected to behave like \( \kappa \propto (J_c - J)^{-1} \). On the other hand, the Drude weight is given by the relation
\[
D = \frac{K_\rho \varphi_c}{\pi},
\]
therefore, it is constant (at least finite) at the phase boundary. In the phase-separated state, the system is separated into an electron rich and a hole rich regions, and the former is regarded as an antiferromagnetic Heisenberg chain with open boundary conditions, so that the dc conductivity in this non-uniform state is expected to be 0. This indicates that the Drude weight changes discontinuously at the phase boundary.

C. Spin systems

For a model of spin systems, we treat the \( XXZ \) spin chain
\[
\mathcal{H} = - \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z). \tag{18}
\]
This model has a massless \( XY \) phase close to the \( \Delta < 1 \), and a ferromagnetic phase for \( \Delta \geq 1 \).

As mentioned in the previous subsection, the Hamiltonian \([18]\) for \( S = 1/2 \) is obtained by the Jordan-Wigner transformation of the \( t-V \) model \([4]\). However, the boundary condition depends on the number of particles in the spinless fermion system: \( S_{L+1}^z = e^{\pm \pi n N} S_1^z \), which changes the selection rule to the bosonic one,
\[
\Delta N = \text{integer}, \quad \Delta D = \text{integer}. \tag{19}
\]
Changing the selection rule, our argument for the spinless fermion also holds in this case. The fact that \( v \propto 1/K \) explains the change of the dispersion curve from the type \( \omega \approx v|q| \) in the \( XY \) region to the \( \omega \propto q^2 \) on the \( SU(2) \) ferromagnet, and that the ground state energy of the ferromagnet does not depend on the system size.

For the general spin \( S \) case, in the \( XY \) phase the fully ferromagnetic states \( (S_1^z = \pm S L) \) have the excited energy
\[
\Delta E_{0,\pm SL} \equiv S^2 L(1 - \Delta)[1 + O(1 - \Delta, 1/L)], \tag{20}
\]
(see Appendix A). Comparing this with the Gaussian model arguments \([3]\), we obtain
\[
\Delta E_{0,\pm m} = \frac{m^2}{L} (1 - \Delta) = \frac{\pi v m^2}{L E K}. \tag{21}
\]
Therefore, assuming \( v \propto 1/K \) near \( \Delta = 1 \), we obtain \( v, 1/K \propto \sqrt{1 - \Delta} \). And the energy gap between the fully ferromagnetic state and the one-spin flip state \( (S_1^z = \pm(SL - 1)) \) is
\[
\Delta E_{0,\pm(j-1)} - \Delta E_{0,\pm j} = \frac{2S L - 1}{L} (1 - \Delta) \approx 2S (1 - \Delta), \tag{22}
\]
which is consistent with the simple spin wave calculation.

For the ferromagnetic region \( (\Delta \geq 1) \), there is a large degeneracy \( O(L) \) in the ground state under the special boundary condition, which reflects the invariance of the Hamiltonian under the quantum group. Physically, this degeneracy is related with the translational invariance of the domain wall.

III. NUMERICAL CALCULATION

To examine the above prediction, we diagonalize the Hamiltonian of the \( t-J \) model \([1]\) using the Lanczos method for 8,12,16,20 sites clusters at quarter filling. In the finite size calculation, the compressibility \( \kappa \) is given by
\[
\kappa = \frac{L}{N^2} \left( \frac{E_0(L; N + 2) + E_0(L; N - 2) - 2E_0(L; N)}{4} \right)^{-1}, \tag{23}
\]
where \( E_0(L; N) \) is the ground state energy of a system with size \( L \) and \( N \) electrons \((n \equiv N/L)\). We choose periodic boundary conditions for \( N = 4m + 2 \) (\( m \): integer) electrons, and antiperiodic boundary conditions for \( N = 4m \) electrons. The reason of this choice is as follows. When the number of electrons are changed by \( 2 \) \((N_c = 2)\) keeping \( S^2 \approx 0 \), the number of up spin changes by \( 1 \) \((\Delta N_u = 1)\). Then, from the selection rule \([15a]\), the possible value of \( \Delta D_c \) shifts by \( 1/2 \). The change of the boundary condition cancels this phase shift, and it makes the ground state always singlet with zero momentum \([13]\).

The Drude weight \([22,23]\) is given with the relation
\[
D = \frac{L}{2} \left. \frac{\partial^2 E_0(\Phi)}{\partial \Phi^2} \right|_{\Phi=0}, \tag{24}
\]
where the flux-dependent ground state energy \( E_0(\Phi) \) is calculated by modifying the hopping part of \([1]\):
\[
- \sum_{j,\sigma} e^{i\Phi/L} c_j^{\dagger} c_{j+1\sigma} + \text{H.c.}. \tag{25}
\]
By fitting the energy difference \( E_0(\Phi) - E_0(0) \) as a function \( A\Phi^2 + B\Phi^4 \), we find that \( A \gg |B| > 0 \). Therefore, the Drude weight \( \Phi^2 \) is well approximated by the linear relation, and we can calculate the Drude weight by the difference of energies (e.g., at \( \Phi = 0 \) and 0.1\( \pi \)). This is a natural consequence in the TLL, because \( \Delta D_c \) is modified as \( \Delta D_c = \Phi/2\pi \) for \( \Phi \neq 0 \), so that \([14a]\) gives only an \( O(\Phi^2) \) dependence if the ground state is singlet. The Drude weight is known exactly at \( J/t = 0 \) as \( D = \sin(\pi n)/\pi \), and at \( J/t = 2 \) from the Bethe ansatz \([24]\).
We have checked the value at these points and confirmed the validity of our calculation.

As we expected, the inverse compressibility \( \kappa^{-1} \) vanishes linearly toward the phase boundary in the TLL region (see FIG.3). The finite size effect is very small, but it has an \( O(L^{-2}) \) size dependence. This correction is explained by the irrelevant fields \( (x = 4) \).

\[
L^{-2} \mathbf{L}^{-2} \mathbf{1}, \quad \{(L^{-2})^2 + (\mathbf{L}^{-2})^2\} \mathbf{1}.
\]  
(26)

Although the compressibility should be non-negative in the thermodynamic limit \( (L \to \infty) \), there exists a region with \( \kappa^{-1} < 0 \). The reason for this phenomenon is considered as follows: we have done the computation under the micro canonical ensemble, while the theory of TLL is constructed in the grand canonical ensemble. The negative inverse compressibility is expected to approach 0 for larger systems (see FIG.3).

FIG.3 shows that the Drude weight decreases to zero as \( J/t \) is increased, but the value remains finite at the phase boundary \( J = J_c \) determined by \( \kappa^{-1} = 0 \). There is also an \( O(L^{-2}) \) size dependence for \( J < J_c \). However, for \( J > J_c \), the slopes of the Drude weight become steeper as the system size increases, and it seems to have a discontinuity in the thermodynamic limit. This is consistent with our discussion that the Drude weight remains finite at the phase-separation boundary.

In order to check the consistency of the relation for the TLL, we compare the charge velocities obtained by the two independent methods (see FIG.3): one is obtained from the low-energy spectrum as

\[
v_c = \frac{E_1(L; N; S = 0) - E_0(L; N)}{2\pi/L},
\]

(27)

where \( E_1(L; N; S = 0) \) is the first singlet excited state for the wave number \( 2\pi/L \), and the other is given by the relation derived from (16) and (17),

\[
v_c = \sqrt{\frac{2D}{\hbar^2 \kappa}}. \quad (28)
\]

We have seen that the Drude weight and the compressibility have the little size dependence for \( J < J_c \). It is natural that the size dependence of the charge velocity obtained by (27) is larger than that of (28), since the former is given by the difference of the energies for discrete wave numbers, but the latter is given by the differentiation of the energy by the continuous quantity \( \Phi \), so that we used finite size data (at \( L = 16 \)) for (28). We find that the charge velocities calculated in the two ways are consistent in the region \( J/t = 2.0-3.0 \), extrapolating (27) as \( v_c(L) = v_c(\infty) + A/L^2 + B/L^4 \).

Finally, to see the degeneracy in the phase-separated region, we do the Legendre transformation \( f = \mu - \mu_n \), where \( \mu \equiv E_0/L \). The chemical potential \( \mu \) is defined by

\[
\mu(L; N) = \frac{E_0(L; N + 2) - E_0(L; N - 2)}{4}, \quad (29)
\]

The \( f \) versus \( J/t \) at quarter-filling is shown in FIG.4. As the system size \( L \) is increased, there appear two regimes with different slopes, and the value \( f \) approaches 0 in the phase-separated region (see also FIG.4). This is the evidence that the transition is the first order. In fact, the phase-separation boundary \( J_c \) can also be defined at the point of \( f = 0 \) which is equivalent to the Maxwell construction. In finite systems, the Maxwell construction tends to estimate the phase boundary at smaller \( J \) than the one determined by \( \kappa^{-1} = 0 \).

FIG.4 shows that \( f \) is almost constant against the change of the electron density in the phase-separated region. This result suggests that the phase-separated state approximately has degeneracy \( O(L) \), which corresponds to the large degeneracy \( O(L) \) in the ferromagnetic region \( (\Delta \geq 1) \) of the spin \( S \) XXZ model.

IV. SUMMARY AND DISCUSSIONS

In this paper, we have studied the instability of the \( c = 1 \) CFT for the U(1) symmetry case. For the spinless fermion (or the \( S = 1/2 \) XXZ spin chain), considering that the excitation energies are limited by the band-width, we showed that the sound velocity is inverse to the Gaussian coupling \( v \propto 1/kL \). In addition, since the transition from the metallic (XY) phase to the phase-separated (ferromagnetic) state is the first order, the spin wave velocity and the Gaussian coupling behave as \( vK \sim \text{Const.}, v/kL \to 1 - \Delta \).

About the 1D \( t-J \) model, since the low-energy behavior of the charge part is described by the \( c = 1 \) U(1) CFT, and the critical exponent \( K_\rho \) diverges near the phase separation, we expected that the compressibility is proportional to \( (J_c - J)^{-1} \), and the Drude weight is constant. The obtained numerical results supports this expectation.

These asymptotic behaviors of the TLL have been observed in many cases; the linear behavior of the inverse compressibility was also observed by Troyer et al. in the 1D extended \( t-J \) model with the (next-)nearest-neighbor repulsion. The discontinuity of the Drude weight (kinetic energy) was found by Sandvik and Sudbø in the case of the 1D two band Hubbard model, with increasing the nearest-neighbor repulsion. Our argument gives a unified interpretation of these behaviors. In particular, the latter phase-separated state is complicated, and similar to the one which was found by Sano and Ono. Although these phase separations are different from the 1D \( t-J \) model, the universality class is expected to be the same, so that our argument can be applied to these cases, and the discontinuity of the Drude weight and other asymptotic behavior can be explained in the same way.

Historically, the similar asymptotic behavior in \( K \to \infty \) was discussed by the g-ology. However, in the exactly solvable electron systems such as the simple Hubbard model or the supersymmetric \( t-J \) model \( (J/t = 2) \), there
is no phase separation, therefore such a possibility has not been considered seriously.

Although our speculation is successful in explanation of the behavior of the TLL with \( K \to \infty \), the higher corrections to \( vK, v/K \) near the critical point are quite ambiguous. There are complicated effects come from the surface energy. It will be useful to investigate this behavior by analyzing the \( t-V \) model where the exact solution is available.

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APPENDIX A

Here we show that the relation (8) applies not only to the integrable case \( S = 1/2 \) but also to the non-integrable case, \( S \) arbitrary.

Close to \( \Delta = 1 \), we can estimate the ground state energy by the perturbation. We treat the SU(2) ferromagnetic term

\[ \mathcal{H}_0 = -\sum_j S_j \cdot S_{j+1}, \]

as a free part, and the anisotropic part

\[ \mathcal{H}_1 = -\sum_i S_{i}^{z} S_{i+1}^{z}, \]

as a perturbation.

The energy of the fully ferromagnetic state \( S_F^z = \pm SL \) is exactly

\[ E_{\text{ferro}} = -\Delta S^2 L. \]

For \( \Delta < 1 \), the ground state has the quantum number \( S_F^z = 0, q = 0 \). At \( \Delta = 1 \), the ground state wave function in the \( S_F^z = 0, q = 0 \) space is derived from the fully ferromagnetic state

\[ |\phi\rangle = (S_F^z)^{SL}|S_F^z = SL\rangle, \]

where \( S_F^\pm = \sum_j S_j^\pm \). The zero-th order energy is given by

\[ \mathcal{H}_0|\phi\rangle = -S^2 L|\phi\rangle. \]

To calculate the first order perturbation, we have to evaluate \( \langle\phi|S_j^z S_{j+1}^z|\phi\rangle \). Since \( |\phi\rangle \) is invariant under the permutation of the lattice sites \( \{ j \} \), we obtain

\[ \langle\phi|S_j^z S_{j+1}^z|\phi\rangle = \text{Const.} \quad \text{for any } i \neq j, \]

therefore,

\[ \langle\phi|\left( \sum_i S_i^z \right)^2|\phi\rangle = 0 \]

\[ = \sum_{i \neq j} \langle\phi|S_i^z S_j^z|\phi\rangle + \sum_i \langle\phi|(S_i^z)^2|\phi\rangle \]

\[ = L(L-1)\langle\phi|S_j^z S_{j+1}^z|\phi\rangle + L\langle\phi|(S_i^z)^2|\phi\rangle. \]

Considering \( \langle\phi|(S_i^z)^2|\phi\rangle/\langle\phi|\phi\rangle \propto S^2 \), we obtain

\[ \langle\phi|S_j^z S_{j+1}^z|\phi\rangle/\langle\phi|\phi\rangle \propto -S^2/L. \]

Then, the first order perturbation is

\[ E_1 = \langle\phi|\mathcal{H}_1|\phi\rangle/\langle\phi|\phi\rangle \]

\[ = -\Delta \sum_j \langle\phi|S_j^z S_{j+1}^z|\phi\rangle/\langle\phi|\phi\rangle \]

\[ \propto -\Delta S^2. \]

Therefore, the energy gap between the singlet ground state and the fully ferromagnetic state is

\[ \Delta E_{0,\pm SL} = S^2(L(1-\Delta)] + O(1-\Delta, 1/L)]. \]
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FIG. 1. Compressibility $\kappa$ as a function of $J/t$ for different system sizes at $n = 1/2$. The size dependence at $J/t = 2.5$ is shown in the inset.

FIG. 2. Size dependence of the inverse compressibility in the phase-separated regime at $n = 1/2$, $J/t =$ 4.

FIG. 3. Drude weight $D$ as a function of $J/t$ for different system sizes at $n = 1/2$. The arrow indicates the critical point determined by $\kappa^{-1} = 0$. The size dependence at $J/t = 2.5$ is shown in the inset.
FIG. 4. Charge velocity $v_c$ derived by (27) for different system sizes, the extrapolated one (lines), and the one derived from (28) by 16 site data ($\times$), as a function of $J/t$ at $n = 1/2$.

FIG. 5. Legendre transformed ground state energy density $f \equiv e - \mu n$ as a function of $J/t$ for different system sizes at $n = 1/2$. The point $f = 0$ corresponds to the phase-separation boundary determined by the Maxwell construction.

FIG. 6. Size dependence of the $f \equiv e - \mu n$ in the phase-separated regime at $n = 1/2$, $J/t = 4$.

FIG. 7. Legendre transformed ground state energy density $f \equiv e - \mu n$ as a function of the electron density $n$ in $L = 16$ system for various values of $J/t$. 