Bosonization study of quantum phase transitions in the one-dimensional asymmetric Hubbard model

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The quantum phase transitions in the one-dimensional asymmetric Hubbard model are investigated with the bosonization approach. The conditions for the phase transition from density wave to phase separation, the correlation functions, and their exponents are obtained analytically. Our results show that the difference between the hopping integrals for up- and down-spin electrons is crucial for the occurrence of the phase separation. When the difference is large enough, the phase separation will appear even if the on-site interaction is small.

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I. INTRODUCTION

The Hubbard model[1] (HM) is one of the simplest nontrivial models of interacting spin-1/2 electrons on a lattice. Its Hamiltonian reads

$$H_{\mathrm{HM}} = -t\sum_{j=1}^{L}\sum_{\delta=\pm 1} c_{j,\sigma}^{\dagger}c_{j+\delta,\sigma} + U\sum_{j} n_{j\uparrow}n_{j\downarrow}, \tag{1}$$

where $c_{j,\sigma}^{\dagger}$ and $c_{j,\sigma}, \sigma=\uparrow,\downarrow$ are creation and annihilation operators for electrons with spin σ at site j, respectively, $n_{\sigma}=c_{\sigma}^{\dagger}c_{\sigma}$, t is the hopping integral, and U denotes the strength of on-site interaction. In one dimension (1D), the HM can be solved exactly by the Bethe-ansatz method.[2,3] The wave function and the energy of $N=N_{\uparrow}+N_{\downarrow}$ electrons on a chain with L sites can be written in terms of N pseudomomentum variables and $N_{\downarrow}$ spin rapidities. Although the energy spectra have been known for many years, the calculation of the correlation functions proved to be a delicate problem.[4–7] The numerical evaluations of the correlation functions[5] and the analytic results[6] indicated clearly that the 1D HM is a Tomonaga-Luttinger liquid (TLL).[8,9] Assuming that the 1D HM is TLL, it then becomes possible to calculate the correlation functions from the knowledge of the energy spectra.[10] Using this procedure, Schulz[11] studied the correlation-function exponents for different U and band fillings n. It is also shown[12] that the large-scale behavior of the spin and charge degrees of freedom can be described by two decoupled boson field theories with dynamics governed by the TLL Hamiltonian in the small and large U regimes.

Another nontrivial model is the Falicov-Kimball model[13] (FKM) which consists of localized ions and itinerant spinless fermions. The Hamiltonian of the FKM reads

$$H_{\mathrm{FKM}} = -t\sum_{j=1}^{L}\sum_{\delta=\pm 1} c_{j}^{\dagger}c_{j+\delta} + U\sum_{j} n_{j}w_{j}, \tag{2}$$

where $c_{j}^{\dagger}$ are creation operators for spinless fermions, and the configuration $\{w_j\}$ denote spatial distribution of ions. Clearly, the FKM can be viewed as a modification of the HM in the sense that the one kind of fermions, such as down-spin fermions, has infinite mass, and hence does not move. Nevertheless, the physics of the FKM is completely different. In the neutral case where each particle concentration equals 1/2, it was[14] proved that the system always orders in an alternating "chessboard" phase below a finite transition temperature in all dimensions greater than 1. This ordered phase can be interpreted from the transition from a high-temperature homogeneous (liquid and/or gas) phase to a low-temperature-ordered (solid) phase. Freericks *et al.*[15] showed that the model (on a hypercubic lattice) also displayed incommensurate order, segregation, or phase separation (PS). The 1D case of the FKM has also been extensively studied. Though there is no finite-temperature phase transition, the system can have phase transition in the ground state. The numerical solutions[16] produced a conjecture for the case $n_e+n_i<1$, with $n_e=N_e/L$ and $n_i=N_i/L$ and the screened Coulomb interaction U is large enough; the system will segregate into an empty lattice (with no ions and all the electrons) and into a full lattice (with all the ions and no electrons). This conjecture was later proven to be true by Lemberger.[17] For any dimensional FKM, Freericks *et al.*[18] gave a theorem that the strong correlation can lead to PS.

The relation between the HM and the FKM is straightforward. In order to have a unified framework, the asymmetric Hubbard model (AHM) has been introduced naturally.[19–22] Its Hamiltonian reads

$$H_{\mathrm{AHM}} = -\sum_{j=1}^{L}\sum_{\delta=\pm 1}\sum_{\sigma} t_{\sigma}c_{j,\sigma}^{\dagger}c_{j+\delta,\sigma} + U\sum_{j=1}^{L} n_{j,\uparrow}n_{j,\downarrow}, \tag{3}$$

where t_{σ} is σ-dependent hopping integral. Clearly, if $t_{\uparrow}=t_{\downarrow}$, the AHM becomes the HM, and if $t_{\downarrow}=0$, it becomes the FKM. The Hamiltonian [Eq. (3)] has $\mathrm{U}(1)\otimes\mathrm{U}(1)$ symmetry for general t_{σ}, and the electron numbers $N_{\downarrow}$ and $N_{\uparrow}$ are conserved. In the condensed matter physics, the AHM is believed to describe many physical phenomena, such as superconductor, valence fluctuating, and heavy fermions.[23,24] In the recent development of the optical lattice, it has been pointed out that the AHM can be used to describe a mixture of two species of fermionic atoms in optical lattices.[25,26]

According to the fact that the ground states of the Hamiltonian [Eq. (3)] in its two limiting cases: the HM ($t_{\uparrow}=t_{\downarrow}$) and the FKM ($t_{\downarrow}=0$) belong to two different universality classes, a quantum phase transition was suggested to happen in the

phase diagram defined in the $U-t_{\downarrow}$ plane.[20,22,25] Nevertheless, the quantitative phase diagram for the case away from half filling had never been obtained until a recent work by Gu *et al.*[26] In their work, the quantum entanglement[27] between a local part and the rest of the system and the structure factor of charge-density wave (CDW) for down-spin electrons are used to identify the transition point. Here, we are going to study the ground-state phase diagram of the AHM away from the half filling with the strategy of bosonization method.[28] Different from the numerical approach[26] which captures the physics from the finite-size analysis for small systems, our work aims to give definite analytical results from the point of view of field theory. This paper is organized as follows. In Sec. II, we derive the bosonized form of the 1D AHM and clarify the role of some terms in the Hamiltonian. In Sec. III, we first diagonalize the effective Hamiltonian in which some irrelevant terms are ignored, then obtain the instability conditions for the PS and compare them with the numerical results of a finite sample. We also obtain the analytical expressions for the correlation functions of charge-density-wave, spin-density-wave (SDW), singlet-superconductivity (SS), triplet-superconductivity (TS) fluctuations, as well as the corresponding exponents. Finally, a brief summary is given in Sec. IV.

II. THE BOSONIZED FORM OF ONE-DIMENSIONAL ASYMMETRIC HUBBARD MODEL

The convenient way to analyze the 1D AHM is to bosonize the Fermi operators and convert them to a quantum theory of two Bose fields.[28,29] In the framework of the standard bosonization method, the AHM is expressed in terms of canonical Bose fields and their dual counterparts as

$$\begin{aligned} H_B = & \frac{v_c}{2}\int dx\left[\frac{1}{K_c}(\partial_x\phi_c)^2 + K_c\pi_c^2\right] \\ & + \frac{v_s}{2}\int dx\left[\frac{1}{K_s}(\partial_x\phi_s)^2 + K_s\pi_s^2\right] \\ & + \delta v\int dx[\pi_c\pi_s + \partial_x\phi_c\partial_x\phi_s] \\ & + \frac{U}{2\pi^2 a}\int dx\cos(\sqrt{8\pi}\phi_s) \\ & + \frac{U}{2\pi^2 a}\int dx\cos[\sqrt{8\pi}\phi_c + 2(k_{F\uparrow}+k_{F\downarrow})x], \end{aligned} \tag{4}$$

with

$$v_c = a\sqrt{t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a)\left[t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a) + \frac{U}{2\pi}\right]}, \tag{5}$$

$$\frac{1}{K_c} = \sqrt{1 + \frac{U}{2\pi[t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a)]}}, \tag{6}$$

$$v_s = a\sqrt{t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a)\left[t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a) - \frac{U}{2\pi}\right]}, \tag{7}$$

$$\frac{1}{K_s} = \sqrt{1 - \frac{U}{2\pi[t_\uparrow\sin(k_{F\uparrow}a) + t_\downarrow\sin(k_{F\downarrow}a)]}}, \tag{8}$$

$$\delta v = a[t_\uparrow\sin(k_{F\uparrow}a) - t_\downarrow\sin(k_{F\downarrow}a)]. \tag{9}$$

Here, the Bose fields ϕ_c and ϕ_s present the charge and spin degrees of freedom, respectively. $k_{F\uparrow}$ and $k_{F\downarrow}$ are the Fermi momentum for up- and down-spin electrons, $k_{F\uparrow}=\pi n_\uparrow/a$ and $k_{F\downarrow}=\pi n_\downarrow/a$, with $n_\uparrow=N_\uparrow/L$ and $n_\downarrow=N_\downarrow/L$ the filling densities for up- and down-spin electrons, respectively, and a is a lattice constant. $v_{c,s}$ are the propagation velocities of the charge and spin collective modes of the decoupled model ($\delta v=0$), and $K_{c,s}$ are the stiffness constants.

Clearly, at unpolarized case where $N_\uparrow=N_\downarrow$, this model is the standard HM with both Bose fields decoupling. If the model is at the half filling, $k_{F\uparrow}+k_{F\downarrow}=\pi/a$, the oscillating factor disappears, the Umklapp term (the last term in H_B) is important, and the HM is in the SDW phase with $U>0$ or in the CDW phase with $U<0$. As the model shifts away from the half-filling band, the Umklapp term has an oscillating factor, which makes the Umklapp term ignorable by appropriate choice of the filling factor. Here, we discuss the quantum phase transition in the case of away from the half filling which means that the Umklapp interaction can be ignored.

The last term in H_B is the spin backscattering term. In general, $t_\uparrow, t_\downarrow > 0$. Then, if $U<0$ and $K_s<1$, the model has attractive on-site interaction and possesses a spin gap at any filling. The term $\cos(\sqrt{8\pi}\phi_s)$ is relevant. Nevertheless, in the parameter region of $U>0$, $K_s>1$, so the term of $\cos(\sqrt{8\pi}\phi_s)$ is irrelevant whenever the system is at unpolarized case with

$N_\uparrow = N_\downarrow$. In the one-loop approximation, we can cancel it directly and get

$$H_{B\,\mathrm{eff}} = \frac{v_c}{2}\int dx\left[\frac{1}{K_c}(\partial_x\phi_c)^2 + K_c\pi_c^2\right] + \frac{v_s}{2}\int dx\left[\frac{1}{K_s}(\partial_x\phi_s)^2 + K_s\pi_s^2\right] + \delta v\int dx[\pi_c\pi_s + \partial_x\phi_c\partial_x\phi_s]. \tag{10}$$

Therefore, the difference between hopping integral and the filling densities of up- and down-spin electrons in the system appears as an effect that breaks the spin-charge separation which reveals the presence of the third term in the last equation.

III. RESULTS AND DISCUSSIONS

The Hamiltonian [Eq. (10)] can be diagonalized in terms of two new phase fields which contains a mixture of spin and charge degrees of freedom. The propagation velocities of these collective modes are

$$v_\pm^2 = \frac{v_c^2 + v_s^2}{2} + \delta v^2 \pm \sqrt{\left(\frac{v_c^2 - v_s^2}{2}\right)^2 + \delta v^2\left[v_c^2 + v_s^2 + v_c v_s\left(K_c K_s + \frac{1}{K_c K_s}\right)\right]}. \tag{11}$$

As $\delta v \to 0$, $v_+ \to \max(v_c, v_s)$ and $v_- \to \min(v_c, v_s)$. As δv increases, v_- decreases until it vanishes at the points

$$\delta v_1^2 = v_c v_s \frac{1}{K_c K_s}, \tag{12}$$

$$\delta v_2^2 = v_c v_s K_c K_s. \tag{13}$$

At these points, the freezing of the lower bosonic mode is accompanied by a divergence in the charge and spin response functions. The static charge compressibility κ diverges at $\delta v = \delta v_1$ or $\delta v = \delta v_2$. It behaves as

$$\kappa = \kappa_0\left[1 - \frac{\delta v}{\delta v_{1(2)}}\right]^{-1}, \quad \kappa_0 = \frac{2K_c}{\pi v_c}. \tag{14}$$

Beyond these points, the susceptibilities become negative. This behavior of the static response functions together with the vanishing of the collective mode velocity indicates that the system becomes unstable[30] and undergoes a first-order phase transition.[31] This instability is known as phase separation and has been shown to occur in the extended HM (Refs. 32 and 33) and in the $t-J$ model.[34,35]

In our case, we obtain

$$\delta v_1 = \sqrt{v_c v_s K_c K_s} = a t_\uparrow \sin(k_{F\uparrow} a) + t_\downarrow \sin(k_{F\downarrow} a), \tag{15}$$

$$\delta v_2 = \sqrt{\frac{v_c v_s}{K_c K_s}} = a t_\uparrow \sin(k_{F\uparrow} a) + t_\downarrow \sin(k_{F\downarrow} a)\sqrt{1 - \left\{\frac{U}{2\pi[t_\uparrow \sin(k_{F\uparrow} a) + t_\downarrow \sin(k_{F\downarrow} a)]}\right\}^2}. \tag{16}$$

It is obvious that $\delta v_1 \geqslant \delta v_2$, so the system is in PS phase state as

$$\delta v \geqslant \delta v_2, \tag{17}$$

i.e.,

$$\frac{t_\uparrow \sin(k_{F\uparrow} a) - t_\downarrow \sin(k_{F\downarrow} a)}{2} \geqslant \frac{t_\uparrow \sin(k_{F\uparrow} a) + t_\downarrow \sin(k_{F\downarrow} a)}{2}\sqrt{1 - \left\{\frac{U}{2\pi[t_\uparrow \sin(k_{F\uparrow} a) + t_\downarrow \sin(k_{F\downarrow} a)]}\right\}^2}. \tag{18}$$

Then, we obtain the condition of PS,

$$[t_\downarrow \sin(k_{F\downarrow}a)][t_\uparrow \sin(k_{F\uparrow}a)] \leqslant \left(\frac{U}{4\pi}\right)^2. \tag{19}$$

Let us now focus our attention on the correlation functions. Our interest in this work is to observe the algebraic decay of the instantaneous correlation functions at zero temperature and to study how the exponents get modified from the standard HM. The operators for CDW, SDW, SS, and TS fluctuations in their bosonized form are[10]

$$O^+_{\mathrm{CDW}}(x) = \Psi^+_{1\uparrow}\Psi_{2\uparrow} = \frac{1}{2\pi\epsilon}\exp[\sqrt{2\pi}i(\phi_\rho + \phi_\sigma) + 2ik_F x],$$

$$O^+_{\mathrm{SDW}}(x) = \Psi^+_{1\uparrow}\Psi_{2\downarrow} = \frac{1}{2\pi\epsilon}\exp\left\{\sqrt{2\pi}i\left[\phi_\rho(x) - \int_{-\infty}^{x} dy\Pi_\sigma(y)\right] - 2ik_F x\right\},$$

$$O^+_{\mathrm{SS}}(x) = \Psi^+_{1\uparrow}\Psi^+_{2\downarrow} = \frac{1}{2\pi\epsilon}\exp\left\{\sqrt{2\pi}i\left[-\int_{-\infty}^{x} dy\Pi_\rho(y) + \phi_\sigma(x)\right]\right\},$$

$$O^+_{\mathrm{TS}}(x) = \Psi^+_{1\uparrow}\Psi^+_{2\uparrow} = \frac{1}{2\pi\epsilon}\exp\left\{\sqrt{2\pi}i\left\{-\int_{-\infty}^{x} dy\Pi_\rho(y) - \int_{-\infty}^{x} dy\Pi_\sigma(y)\right]\right\}, \tag{20}$$

which represent fluctuations of CDW, SDW, SS, and TS phases, respectively. The correlation functions are defined as

$$R_i(x) = \langle : O_i(x)O_i^+(0) : \rangle. \tag{21}$$

After some calculation, we find that the correlation functions behave as

$$R_i(x) \sim |x|^{-2+\alpha_i}. \tag{22}$$

The exponents α_i's determine the divergence of the corresponding phase. The expressions obtained for the α_i are

$$\alpha_{\mathrm{CDW}} = 2 - K_c\nu^c - K_s\nu^s, \tag{23}$$

$$\alpha_{\mathrm{SDW}} = 2(1 + |\gamma|^s) - K_c\nu^c - \mu^s/K_s, \tag{24}$$

$$\alpha_{\mathrm{SS}} = 2(1 + |\gamma|^c) - \mu^c/K_c - K_s\nu^s, \tag{25}$$

$$\alpha_{\mathrm{TS}} = 2 - \mu^c/K_c - \mu^s/K_s. \tag{26}$$

with

$$\mu_c = \frac{v_c}{v_+ + v_-}\left[1 + \frac{v_s^2}{v_+v_-}\left(1 - \frac{\delta v^2}{\delta v_2^2}\right)\right], \tag{27}$$

$$\mu_s = \frac{v_s}{v_+ + v_-}\left[1 + \frac{v_c^2}{v_+v_-}\left(1 - \frac{\delta v^2}{\delta v_1^2}\right)\right], \tag{28}$$

$$\nu_c = \frac{v_c}{v_+ + v_-}\left[1 + \frac{v_s^2}{v_+v_-}\left(1 - \frac{\delta v^2}{\delta v_1^2}\right)\right], \tag{29}$$

$$\nu_s = \frac{v_s}{v_+ + v_-}\left[1 + - \frac{v_c^2}{v_+v_-}\left(1 - \frac{\delta v^2}{\delta v_2^2}\right)\right], \tag{30}$$

$$\gamma_c = \frac{\delta v}{v_+ + v_-}\left(1 + \frac{\delta v_2^2 - \delta v^2}{v_+v_-}\right), \tag{31}$$

$$\gamma_s = \frac{\delta v}{v_+ + v_-}\left(1 + \frac{\delta v_1^2 - \delta v^2}{v_+v_-}\right). \tag{32}$$

The ground state is controlled and named by the most divergent correlation function, i.e., with the largest α_i.

To have a deep understanding of the PS, it is very useful to study the structure factor of the CDW. Since the dominating configuration of electrons with spin down is quite different in two phases, we introduce the following structure of down-spin electrons;

$$S_{\mathrm{CDW}}(q) = \frac{1}{L}\sum_{jl} e^{iq(j-l)}(\langle n_{j,\downarrow}n_{l,\downarrow}\rangle - \langle n_\downarrow\rangle^2), \tag{33}$$

where $q=2n\pi/L$, $n=0,1,\ldots,L$. From the point of view of the bosonization approach, the density-density correlation in Eq. (33) can be evaluated from Eq. (20). We show the structure fact as a function of $t=t_\downarrow/t_\uparrow$ at a given $U/t_\uparrow=0.5$ for two different modes $q=2\pi/L$ and $q=2N_\downarrow\pi/L$ in Fig. 1. From the

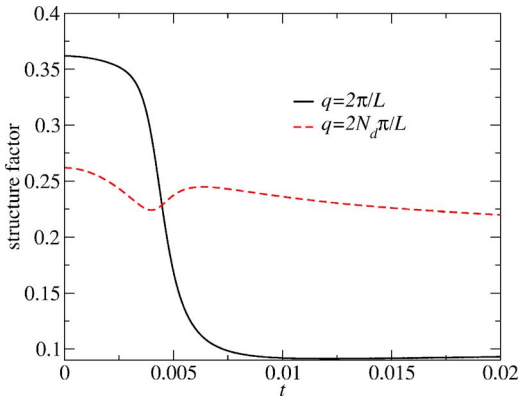

FIG. 1. (Color online) The structure factor of the CDW for two different modes $q=2\pi/L$ and $q=2N_\downarrow\pi/L$ at given $U/t_\uparrow=0.5$. Here $L=10, N_\uparrow=N_\downarrow=2, t=t_\downarrow/t_\uparrow$, and N_d denotes $N_\downarrow$.

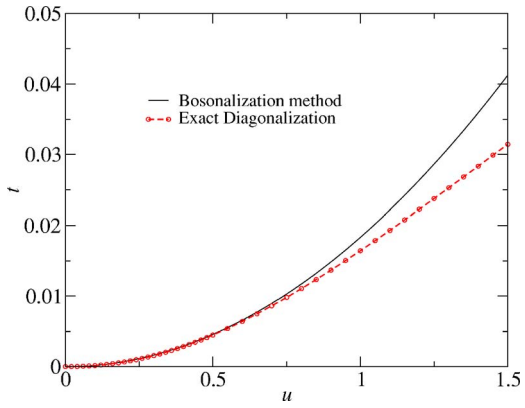

FIG. 2. (Color online) The boundary line between the density wave and phase separation predicted by the bosonization method (solid line) and exact diagonalization (dotted line for $N=10$, $N_\uparrow=N_\downarrow=2$) at a given concentration $n=2/5$. Here, $t=t_\downarrow/t_\uparrow$ and $u=U/t_\uparrow$.

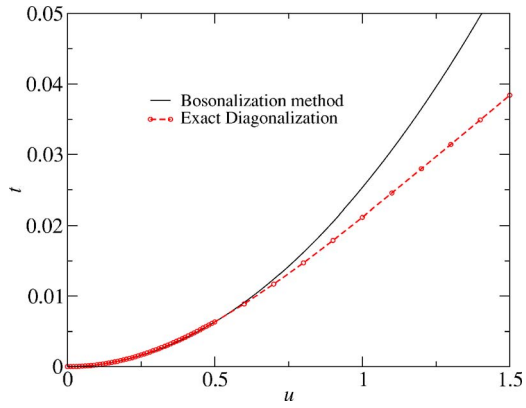

FIG. 3. (Color online) The boundary line between the density wave and phase separation predicted by the bosonization method (solid line) and exact diagonalization (dotted line, $N=12$, $N_\uparrow=N_\downarrow=2$) at a given concentration $n=1/3$. Here, $t=t_\downarrow/t_\uparrow$ and $u=U/t_\uparrow$.

figure, we find that in the small t limit, $S(2\pi/L)$ dominates (this fact manifest the phase separation), while in a relatively larger t region, $S(2N_\downarrow\pi/L)$ dominates [this suggests the density-wave (DW) state]. Thus, we can use the intersection point of the structure factors of two different modes to determine the transition point. In Figs. 2 and 3, we show the phase diagram for different concentrations $n=2/5$ and $1/3$ in the small U region. The results are very impressive. In both figures, we can see that if $U<0.5$, the numerical results from the exact diagonalization method agree with Eq. (19) excellently. That is, the phase boundary in the small U regime is proportional to U^2. However, when U becomes large, say, $U>1$, the bosonization results deviate from the numerical results apparently. We interpret it as due to the fact that the bosonization method becomes invalid in the large U region. On the other hand, the excellent agreement between the results obtained from two approaches suggests that finite-size correction to the numerical data for a finite sample in the small U region is very small.

Therefore, the bosonization results are wonderful in the small U region and low concentration conditions. Since the 1D AHM is equivalent to the FKM if $t_\downarrow=0$ (or $t_\uparrow=0$), this has proven that there exists PS phase at infinite-U limit when the system shifts away from half filling. From Eq. (19), we find that the PS phase always appears in the 1D FKM whenever the onsite interaction is small or large as the system shifts away from half filling. On the other hand, the numerical studies[26] suggest that there might exist a critical U if the density of electrons is close to half filling. This inconsistency may due to the effect of Umklapp process around half filling.

IV. SUMMARY

In summary, we have studied the quantum phase transitions in the 1D AHM with the bosonization approach. In the framework of standard bosonization method, we first obtained an effective Hamiltonian of 1D AHM. Then, we diagonalized the Hamiltonian and obtained the propagation velocities of the collective modes for both spin and charge degrees of freedom. Based on the instability condition, we got the final conditions of the phase transition from DW to PS. We also obtained the analytical expressions for the correlation functions of CDW, SDW, SS, and TS fluctuations, as well as the corresponding exponents.

Our results show that the difference between the hopping integrals for up- and down-spin electrons is crucial for the occurrence of the PS. When the difference is large enough, the phase separation will appear even if the on-site interaction is small. In the small-U and low concentration regions, the phase boundary which scales like $t_\downarrow \propto U^2$ agrees with the numerical results excellently.

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