Phase Diagram of the $t-U-V_1-V_2$ Model at Quarter Filling

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We examine the ground-state properties of the one-dimensional Hubbard model at quarter filling with Coulomb interactions between nearest-neighbors $V_1$ and next-nearest neighbors $V_2$. Using the density-matrix renormalization group and exact diagonalization methods, we obtain for $U = 10t$ three different phases in the $V_1-V_2$ plane: 2$k_F$- and 4$k_F$-charge-density-wave (CDW) and a broad metallic phase in-between. Assuming that the metal is a Tomonaga-Luttinger liquid (TLL), we calculate the TLL parameter $K_\rho$. It is largest when $V_1$ and $V_2$ are frustrated, and $K_\rho = 0.25$ at the boundaries between the metallic phase and each of the two CDW phases.

PACS numbers: 71.10.Fd 71.30.+h 71.10.Hf

The low-energy physics of one-dimensional correlated electron system can be described by the Tomonaga-Luttinger liquid theory. In general, the Green function and various correlation functions show a power-law behavior as a function of momentum $k$ and frequency $\omega$. The decay of the correlation functions is determined by the so-called TLL parameter $K_\rho$ which depends on the strength of the interactions. Numerous experiments as well as theoretical studies have been performed on a variety of systems in order to determine $K_\rho$ for one-dimensional metallic systems.

Most features of a recent angle-resolved photoemission spectroscopy (ARPES) experiment for the quasi one-dimensional organic conductor TTF-TCNQ can be explained by the photoemission spectral function of the one-dimensional Hubbard model with only on-site interactions. However, the Hubbard model yields $K_\rho \geq 0.5$, in contrast to $K_\rho \approx 0.18$ as deduced from angle-integrated data for the density of states which suggest a power-law behavior of the density of states near the Fermi level, $\rho(\omega) \propto \omega^\alpha$, where $\alpha = (K_\rho + K_\rho^{-1} - 2)/4$ with $\alpha \approx 1$. Another example of a small $K_\rho$ is the quasi one-dimensional organic conductor (TMTSF)$_2$X, where X=PF$_6$, ASF$_6$, or ClO$_4$. In this system, the parameter $K_\rho$ was estimated to be $K_\rho \approx 0.23$ from the power-law dependence dominating in the higher-energy part of the optical conductivity, $\sigma(\omega) \sim \omega^a K_\rho^{-5}$, where $a$ is the order of the commensurability ($a = 1$ for half filling; $a = 2$ for quarter filling). This value is consistent with ARPES measurements. TLL behavior was also suggested for the strongly anisotropic transition-metal oxide PrBa$_2$Cu$_4$O$_8$; the parameter was estimated to be $K_\rho \approx 0.24$ from both the optical conductivity and the ARPES study of Zn-doped PrBa$_2$Cu$_4$O$_8$.

Common features of all the materials mentioned above are that the filling of the conduction band is near one quarter, $n \approx 1/4$. Consequently, they are close to a charge-density-wave (CDW) instability. In addition, the parameter $K_\rho$ is rather small, which is incompatible with the result from a simple one-dimensional Hubbard model and shows that the long-range Coulomb interactions between carriers is relevant. Therefore, we examine the one-dimensional Hubbard model with interactions to nearest and next-nearest neighbors,

$$\hat{H} = -t \sum_{i,\sigma} (\hat{c}^\dagger_{i,\sigma} \hat{c}^\uparrow_{i+1,\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

$$+ V_1 \sum_{i,\sigma,\sigma'} (\hat{n}_{i,\sigma} - \frac{1}{2}) (\hat{n}_{i+1,\sigma'} - \frac{1}{2})$$

$$+ V_2 \sum_{i,\sigma,\sigma'} (\hat{n}_{i,\sigma} - \frac{1}{2}) (\hat{n}_{i+2,\sigma'} - \frac{1}{2}) , \quad (1)$$

where $\hat{c}^\dagger_{i,\sigma}$ ($\hat{c}_{i,\sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma (=\uparrow,\downarrow)$ at site $i$ and $\hat{n}_{i,\sigma} = \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma}$ is the number operator. $t$ is the hopping integral between neighboring sites, $U$ is the strength of the Hubbard interaction, and the charge frustrating interactions $V_1$ and $V_2$ determine the nearest-neighbor and next-nearest-neighbor Coulomb repulsion. We restrict ourselves to the case of quarter filling ($n = 1/2$), and strong coupling, $U = 10t$.

![FIG. 1: Phase diagram of the one-dimensional $t-U-V_1-V_2$ model for $U = 10t$ at quarter filling. The curves show the contours of constant TLL parameter $K_\rho$. Bold lines represent the boundary of the metal-insulator (CDW) transition and the dotted line corresponds to $V_2/t = V_1/(2t)$.](image-url)
So far several theoretical studies have been made on this and similar models. In the ground state there exist two CDW phases with wavenumbers $q = 2k_F$ and $4k_F$. Between the two CDW phases there appears a wide region of a vanishing charge gap which results from the geometrical frustration of the long-range Coulomb interactions. If we assumed the inter-site Coulomb repulsions to be inversely proportional to the inter-site distance, we would find $V_1 = 2V_2$, so that neither of the two CDW instabilities dominates in the atomic limit, $t = 0$. Hence, one can easily imagine that the phase diagram contains a metallic region as soon as a finite $t$ is introduced. However, little is known about the physical properties of this metallic state. It is the purpose of this paper to obtain an accurate ground-state phase diagram of the $t$-$U$-$V_1$-$V_2$ model, including the TLL parameter $K$, whereby we make the natural assumption that the metallic phase is a Tomonaga-Luttinger liquid. Our phase diagram is shown in Fig. 1.

We apply the density-matrix renormalization group (DMRG) method for the calculation of the ground-state energy. We study chains with up to 256 sites with open boundary conditions and keep up to $m = 2000$ density-matrix eigenstates so that the maximum truncation error is about $10^{-5}$. We use periodic boundary conditions for the calculation of charge excitations with the Lanczos exact diagonalization technique.

In order to determine the metallic region in the phase diagram, we calculate the two-particle charge gap,

$$\Delta_c^{(2)}(L) = E_0(N_{\uparrow} + 1, N_{\downarrow} + 1, L) + E_0(N_{\uparrow} - 1, N_{\downarrow} - 1, L) - 2E_0(N_{\uparrow}, N_{\downarrow}, L),$$

where $E_0(N_{\uparrow}, N_{\downarrow}, L)$ denotes the ground-state energy of a chain of length $L$ with $N_{\uparrow}$ spin-up electrons and $N_{\downarrow}$ spin-down electrons. When pairing is absent, in the thermodynamic limit the two-particle charge gap becomes twice the single-particle charge gap, $\lim_{L \to \infty} \Delta_c^{(2)}(L) = 2\lim_{L \to \infty} \Delta_c(L)$. We find that $\Delta_c^{(2)}(L)$ decreases monotonically with increasing $L$, so that we can extrapolate it to the thermodynamic limit systematically by performing a polynomial fitting in $1/L$. Note that we need relatively large system sizes to obtain an accurate phase boundary. The extrapolated results $\Delta_c^{(2)}(t)$ at $U/t = 10$ and $V_1/t = 4$ are shown in Fig. 2.

It is evident that $\Delta_c^{(2)}(t)$ is finite for both small $V_2/t \leq 0.66$ and large $V_2/t \geq 3.43$, i.e., the system is insulating, and $\Delta_c^{(2)}(t)$ vanishes in a wide range of $V_2/t$, i.e., $0.66 \leq V_2/t \leq 3.43$, within the accuracy of the extrapolation (error smaller than $10^{-4}$). We find similar situations for other values of $V_1/t$ as well, which demonstrates that a stable metallic phase indeed exists between two insulating phases as shown in Fig. 1. This result is consistent with other studies.

In the Tomonaga-Luttinger phase, the dominant correlations are determined by a single parameter $K$, which is given by

$$K = (\pi/2)n^2\kappa v_c,$$

where $\kappa$ and $v_c$ are the compressibility and the charge velocity, respectively. To estimate $K$ numerically, we calculate the compressibility $\kappa$ from the charge gap,

$$\Delta_c^{(2)}(L) = 4/(n^2L\kappa(L)),$$

and the velocity of the charge excitations $v_c$ from

$$E_{1\rho}(N_{\uparrow}, N_{\downarrow}, L) - E_0(N_{\uparrow}, N_{\downarrow}, L) = 2\pi v_c(L)/L,$$

where $E_{1\rho}(N_{\uparrow}, N_{\downarrow}, L)$ is the lowest excitation energy with momentum $k = 2\pi/L$ and total spin $S = 0$ for finite system size $L$. As shown in Fig. 3 both of the quantities are monotonous functions of $1/L$ for all parameter sets and can be fitted to a polynomial function

$$f(L) = a_1L^{-1} + a_2L^{-2} + \cdots.$$

Therefore, we obtain

$$\kappa = \lim_{L \to \infty} \kappa(L) = 16/a_1^{(\kappa)} ,$$

$$v_c = \lim_{L \to \infty} v_c(L) = a_1^{(v_c)}/2\pi ,$$

FIG. 2: Charge gap $\Delta_c^{(2)}/(2t)$ (squares) and TLL parameter $K$ (circles) in the one-dimensional $t$-$U$-$V_1$-$V_2$ model at quarter filling for $U/t = 10$ and $V_1/t = 4$. Lines are guides to the eye.

FIG. 3: Scaling of the ground-state energy differences from Eq. 1 and the excitation energy from Eq. 5 as a function of $1/L$ at $U/t = 10$, $V_1/t = 1$ and $V_2/t = 1$. The lines indicate the polynomial fits by Eq. 6 to the data.
so that the TLL parameter can be estimated as

\[ K_\rho = \frac{a_1}{a_1^{(s)}} \]  

(9)

in the thermodynamic limit. For the compressibility we can use DMRG for up to 128 sites. The extrapolation is very well behaved, and a reliable extrapolation could have been obtained from the results for much smaller systems. This makes us confident that the extrapolation for the charge velocity is meaningful despite the fact that exact diagonalization is limited to \( L \leq 20 \). A comparison with the exact \( K_\rho^{\text{exact}} \) for the one-dimensional Hubbard model (\( V_1 = V_2 = 0 \)) shows that relative errors \( |K_\rho^{\text{DMRG}} - K_\rho^{\text{exact}}|/K_\rho^{\text{exact}} \) are below 1%. For finite \( V_1 \) and/or \( V_2 \), our results are consistent with other estimates using the charge structure factor.25,26,27

In Fig. 2 the parameter \( K_\rho \) is plotted as a function of \( V_2/t \) at fixed \( U/t = 10 \) and \( V_1/t = 4 \). We see that \( K_\rho > 0.25 \) when the charge gap is zero and \( K_\rho > 0.25 \) at the critical points. We have confirmed numerically that \( K_\rho \) is always 0.25 at the CDW critical points for all finite values of \( U \). \( K_\rho \) reaches its maximum value around \( V_1 = 2V_2 \), i.e., the density-density correlations decay most rapidly when \( V_1 \) and \( V_2 \) maximally frustrate each other. In general, long-range Coulomb repulsions are expected to suppress the value of \( K_\rho \). This is consistent with our results because \( K_\rho \) decreases when the values of \( V_1 \) and \( V_2 \) deviate from the relation \( V_1 \approx 2V_2 \), whereby the effective interaction strength increases. Apparently, the line \( V_1 = 2V_2 \) goes along the ridges of the contour line of \( K_\rho \) in Fig. 2. This has been already suggested in the spinless fermion case and similar models.21

As in the case of charge gap, the extrapolation to the thermodynamic limit is straightforward. In the \( 2k_F \)-CDW phase, we find that \( \Delta_s \) is always finite because the system contains separated spin singlet pairs. For fixed \( V_1 \), \( \Delta_s \) increases as a function of \( V_2 \) and eventually saturates at \( \Delta_s = 4t^2/(U - V_1) \) in the limit \( V_2 \to \infty \). This is readily understood because, for \( U, V_2 \gg V_1 \), the system can be mapped to an effective spin Hamiltonian \( H = J_{2k_F} \sum_i \hat{S}_{4i} \cdot \hat{S}_{4i+1} \) with \( J_{2k_F} = 4t^2/(U - V_1) \). This model is trivial and the spin gap is the energy difference between the singlet and triplet state at each bond, \( \Delta_s = 4t^2/(U - V_1) \).

In the \( 4k_F \)-CDW phase, we find that \( \Delta_s \) is always zero, because a charged site and a vacant site come alternately and the spin degrees of freedom can be described in terms of a one-dimensional uniform Heisenberg model. In fact, for \( U > V_1/2 \gg V_2 \), the effective spin Hamiltonian can be written as \( H = J_{4k_F} \sum_i \hat{S}_{2i} \cdot \hat{S}_{2i+2} \) with \( J_{4k_F} = 4 (t^2/(V_1 - 2V_2))^2 [(1/(U - V_2) + 2/(U - 2V_2))] \). This effective Heisenberg model displays gapless spin excitations, in agreement with our numerical results.

Lastly, in Fig. 3 we plot the TLL parameter \( K_\rho \) as a function of \( V_1/t \) for fixed \( V_1 = 2V_2 \) and several values of \( U \). For large \( U \), \( K_\rho \) decreases as a function of \( V_1/t \) and eventually crosses \( K_\rho = 0.25 \) at some finite value of \( V_1/c \). As shown above, \( K_\rho \geq 0.25 \) for a metallic phase, so that the Tomonaga-Luttinger liquid turns into the \( 4k_F \)-CDW at \( V_1/c \). For small \( U \), e.g., \( U = 2t \) in Fig. 3, \( K_\rho \) decreases as a function of \( V_1 \), displays a minimum around \( V_1/t \approx \mathcal{O}(U/t) \) with \( K_{\rho,\text{min}} \geq 0.25 \), and increases again. This results from the fact that \( V_1 \) overcomes the Hubbard interaction \( U \) and electrons with opposite spin gain energy from on-site pairing. Eventually, \( K_\rho \) can become

\[ \Delta_s(L) = E_0(N_1 + 1, N_1 - 1, L) - E_0(N_1, N_1, L). \]  

(10)
larger than unity and superconducting correlations are dominant. As seen from Fig. 5, the ground-state phase diagram in Fig. 11 is representative for all $U \gtrsim 4t$ when a superconducting phase does not interfere. The ridge of $K_p$ goes along the line $V_1 = 2V_2$ and $K_p$ decreases as the value of $V_1$ and $V_2$ deviate from this line.

In conclusion, we obtained an accurate ground-state phase diagram of the $t-U-V_1-V_2$ model at quarter filling using DMRG and exact diagonalization methods. For intermediate to large Hubbard interaction $U \gtrsim 4t$, the system has CDW phases with $q = 2k_F$ and $4k_F$ between which there appears a broad region of a Tomonaga-Luttinger liquid. Because of the geometrical frustration of the long-range Coulomb interactions, $K_p$ is maximum around $V_2 = V_1/2$. It is smallest at the phase boundaries, $K_p = 0.25$, which appears to be universal for transitions between the metallic and the CDW phases.

Acknowledgments

We are grateful to E. Jeckelmann, G. Japaridze, and P. Schmitteckert for helpful discussions. We acknowledge support by the Central Institute for Applied Mathematics at Research Centre Jülich. S.E. is supported by the Honjo International Scholarship Foundation. Also acknowledged is partial support by Grants-in-Aid for Scientific Research from the Ministry of Education, Science, Sports, and Culture of Japan. A part of computations was carried out at the computer centers of the Institute for Molecular Science, Okazaki, and the Institute for Solid State Physics, University of Tokyo.

1. K. Schönhammer in *Strong Interactions in Low Dimensions*, Physics and Chemistry of Materials with Low-Dimensional Structures, Vol. 25, ed. by D. Baeriswyl and L. Degiorgi (Springer, Berlin, 2004); e-print cond-mat/0305035
2. R. Claessen, M. Sing, U. Schwingenschlög¹, P. Blaha, M. Dressel, and C.S. Jacobsen, Phys. Rev. Lett. 88, 096402 (2002).
3. H. Benthien, F. Gebhard, and E. Jeckelmann, Phys. Rev. Lett. 92, 256401 (2004).
4. V. Emery in *Highly Conducting One-dimensional Solids*, ed. by J.T. Devreese et al. (Plenum, New York, 1979), p. 327.
5. J. Sólyom, Adv. Phys. 28, 209 (1979).
6. F. Zwick, S. Brown, G. Margaritondo, C. Merlic, M. Onelion, J. Voit, and M. Grioni, Phys. Rev. Lett. 79, 3982 (1997).
7. K. Takenaka, K. Nakada, A. Osuka, S. Horii, H. Ikuta, I. Hirabayashi, S. Sugai, and U. Mizutani, Phys. Rev. Lett. 85, 5428 (2000).
8. T. Mizokawa, A. Ino, T. Yoshida, A. Fujimori, C. Kim, H. Eisaki, Z.-X. Shen, S. Horii, T. Takeshita, S. Uchida, K. Tomimoto, S. Tajima, and Y. Yamada, in *Stripes and Related Phenomena*, ed. by A. Bianconi and N.L. Saini (Plenum, New York, 2000).
9. T. Mizokawa, K. Nakada, C. Kim, Z.-X. Shen, T. Yoshida, A. Fujimori, S. Horii, Y. Yamada, H. Ikuta, and U. Mizutani, Phys. Rev. B 65, 193101 (2002).
10. M. Sing, U. Schwingenschlög¹, R. Claessen, P. Blaha, J.M. P. Carmelo, L.M. Martelo, P.D. Sacramento, M. Dressel, and C.S. Jacobsen, Phys. Rev. B 68 125111 (2003).
11. C. Bourbonnais and D. Jérome, *Advances in Synthetic Metals, Twenty Years of Progress in Science and Technology*, ed. by P. Bernier, S. Lefrant, and G. Bidan (Elsevier, New York, 1999), p. 206.
12. R. Claessen, private communication (2004).
13. F. Nad, P. Monceau, C. Carcel, and J.M. Fabre, Phys. Rev. B 62, 1753 (2000).
14. D.S. Chow, F. Zamborszky, B. Alavi, D.J. Tantillo, A. Baur, C.A. Merlic, and S.E. Brown, Phys. Rev. Lett. 85, 1698 (2000).
15. S. Fujiyama, M. Takigawa, and S. Horii, Phys. Rev. Lett. 90, 147004 (2003).
16. H. Yoshioka, M. Tsuchiizu, and Y. Suzumura, J. Phys. Soc. Jpn. 70, 762 (2001).
17. D. Poilblanc, S. Yunoki, S. Maezawa, and E. Dagotto, Phys. Rev. B 56, R1645 (1997).
18. H. Seo and M. Ogata, Phys. Rev. B 64, 113103 (2001).
19. S. Nishimoto and Y. Ohta, Phys. Rev. B 68, 235114 (2003).
20. A.K. Zhuravlev, M.I. Katsnelson, and A.V. Trefilov, Phys. Rev. B 56, 12939 (1997); A.K. Zhuravlev and M.I. Katsnelson, *ibid.* 61, 15534 (2000).
21. P. Schmitteckert and R. Werner, Phys. Rev. B 69, 195115 (2004).
22. H.J. Schulz, Phys. Rev. Lett. 64, 2831 (1990).
23. N. Kawakami and S.-K. Yang, Phys. Lett. A 148, 359 (1990).
24. H. Frahm and V.E. Korepin, Phys. Rev. B 42, 10553 (1990).
25. S. Daul and R.M. Noack, Phys. Rev. B 58, 2635 (1998).
26. R.T. Clay, A.W. Sandvik, and D.K. Campbell, Phys. Rev. B 59, 4665 (1999).
27. S. Ejima, S. Nishimoto and F. Gebhard, in preparation.