Mechanism of CDW-SDW Transition in One Dimension

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The phase transition between charge- and spin-density-wave (CDW, SDW) phases is studied in the one-dimensional extended Hubbard model (EHM) has curious properties. The Hamiltonian of this model is given by

\[ H = -t \sum_{i} (c_{i\uparrow} c_{i+1\uparrow} + H.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + V \sum_{i} n_{i\uparrow} n_{i+1\uparrow}. \]  

From the strong coupling theory, it has been shown that the first-order transition takes place near \( U = 2V \). On the other hand, the weak coupling theory predicts that the transition is the second order on the same line. This means that there exist a crossover between these two transitions while, in more than two dimension, the third phase exists between the CDW and the SDW states. Our results are also consistent with those of the strong-coupling perturbative expansion and of the direct evaluation of order parameters.

It has been pointed out that the phase transition of 1D electron systems can be described as Tomonaga-Luttinger (TL) liquids. In the TL liquid (bosonization) theory, the continuous fermion fields are defined by \( c_{i\sigma} \rightarrow \psi_{L\sigma}(x) + \psi_{R\sigma}(x) \) with

\[ \psi_{r\sigma}(x) = \frac{1}{\sqrt{2\pi\alpha}} e^{i \frac{r}{\alpha} \frac{\pi}{2}} \left[ \nu_{r\sigma} x \right] + \frac{\nu_{r\sigma}}{\sqrt{2\pi\alpha}} \left[ \nu_{r\sigma} x \right] \]  

where \( r = R, L \) and \( \sigma = \uparrow, \downarrow \) refer to +, − in that order. \( k_F \) is the Fermi wave number. The field \( \phi_{\sigma} \) and dual field \( \theta_{\sigma} \) of the charge \( (\nu = \rho) \) and spin \( (\nu = \sigma) \) degrees of freedoms satisfy the relation \( \left[ \phi_{\rho}(x), \theta_{\sigma}(x') \right] = -i \pi \delta_{\rho\sigma} \operatorname{sign}(x - x')/2 \). Then the effective Hamiltonian for the system with length \( L \) is given by the sine-Gordon model:

\[ H = \sum_{\nu=\rho,\sigma} \frac{v_{\nu}}{2\pi} \int_{0}^{L} dx \left[ K_{\nu}(\partial_x \theta_{\nu})^2 + K^{-1}_{\nu}(\partial_x \phi_{\nu})^2 \right] + \frac{2g_{3\nu}}{(2\pi\alpha)^2} \int_{0}^{L} dx \cos[\sqrt{8} \phi_{\nu}] + \frac{2g_{1\nu}}{(2\pi\alpha)^2} \int_{0}^{L} dx \cos[\sqrt{8} \theta_{\nu}], \]  

where \( v_{\nu} \) and \( K_{\nu} \) denote the sound velocity and the Gaussian coupling, respectively, for each sector. The nonlinear terms in eq. (3) are originated from the Umklapp (charge) and the backward (spin) scattering effects which can cause the charge- and the spin-gap instabilities. If these non-linear terms are irrelevant, the excitation spectra and their wave numbers in this system are given by the relation

\[ \Delta E = \frac{2\pi v_{\nu}}{L} x_{\nu} + \frac{2\pi v_{\sigma}}{L} x_{\sigma}, \]  

\[ k = \frac{2\pi}{L} (s_{\rho} + s_{\sigma}) + 2m_{\nu} k_F, \]  

where \( x_{\nu} = (n_{\nu}^2/K_{\nu} + m_{\nu}^2 K_{\nu})/2 \) are the scaling dimensions and \( s_{\nu} = n_{\nu} m_{\nu} \) are the conformal spins. The integers \( n_{\nu} \) and \( m_{\nu} \) are quantum numbers for the particle numbers and the current excitations, respectively. The
scaling dimensions are related to the critical exponents for the correlation functions as

$$\langle O(r)O(r') \rangle \sim |r-r'|^{-2(x_{\mu}+x_{\nu})}. \quad (6)$$

Therefore, there is one to one correspondence between the excitation spectra and the operators.

In our analysis we turn our attention on excitation spectra which correspond to the following operators:

$$O_{\nu,1} \equiv \sqrt{2} \cos(\sqrt{2}\phi_{\nu}), \quad (7a)$$
$$O_{\nu,2} \equiv \sqrt{2} \sin(\sqrt{2}\phi_{\nu}), \quad (7b)$$
$$O_{\nu,3} \equiv \exp(\pm i\sqrt{2}\theta_{\nu}). \quad (7c)$$

For the spin sector ($\nu = \sigma$) which have an SU(2) symmetry, the operators (7a) and (7b) form singlet and triplet states, respectively. In this case, the level crossing of these spectra ($x_{\nu,1} = x_{\nu,2}$) gives the spin-gap phase boundary [3,4]. On the other hand, the charge sector ($\nu = \rho$) is U(1) symmetric. Then the operators of eqs. (7) correspond to “Néel,” “dimer,” and “doublet” states in that order, borrowing the terminology of anisotropic spin chains. In this case the level-crossing of “Néel” and “dimer” excitations ($x_{\rho,1} = x_{\rho,2}$) gives the Gaussian transition [13,17], which means a second order transition between two massive states with different fixed points ($g_{\lambda} \rightarrow \pm \infty$). Note that these excitation spectra can be extracted when we choose anti-periodic boundary conditions (BC = -1, see Tab. 1), reflecting the selection rule of the quantum numbers [14]. In the weak-coupling limit, the Gaussian and the spin-gap transition take place simultaneously, because $g_{\lambda} = g_{\lambda} = U = 2V$. However, there is no guarantee for the synchronization except for this limit.

In addition to the above effective Hamiltonian [3], there exists the following Umklapp operator transferring finite spin [14,18,19]:

$$\mathcal{H}' = \frac{2g_{\|}}{(2\pi)^2} \int_0^L dx \cos(\sqrt{2}\rho_{\rho}) \cos(\sqrt{2}\rho_{\sigma}). \quad (8)$$

In the weak coupling limit, the coupling constant is assigned as $g_{\|} = -2V$, so that it remains finite on the $U = 2V$ line. Therefore, we should consider the possibility that the charge and the spin degrees of freedom is not separated, and a direct transition between the CDW and the SDW phases takes place. To examine this possibility, we also observe the level-crossing of excitation spectra of the CDW and the SDW operators which consist of both charge and spin components (see Tab. I). These excitation spectra can be obtained in periodic boundary conditions (BC = 1) with the wave number $2k_F = \pi$.

The excitation spectra correspond to the above operators can be identified according to their discrete symmetries. The wave functions for the excited states can change their signs under particle-hole ($C$: $c_{is} \leftrightarrow (-1)^i c_{is}$), space-inversion ($P$: $R \leftrightarrow L$), and spin-reversal ($T$: $\uparrow \leftrightarrow \downarrow$) transformations. It follows from eq. (3), that the phase fields $\phi_{\nu}$ change by these transformations as follows:

$$C,P : \phi_{\sigma} \rightarrow -\phi_{\sigma}, \quad \phi_{\rho} \rightarrow \pi/\sqrt{2} - \phi_{\rho} \quad (9a)$$
$$T : \phi_{\sigma} \rightarrow -\phi_{\sigma}. \quad (9b)$$

Here, $CP = 1$ is always satisfied, so that independent discrete symmetries are $P$ and $T$. The boson representation of the operators and their symmetries are summarized in Tab. I [19]. In the present numerical calculation based on the Lanczos algorism, the identification is done by projecting the initial vector as

$$|\Psi_{\text{init}}\rangle = \frac{1}{2}(1 \pm P)(1 \pm T)|i\rangle, \quad (10)$$

where the signs in front of the operators correspond to their eigen values, and $|i\rangle$ is some configuration which satisfies $P,T|i\rangle \neq \pm |i\rangle$. Furthermore, $|i\rangle$ is classified by the wave numbers $k = 0, \pi$.

The critical lines obtained by the above explained way with the exact diagonalization of the $L = 8,10,12,14$ systems are shown in Fig. 1. For the Gaussian transition line, the finite-size effect is small for all region (see Fig. 2(a)). On the other hand, for the spin-gap transition line, the finite-size effect is small in the weak-coupling regime (see Fig. 2(b)), but large in the intermediate- and the strong-coupling regime. The CDW-SDW transition line lies between the above two lines [20]. Its finite-size effect is large for all region.

In order to check the consistency of our argument, we confirm the relations between the scaling dimensions for each instability. The relation on the Gaussian critical line [13] and that near the spin-gap transition [13,14] are given by

$$\frac{x_{\rho,1} + x_{\rho,2} x_{\rho,3}}{2} = \frac{1}{4}, \quad (11)$$
$$\frac{x_{\nu,1} + 3x_{\nu,2} x_{\nu,3}}{4} = \frac{1}{2}. \quad (12)$$

The numerical results are shown in Figs. 1 and 2. The Gaussian and the spin-gap transition lines satisfy the consistency of our theoretical scheme from the weak- to the intermediate coupling region.

Moreover, in order to back up the present result from the strong coupling theory, we compare above result to the critical line obtained by the strong coupling expansions. In this limit, the phase boundary between the CDW and the SDW states can be determined by equating energies of these states. This calculation has already been done by Hirsch [2] and van Dongen [3] up to second and forth order, respectively, using the Bethe-ansatz results. Among the three transition lines we assumed, van Dongen’s result shows good agreement with the Gaussian transition in the charge part up to $U/t \sim 6$. We should
also note that our Gaussian critical point agrees with the Cannon et al.’s result obtained by the direct evaluation of the CDW order parameter: \( V_c/t = 1.65^{+0.10}_{-0.05} \) for \( U/t = 3 \) \( V_c/t = 2.92 \pm 0.04 \) for \( U/t = 5.5 \) (see Fig. 2 and 3a).

From the above evidence, we conclude that the actual transition near \( U = 2V \) line is not direct transition between the CDW and the SDW states, but independent Gaussian and spin-gap transitions at least from the weak to the intermediate-coupling region. In the strong coupling regime, these two boundaries approach and coincide at the finite strength of the coupling. Unfortunately, in the present analysis, we cannot determine this point, but it is considered to be identical to the crossover point between the second and the first order transitions. In this way, our analysis suggests that the crossover along the \( U = 2V \) line is closely related to the validity of the charge-spin separation.

Our result also means that there is a finite region with charge- and spin-gapped state which has different symmetries from the CDW state. This third phase is considered as a bond-order-wave (BOW) state with LRO which is characterized by the following operator:

\[
O_{\text{BOW}} = \left(-\frac{1}{2}\right) \sum_s \left[c_{s+1}^\dagger c_{s}^\dagger c_s c_{s+1} + c_s^\dagger c_{s+1}^\dagger c_{s+1} c_s\right].
\]

Therefore the direct evaluation of this order parameter may possible. The existence of the BOW state can be more clarified by extending the EHM. According to the bosonization analysis of the EHM with correlated-hopping interactions \[22\], a finite BOW region remains even in the weak coupling limit \((g_{1\perp} < g_{3\perp})\). On the other hand, if the Gaussian and the spin-gap transitions take place in the opposite order \((g_{1\perp} > g_{3\perp})\), there appears a bond-spin-density-wave (BSDW) phase which has massive charge sector and massless spin sector.

Finally, we refer to other examples of the crossover similar to that in the EHM. This type of phenomenon has also been observed in the transition between the singlet and the Haldane phases in the \( S = 1/2 \) frustrated spin-ladder model \[22\]. Our result would also shed light on such a transition.

In summary, we have studied the CDW-SDW transition in the EHM along the \( U = 2V \) line, and shown that there exist the Gaussian and the spin-gap transitions in the charge and the spin degrees of freedom, respectively, and there is the BOW state between them. The crossover from the second to the first order transition is suggested to be related with the validity of the charge-spin separation.

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FIG. 1. Possible three transitions (Gaussian, spin-gap, and CDW-SDW transitions) along $U = 2V$ line of the EHM calculated in $L = 8, 10, 12, 14$ systems. The result of the strong coupling expansion agrees with the Gaussian transition. This means that the actual transitions are the Gaussian and the spin-gap transitions, and a BOW state exists between them.

FIG. 2. Size dependence of the critical points for the (a) Gaussian transition at $U/t = 3$, and the (b) spin-gap transition at $U/t = 2$. The former agrees with the Cannon et al.’s result that $V_c/t = 1.69_{-0.05}^{+0.16}$.

FIG. 3. Product of the scaling dimensions on the Gaussian critical line (eq.(11)). The TL liquid theory predicts the value takes $1/4$.

FIG. 4. Averaged scaling dimension of the spin sector near the spin-gap critical point at $U/t = 2$ (eq.(12)). The TL liquid theory predicts the value takes $1/2$. 
| operators                  | C | P | T | k | BC |
|---------------------------|---|---|---|---|----|
| G.S.                      | 1 | 1 | 1 | 0 | ±1 |
| marginal                  | $-\frac{4}{3}\partial \phi_{\nu} \partial \phi_{\nu}$ | 1 | 1 | 1 | 0 | ±1 |
| BOW                       | $\sin \sqrt{2} \phi_{\rho} \cos \sqrt{2} \phi_{\sigma}$ | 1 | 1 | 1 | $2k_{F}$ | ±1 |
| SDW$_{zz}$                | $\sin \sqrt{2} \phi_{\rho} \sin \sqrt{2} \phi_{\sigma}$ | -1 | -1 | -1 | $2k_{F}$ | ±1 |
| SDW$_{xx}$                | $\sin \sqrt{2} \phi_{\rho} \exp \pm i \sqrt{2} \theta_{\sigma}$ | * | 1 | * | $2k_{F}$ | ±1 |
| CDW                       | $\cos \sqrt{2} \phi_{\rho} \cos \sqrt{2} \phi_{\sigma}$ | -1 | -1 | 1 | $2k_{F}$ | ±1 |
| BSDW$_{zz}$               | $\cos \sqrt{2} \phi_{\rho} \sin \sqrt{2} \phi_{\sigma}$ | 1 | 1 | -1 | $2k_{F}$ | ±1 |
| BSDW$_{xx}$               | $\cos \sqrt{2} \phi_{\rho} \exp \pm i \sqrt{2} \theta_{\sigma}$ | * | -1 | * | $2k_{F}$ | ±1 |
| SS                        | $\exp \pm i \sqrt{2} \theta_{\rho} \cos \sqrt{2} \phi_{\sigma}$ | * | 1 | 1 | 0 | ±1 |
| TS$_{0}$                  | $\exp \pm i \sqrt{2} \theta_{\rho} \sin \sqrt{2} \phi_{\sigma}$ | * | -1 | -1 | 0 | ±1 |
| TS$_{1}$                  | $\exp \pm i \sqrt{2} \theta_{\rho} \exp \pm i \sqrt{2} \theta_{\sigma}$ | * | 1 | * | 0 | ±1 |
| 4k$_{F}$-CDW              | $\cos 2 \sqrt{2} \phi_{\rho}$ | * | -1 | * | $4k_{F}$ | ±1 |

TABLE I. Discrete symmetries of wave functions which correspond to several excitation spectra (C: charge conjugation, P: space inversion, T: spin reversal, and k: wave number). The upper (lower) sign of boundary conditions (BC) denotes $N/2 =$odd (even) cases. The upper 12 states are “physical” states which appear in the same boundary conditions as the ground state. The lower 6 states are the “artificial” ones which are extracted by twisting the boundary conditions respect to the ground state.
\[
\frac{(V-U/2)}{t} / \frac{U}{(U+4t)}
\]

Gaussian

CDW-SDW

spin-gap

\[ L = 8 \]

\[ L = 10 \]

\[ L = 12 \]

\[ L = 14 \]