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Density matrix spectra and order parameters in the 1D extended Hubbard model

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Abstract. Without any knowledge of the symmetry existing in a system, we derive the exact forms of the order parameters which show long-range correlations in the ground state of the one-dimensional (1D) extended Hubbard model using a quantum information approach. Our work demonstrates that the quantum information approach can help us to find the explicit form of the order parameter, which could not be derived systematically via traditional methods in the condensed matter theory.

1 Introduction

In many-body physics, the correlation function plays a fundamental role. The understanding of many physical phenomena are based on calculations of the corresponding correlation functions [1,2] especially in theoretical studies. For instance, to investigate the magnetic properties of a system, people often calculate the spin-spin correlation function to learn the possible magnetic order. In the one-dimensional case, the system has a ferromagnetic long range order if the zero mode of momentum is dominant, and an anti-ferromagnetic qausi-long range order (QLRO) if the π mode is dominant. The long-range behavior of the correlation function is associated with symmetry-breaking in the system, which is an important concept in understanding continuous phase transitions. For a certain operator, its non-vanishing value at a long distance denotes a symmetry-broken phase which usually occurs in the thermodynamic limit. Mathematically, if the correlation function

$$C(0,r) = \langle O_0 O_r \rangle - \langle O_0 \rangle \langle O_r \rangle \tag{1}$$

is a constant or decays algebraically in the infinite r limit, we say that the state has a long-range order or QLRO respectively. The operator O can then be taken as the order parameter to describe the corresponding phase.

Traditionally, to find an appropriate order parameter corresponding to a certain phase, people often rely on physical intuition or resort to methods such as group theory and the renormalization group analysis. However, there is no guarantee that these methods always apply. Hence it is desirable to develop a systematic way to derive the order parameter. Using the variational approach, Furukawa et al. [3] proposed a scheme, which was later improved by Henley and Changlani [4], to derive the order parameter. While the improved scheme is promising, it still needs the knowledge of a set of low-energy quasi-degenerate states that lead to the symmetry breaking in the thermodynamic limit. Another scheme was proposed by Cheong and Henley [5] where one applies the singular-value decomposition to the correlation density matrix to gain information on the correlation functions and order parameters. Recently, we have also proposed a scheme to derive the order parameter from the spectrum of the reduced density matrix of the ground state directly [6]. This scheme is non-variational and needs only the knowledge of the ground state. Moreover, our scheme establishes a connection between the mutual information and the order parameters and is relatively more intuitive to apply.

In this paper, we apply our proposed scheme, for the first time, to a realistic many-body model, the 1D extended Hubbard model (EHM). The model has been widely studied in the research of quasi one-dimensional organic solids such as conjugated polymers [7,8] and charge transfer crystals [9]. In Section 2, we outline the scheme for deriving the order parameters proposed in reference [6]. We then demonstrate how to derive the order parameters in the 1D EHM in Section 3. We show that even without any prior knowledge of the symmetry of the system, we can derive the exact forms of the order parameters, which show long-range correlations in the ground state. A summary is given in Section 4.

2 Outline of the scheme

To find the order existing in the ground state of the model, we need to first examine if there exists a long-range

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correlation in the ground state or not. Even if we do not know the form of any order parameters, we can still use the mutual information, a concept borrowed from quantum information science, to measure the total correlation between two arbitrary blocks in the system. The mutual information is defined as:

$$S(i|j) = S(\rho_i) + S(\rho_j) - S(\rho_{i\cup j}), \tag{2}$$

where $S(\rho_i) = -\mathrm{tr}(\rho_i \log_2 \rho_i)$ is the von-Neumann entropy of the block i. ρ_i is the reduced density matrix obtained by tracing out all other degrees of freedom except those of the block i, i.e. $\rho_i = \mathrm{tr}\,|\Psi_0\rangle\langle\Psi_0|$ where $|\Psi_0\rangle$ is the ground state of the system. It has been shown that the mutual information is non-vanishing at a long distance if and only if there exists a long-range order (or QLRO) in the system [10,11].

After finding a block of minimum size in which the mutual information does not vanish at a long distance, we compute the eigenvalues and eigenvectors of the reduced density matrices. Depending on the bases of the reduced density matrix, it is possible to have diagonal and off-diagonal long-range orders. For the diagonal long-range order, the order parameter is defined as

$$O_i^d = \sum_{\mu\leq\xi} w_\mu a_{i\mu}^\dagger a_{i\mu}, \tag{3}$$

where $a_{i\mu}^\dagger(a_{i\mu})$ is the creation (annihilation) operator for the state $|\mu\rangle$ localized at the block i and ξ is the rank of ρ_i. The coefficients w_μ could be fixed by the traceless condition $\mathrm{tr}(\rho_i O_i^d) = 0$ and the cut-off condition $\max(\{w_\mu\}) = 1$.

If the two-block reduced density matrix $\rho_{i\cup j}$ is not diagonal in the eigen-bases of $\rho_i \otimes \rho_j$, there exists off-diagonal long-range order in the system. The corresponding order operator is defined by

$$O_i^o = \sum_{\langle\mu,\nu\rangle} w_{\mu\nu} a_{i\mu}^\dagger a_{i\nu} + w_{\mu\nu}^* a_{i\nu}^\dagger a_{i\mu}, \tag{4}$$

where $\mu \neq \nu$ and the sum is over all the pairs of μ, ν that correspond to the non-zero off-diagonal matrix elements in $\rho_{i\cup j}$. With the derived order parameters, one could calculate the correlation functions and study the dominating mode of momentum.

3 Deriving the order parameter

The Hamiltonian of the 1D extended Hubbard model reads

$$H = -t\sum_{\sigma,j}\left(c_{j,\sigma}^\dagger c_{j+1,\sigma} + h.c.\right) + U\sum_j n_{j,\uparrow}n_{j,\downarrow} + V\sum_j n_j n_{j+1}, \tag{5}$$

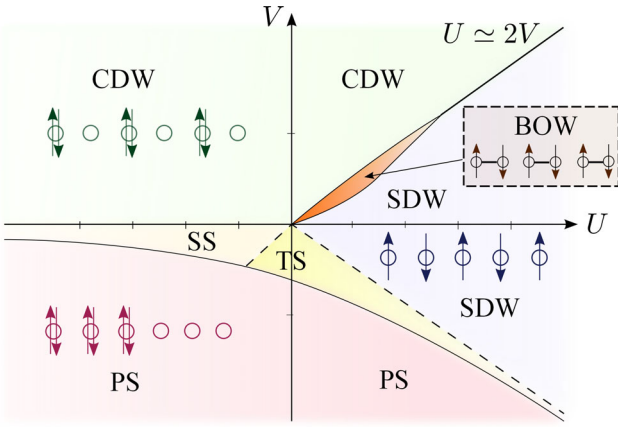

Fig. 1. Schematic drawing of the ground state phase diagram of the 1D extended Hubbard model at half-filling.

where $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ ($\sigma = \uparrow, \downarrow$) are creation and annihilation operators of electrons with a spin σ at the site j respectively, $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$, and $n_j = n_{j,\uparrow} + n_{j,\downarrow}$. U and V is the strength of the on-site and the nearest-neighbor Coulomb interaction respectively. t is the hopping integral and is taken to be unity for convenience. The case of half-filling is being considered in the following discussion.

Interestingly, this model exhibits a very rich phase diagram (see Fig. 1). Both analytical [12–16] and numerical [17–21] studies have shown that the phase diagram consists of spin-density waves (SDW), charge-density waves (CDW), phase separation (PS), a singlet superconducting (SS) phase and a triplet superconducting (TS) phase. By studying the excitation spectra with numerical exact diagonalization, Nakamura pointed out that there also exists a spontaneous dimerized phase, the bond-order wave (BOW) phase, in a narrow region between the SDW and CDW phases up to a tricritical point [22,23]. On the other hand, Jeckelmann argued that the BOW phase only exists on a short segment of the critical line, rather than a stripe, of the CDW-SDW transition from DMRG studies [24,25]. Subsequent efforts using quantum Monte Carlo simulation [26,27], density matrix renormalization group [28,29], and analytical methods [30,31] have been devoted to clarify the ground state phase diagram of the model. Recently, the concept from quantum information science, namely the entanglement entropy, was also used to explore the problem [32–34]. Although studies have confirmed the existence of the BOW phase, the boundary of it still has not settled with agreement. Most of the studies found that the first order CDW-SDW transition line bifurcates into a CDW-BOW and a BOW-SDW transition line and the transition along the CDW-BOW line changes from a first order to continuous. However, the location of the bifurcation point and the position on the CDW-BOW transition line in which the transition changes order remain controversial and are still under active research.

In the following, we assumed to know nothing about the phase diagram of the model and derive the order parameters by investigating the reduced density matrix spectrum.

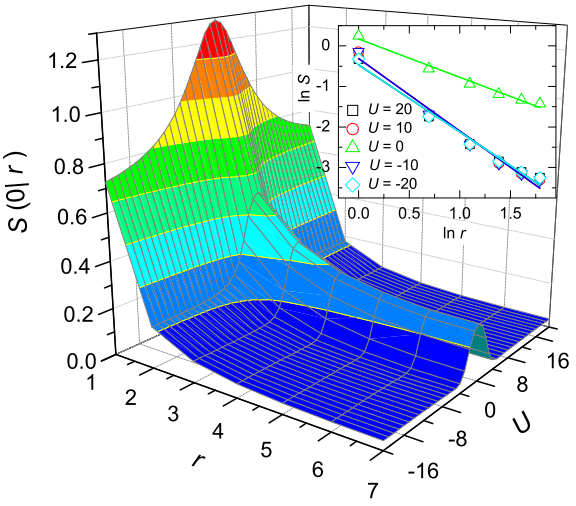

Fig. 2. The mutual information as a function of $r = |i - j|$ and U in the Hubbard model. The inset shows that the mutual information decays algebraically with r and thus long-range correlation is presented in the system. Here the block size $N_B = 1$.

3.1 Case I: $V = 0$

Let us start with the simplest case where $V = 0$, and the model is reduced to the conventional Hubbard model [35–37]. Consider a block consists of one site, i.e. $N_B = 1$. In the bases of local states $\{|\mu\rangle\} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$, ρ_i is found to be diagonal, i.e.

$$\rho_i = u\,|0\rangle\langle 0| + v\,|\uparrow\rangle\langle\uparrow| + v\,|\downarrow\rangle\langle\downarrow| + u\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow|, \qquad (6)$$

where u and v are some positive real numbers. The two-site reduced density matrix $\rho_{i\cup j}$ is a block-diagonal matrix in the bases $\{|\mu\nu\rangle\} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\} \otimes \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$.

Figure 2 shows the dependence of the mutual information $S(0|r)$ as a function of $r = |i - j|$ and U calculated for a 14-site system. Periodic boundary condition is used. From the inset, we see that $S(0|r)$ decays algebraically with r and we could judge that there exist a certain kind of long-range correlation in the ground state [10,11] though we do not know the explicit form of the order parameter yet.

Diagonal order parameter: to single out the correlated elements in ρ_i, we calculated the difference between the diagonal matrix elements of $\rho_{i\cup j}$ and that of $\rho_i \otimes \rho_j$ as a function of r. Figure 3 shows a plot of $\rho_{0r}^{\mu\nu,\mu\nu} - \rho_0^{\mu,\mu}\rho_r^{\nu,\nu}$ as a function of r. For convenience, $\rho_{0\cup r}$ is written as ρ_{0r}. From the figure, we clearly see that $\rho_{0r} \neq \rho_0 \otimes \rho_r$ which is consistent with $S(0|r) \neq 0$. Moreover, for $U = -20$, the difference in the diagonal matrix elements for $\{\mu, \nu\} \in \{|0\rangle, |\uparrow\downarrow\rangle\}$ decays algebraically with r while it is almost zero for the others. We can then argue that the vacant state and the double occupancy state of the two blocks are correlated in this case. For the case of $U = 20$, $\rho_{0r}^{\mu\nu,\mu\nu} - \rho_0^{\mu,\mu}\rho_r^{\nu,\nu}$ are almost zero unless $\{\mu, \nu\} \in \{|\uparrow\rangle, |\downarrow\rangle\}$. In this limit, the spin up and spin down states are correlated.

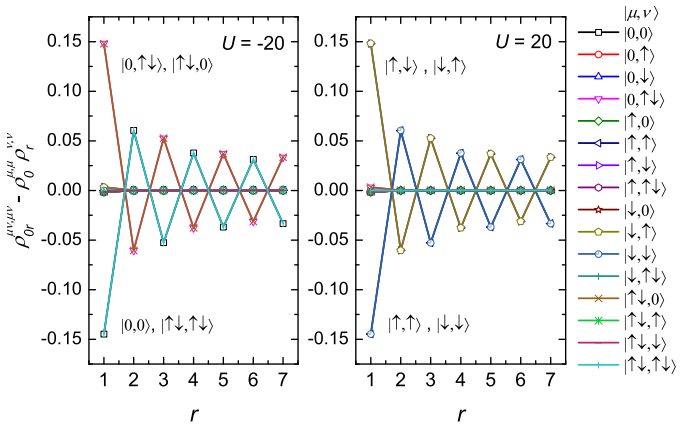

Fig. 3. A plot of $\rho_{0r}^{\mu\nu,\mu\nu} - \rho_0^{\mu,\mu}\rho_r^{\nu,\nu}$ as a function of r for two limiting cases of $U = -20, 20$ in the Hubbard model. For $U = -20$ (left), the charge degrees of freedom ($\{\mu, \nu\} \in \{|0\rangle, |\uparrow\downarrow\rangle\}$) are correlated, while for $U = 20$ (right) the spin degrees of freedom ($\{\mu, \nu\} \in \{|\uparrow\rangle, |\downarrow\rangle\}$) are correlated.

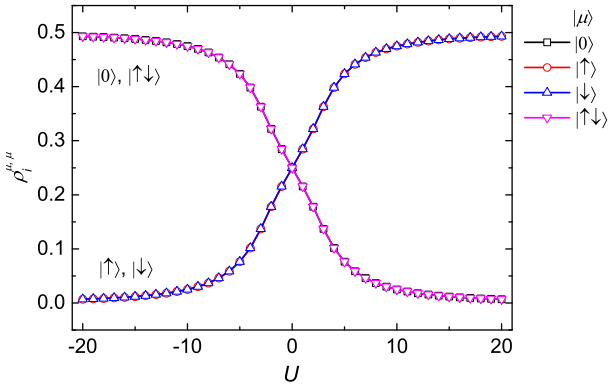

Fig. 4. The diagonal matrix elements, which is also the eigenvalues, of ρ_i as a function of U in the Hubbard model. For the negative U case, the eigenstates $|0\rangle$ and $|\uparrow\downarrow\rangle$ have dominate weights while for positive U, the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ have dominant weights.

In Figure 4, we show the dependence of the eigenvalues of ρ_i on the interaction U. In the large U limit, the reduced density matrix becomes

$$\rho_i = \frac{1}{2}\,|\uparrow\rangle\langle\uparrow| + \frac{1}{2}\,|\downarrow\rangle\langle\downarrow|. \qquad (7)$$

In the bases of $\rho_i \otimes \rho_j$, we show the non-zero diagonal and off-diagonal elements of $\rho_{i\cup j}$ in Figures 5 and 6 respectively. From the figures, we find that ρ_{0r} takes the form

$$\rho_{0r} = \begin{pmatrix} u & 0 & 0 & 0 \\ 0 & v & z & 0 \\ 0 & z & v & 0 \\ 0 & 0 & 0 & u \end{pmatrix} \qquad (8)$$

in the large U limit in the bases of $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. From equation (3), the order parameter is defined as

$$O_i^d = w_1\,|\uparrow\rangle\langle\uparrow| + w_2\,|\downarrow\rangle\langle\downarrow|. \qquad (9)$$

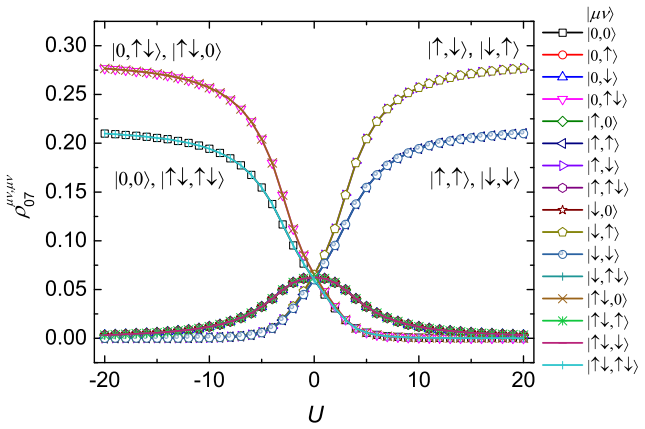

Fig. 5. The diagonal elements of ρ_{ij} as a function of U in the Hubbard model for $r = |i - j| = 7$. In the negative U limit, only the matrix elements corresponding to the bases $\{\mu, \nu\} \in \{|0\rangle, |\uparrow\downarrow\rangle\}$ is non-vanishing. In the positive U limit, only the matrix elements corresponding to the bases $\{\mu, \nu\} \in \{|\uparrow\rangle, |\downarrow\rangle\}$ is non-vanishing.

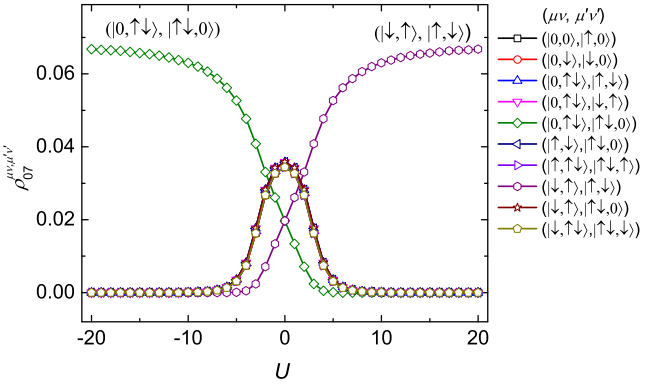

Fig. 6. The non-zero off-diagonal elements of ρ_{ij} as a function of U in the Hubbard model for $r = 7$. The matrix elements for $(\mu\nu, \mu'\nu')$ is the same as $(\mu'\nu', \mu, \nu)$.

According to the traceless condition $\mathrm{tr}(O_i^d \rho_i) = 0$, we have $w_1 = -w_2$. Let $w_1 = 1$, then the order parameter becomes

$$O_i^d = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|, \tag{10}$$

and let us denote it as σ_i^z.

Similarly, for the case of negative U, we can find that

$$O_i^d = |0\rangle\langle 0| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow|, \tag{11}$$

and let us denote it as η_i^z.

Off-diagonal order parameter: from equation (8), we find that ρ_{0r} is not a diagonal matrix. This means that there exists off-diagonal long-range correlations in the ground state of the system. The off-diagonal order parameter can be defined as

$$O_i^o = w|\uparrow\rangle\langle\downarrow| + w^*|\downarrow\rangle\langle\uparrow|.$$

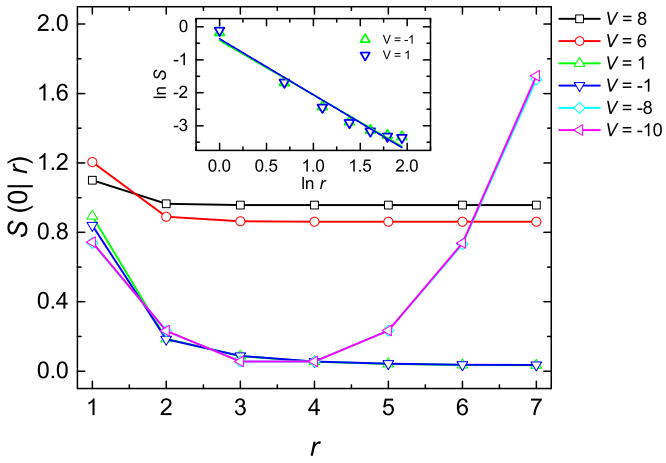

Fig. 7. The mutual information as a function of $r = |i - j|$ for $U = 10$ in EHM. The inset shows a plot of the mutual information versus r on a natural logarithmic scale for $V = \pm 1$.

Here w is complex. Separating the real and the imaginary part in the operator, we have

$$O_i^o = xO_i^x - yO_i^y \tag{12}$$

with

$$O_i^x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|,$$
$$O_i^y = -i(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|).$$

Obviously, $\langle O_i^x\rangle = \langle O_i^y\rangle = 0$ and $\langle O_i^x O_j^x\rangle = \langle O_i^y O_j^y\rangle = 2z$. So we can treat either O_i^x, O_i^y or their linear combination as the off-diagonal order operator. Let us denote O_i^x and O_i^y as σ_i^x and σ_i^y respectively.

Similarly, in the negative U limit, we can also derive the off-diagonal order parameter as

$$O_i^x = |0\rangle\langle\uparrow\downarrow| + |\uparrow\downarrow\rangle\langle 0|,$$
$$O_i^y = -i(|0\rangle\langle\uparrow\downarrow| - |\uparrow\downarrow\rangle\langle 0|).$$

We denote them as η_i^x and η_i^y, respectively. The order parameters we derived are in fact the well-known Pauli matrices and the eta-spin operators which satisfies the SU(2) Lie algebra.

3.2 Case II: $V \neq 0$, $U = 10$

Now, let us also include the next-nearest neighbor interaction in the system. Figure 7 shows a plot of the mutual information as a function of r. Obviously, the mutual information is non-vanishing at a large r for $V = -10, \pm 8, 6$. For the intermediate case, we can see from the inset that the mutual information shows a power law decaying behavior. One can then safely argue that the system exhibits certain kind of long-range correlations and we can go on to investigate the spectrum of the reduced density matrix to derive the potential order parameters.

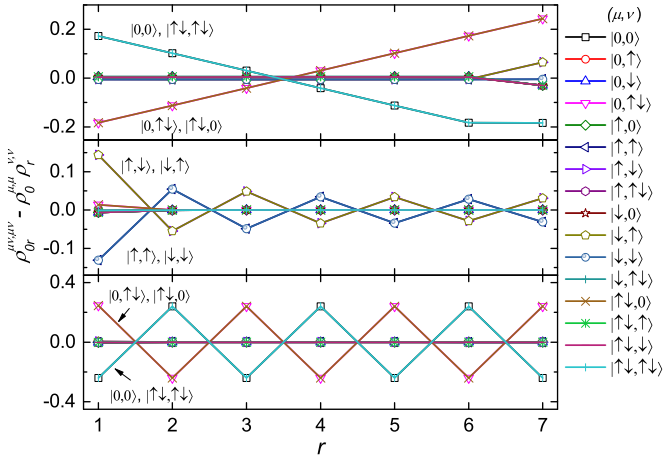

Fig. 8. A plot of $\rho_{0r}^{\mu\nu,\mu\nu} - \rho_0^{\mu,\mu}\rho_r^{\nu,\nu}$ as a function of r for $V = -8$ (top panel), $V = 1$ (middle panel), and $V = 8$ (bottom panel) in EHM for $U = 10$. For $V = \pm 8$, the charge degrees of freedom ($\{\mu,\nu\} \in \{|0\rangle, |\uparrow\downarrow\rangle\}$) are correlated, while for $V = 1$ the spin degrees of freedom($\{\mu,\nu\} \in \{|\uparrow\rangle, |\downarrow\rangle\}$) are correlated.

Using the same bases as that for the Hubbard model in Section 3.1, we calculated the single-site and two-sites reduced density matrices. ρ_i is diagonal and takes the form of equation (6). Figure 8 shows a plot of the difference between the diagonal matrix element of ρ_{0r} and the product of the diagonal matrix elements of ρ_0 and ρ_r with the corresponding bases as a function of r. The finite difference in $\rho_{0r}^{\mu\nu,\mu\nu} - \rho_0^{\mu,\mu}\rho_r^{\nu,\nu}$ for some particular μ and ν indicates that $\rho_{0r} \neq \rho_0 \otimes \rho_r$. For $V = -8$ and $V = 8$, we see that the main contributors to the correlation of two sites separated by a large distance are the states $|0\rangle$ and $|\uparrow\downarrow\rangle$. While for the case of $V = 1$, the $|\uparrow\rangle$ and $|\downarrow\rangle$ states play the same role.

Figure 9 shows the eigenvalues of the single-site reduced density matrix as a function of V. The crossings of the eigenvalues of ρ_i separate the system into three different regimes corresponding to $V \lesssim -7$, $-7 \lesssim V \lesssim 5$, and $V \gtrsim 5$. In each of the regimes, the kind of correlation existing in the system is qualitatively different, as one can judge from the nature of the dominating eigenstates. Following similar argument in Section 3.1, one can find, respectively the order parameters to be σ_i^z for $-7 \lesssim V \lesssim 5$, and η_i^z for $V \lesssim -7$ and $V \gtrsim 5$.

Here we obtained the same order parameter for both regimes where $V \lesssim -7$ and $V \gtrsim 5$. However, recall from Figure 7 that the mutual information as a function of r shows qualitatively different behavior in these two ranges. For $V \gtrsim 5$, the mutual information almost remains constant as r increases. On the other hand, for $V \lesssim -7$, the mutual information first decreases and then increases to a maximum value upon reaching $r = 7$, where the middle of the chain is. It is reasonable to suspect that the ground state of the system is qualitatively different in these two regimes. To further distinguish between them, it is worth studying the dominating mode of momentum of the correlation function.

Figure 10 shows a plot of the correlation function as a function of the momentum wavevector k. The correlation function peaks at $k = \pi$ for $V = 8$. One can expect this holds true for the whole range of $V \gtrsim 5$. Together with the form of the derived order parameter, we may conclude that the dominating configuration in the ground state of the system consists of alternating vacant and double occupancy states. This is in fact the well-known CDW states.

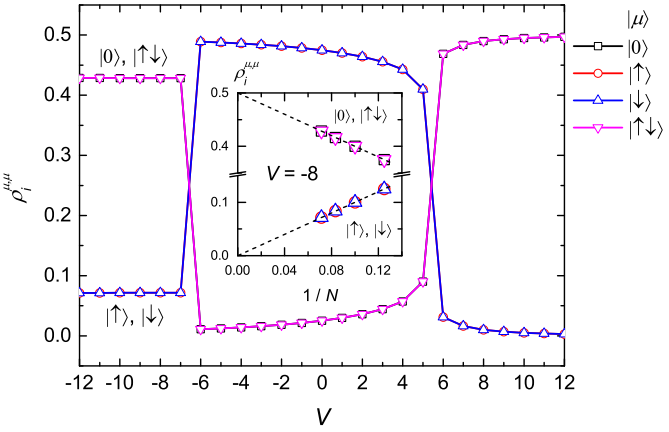

Fig. 9. A plot of the eigenvalues of ρ_i as a function of V for $U = 10$ in EHM. The inset shows the size dependence of the eigenvalues of ρ_i for $V = -8$. From linear fitting, the eigenvalues corresponding to $|0\rangle$ and $|\uparrow\downarrow\rangle$ tend to 0.5 while that corresponding to $|\uparrow\rangle$, and $|\downarrow\rangle$ tend to 0 in the thermodynamic limit. For $V \lesssim -7$ and $V \gtrsim 5$, the eigenstates $|0\rangle$ and $|\uparrow\downarrow\rangle$ have dominate weights. For $-7 \lesssim V \lesssim 5$, the eigenstates $|\uparrow\rangle$, and $|\downarrow\rangle$ are dominated.

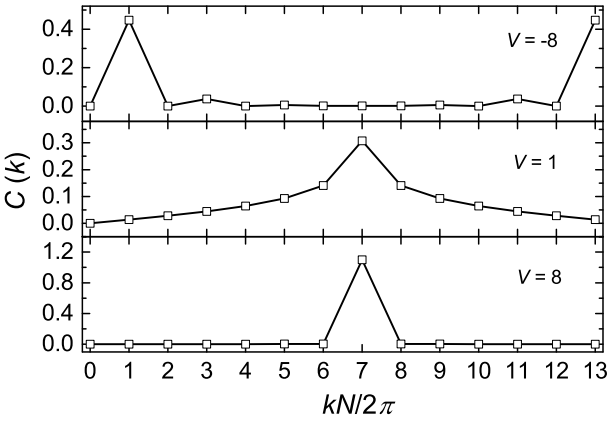

Fig. 10. The correlation function calculated from the derived order operators in the momentum space as a function of k in EHM. Here $U = 10$ and $V = -8$ (top panel), $V = 1$ (middle panel), and $V = 8$ (bottom panel) respectively.

For $V \lesssim -7$, the dominating modes are $k = 2\pi/N$ and $2\pi(N-1)/N$. The second peak in the correlation function is just a result from the periodic boundary conditions. In this regime, one can deduce that the dominating ground state configuration has a period of half of the lattice in the real space. They are the PS states $|0,\ldots,0,\uparrow\downarrow,\ldots,\uparrow\downarrow\rangle$ and the translations of it. This also explains why the mutual information is maximum for the sites separated by half of the lattice. Since any of the translation of the above states

are equally weighted in the ground state before symmetry is broken, only the local states separated by half of the lattice can be confidently determined once we know one of them.

For completeness, we also showed $C(k)$ for $-7 \lesssim V \lesssim 5$ in the middle panel of Figure 10. The maximum of the correlation function occurs at $k = \pi$ and with the form of the derived order parameter, we can deduce that this is a SDW state. The obtained results are consistent with previous studies [20].

3.3 Case III: $V \neq 0$, $U = 4$

Let us consider a block size of two sites, i.e. $N_B = 2$. In the following, we will use i to denote a single-site and $\tilde{i}$ to denote a single-block consisting of two neighboring sites. In the bases of $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\} \otimes \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$, the eigenstates of $\rho_{\tilde{i}}$ have the form of

$$
\begin{aligned}
|\phi_A\rangle &= |\uparrow\downarrow,\uparrow\downarrow\rangle,\\
|\phi_B\rangle &= |0,0\rangle,\\
|\phi_C\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow,\downarrow\rangle + |\downarrow,\uparrow\downarrow\rangle\big),\\
|\phi_D\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow,0\rangle - |0,\uparrow\rangle\big),\\
|\phi_E\rangle &= \frac{1}{\sqrt{2}}\big(|\downarrow,0\rangle - |0,\downarrow\rangle\big),\\
|\phi_F\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow,\uparrow\rangle + |\uparrow,\uparrow\downarrow\rangle\big),\\
|\phi_G\rangle &= \alpha\big(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\big) - \beta\big(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\big),\\
|\phi_H\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\big),\\
|\phi_I\rangle &= |\uparrow,\uparrow\rangle,\\
|\phi_J\rangle &= |\downarrow,\downarrow\rangle,\\
|\phi_K\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow,\downarrow\rangle - |\downarrow,\uparrow\downarrow\rangle\big),\\
|\phi_L\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow,0\rangle + |0,\uparrow\rangle\big),\\
|\phi_M\rangle &= \frac{1}{\sqrt{2}}\big(|\downarrow,0\rangle + |0,\downarrow\rangle\big),\\
|\phi_N\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow,\uparrow\rangle - |\uparrow,\uparrow\downarrow\rangle\big),\\
|\phi_O\rangle &= \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle\big),\\
|\phi_P\rangle &= \gamma\big(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\big) + \delta\big(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\big), \quad (13)
\end{aligned}
$$

where $\alpha, \beta, \gamma, \delta$ are positive real numbers and the expression is consistent with that obtained in reference [38].

Figure 11 shows a plot of the eigenvalues of the corresponding eigenstates in equation (13) as a function of V. From the figure, we can see that some of the states, for examples, states $\{|\phi_C\rangle, |\phi_D\rangle, |\phi_E\rangle, |\phi_F\rangle\}$ and states $\{|\phi_K\rangle, |\phi_L\rangle, |\phi_M\rangle, |\phi_N\rangle\}$, are degenerated respectively.

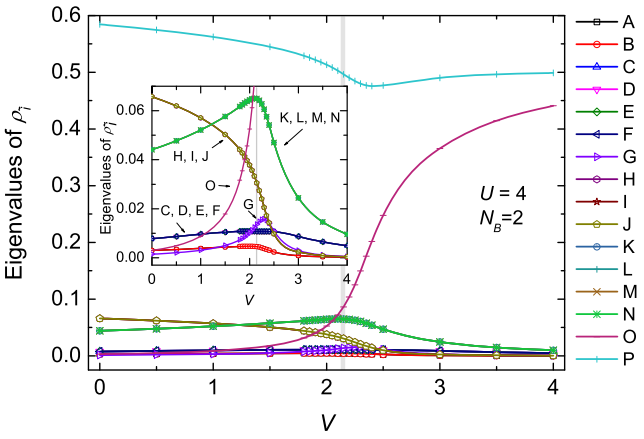

Fig. 11. The eigenvalues of the single-block (two-site) reduced density matrix $\rho_{\tilde{i}}$ as a function of V in the 1D extended Hubbard model for $U = 4$. The inset shows a close-up of the low-lying states. The grey region indicates the range of values of V in which the BOW exists in the thermodynamic limit as obtained in reference [33].

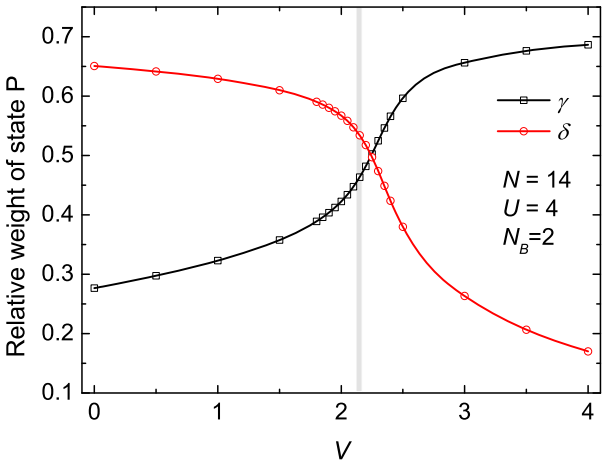

Fig. 12. The relative weight of the γ and δ in the eigenstate $|\phi_P\rangle$ of the single-block reduced density matrix as a function of V. Here $U = 4$, and $N_B = 2$.

The degeneracy tells us that there are spin-up-down and charge symmetries in the system.

Among all the eigenstates, the weight of the state $|\phi_P\rangle$ dominates for the whole range of values of V shown. The weights of the charge part γ and the spin part δ in $|\phi_P\rangle$ are plotted as a function of V in Figure 12. There is a crossing between the two magnitudes around $V = 2$. For $V \gg 2$, the relative weight of the charge part is much greater than that of the spin part. Besides, considering the region $V \gg 2$ in Figure 11 again, the second dominating state is $|\phi_O\rangle$ which overwhelms all other eigenstates except $|\phi_P\rangle$. From equation (13), we also notice that the state $|\phi_O\rangle$ only consists of the charge part. As a result, we may argue that in this region, the charge part is decoupled from the spin part. The reduced density matrix can be reduced to the form in equation (8) with bases $\{|0\rangle\,|0\rangle, |0\rangle\,|\downarrow\uparrow\rangle, |\downarrow\uparrow\rangle\,|0\rangle, |\downarrow\uparrow\rangle\,|\downarrow\uparrow\rangle\}$.

Similarly, for $V \ll 2$, the spin part in $|\phi_P\rangle$ outweighs the charge part as one can realize from Figure 12. The eigenvalues for $|\phi_H\rangle$, $|\phi_I\rangle$, and $|\phi_J\rangle$ also dominate in the low-lying eigenstates. The spin degree of freedom is singled out in this regime and the reduced density matrix can be effectively expressed as in equation (8).

Following similar analysis in the previous sections, we can find that the order operators are σ_i^z and η_i^z, which characterize the SDW and CDW respectively, in these two regions.

Around $V = 2$, the eigenvalue of $|\phi_P\rangle$ shows a drop and there is also a relatively large rise in the weight of the eigenstates $|\phi_K\rangle$, $|\phi_L\rangle$, $|\phi_M\rangle$ and $|\phi_N\rangle$. In addition, the magnitudes of γ and δ in $|\phi_P\rangle$ become comparable in this intermediate value. These observations suggest that the spin part and the charge part are coupled around $V = 2$. Let us try to see if there exist some other kind of long-range correlation other than SDW and CDW in this intermediate region.

Rearranging the single-block reduced density matrix from the bases of $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}_i \otimes \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}_{i+1}$ to $\{|0,0\rangle, |0,\uparrow\rangle, |\uparrow,0\rangle, |\uparrow,\uparrow\rangle\}_{\tilde{i}} \otimes \{|0,0\rangle, |0,\downarrow\rangle, |\downarrow,0\rangle, |\downarrow,\downarrow\rangle\}_{\tilde{i}}$. The purpose of doing this is that we want to filter out the spin-down degree of freedom from the spin-up degree of freedom (or vice versa). After the rearrangement, we traced out the spin-down degree of freedom. The resulting reduced density matrix $\rho_{\tilde{i}\uparrow}$ has the form of equation (8) with bases $\{|0,0\rangle, |0,\uparrow\rangle, |\uparrow,0\rangle, |\uparrow,\uparrow\rangle\}_{\tilde{i}}$. Similarly, if we trace out the degree of freedom for spin-up, the reduced density matrix $\rho_{\tilde{i}\downarrow}$ also has the form of equation (8) but with bases of $\{|0,0\rangle, |0,\downarrow\rangle, |\downarrow,0\rangle, |\downarrow,\downarrow\rangle\}_{\tilde{i}}$.

Next, we would like to compare the off-diagonal matrix elements z in $\rho_{\tilde{i}\uparrow}$ and $\rho_{\tilde{i}\downarrow}$ with that corresponding to SDW and CDW. The weight of SDW is given by the coefficient of $|\uparrow,\downarrow\rangle\langle\uparrow,\downarrow|$ or $|\downarrow,\uparrow\rangle\langle\downarrow,\uparrow|$ (the notation here is in the form of $|i,i+1\rangle\langle i,i+1|$). From equation (13), it can be obtained by

$$P_{\mathrm{SDW}} = \delta^2 p_P + 0.5 p_H + \beta^2 p_G, \tag{14}$$

where the p's are the eigenvalues of the corresponding eigenstates in equation (13). For the weight of CDW, we obtained it by considering the matrix element corresponding to $|0,\uparrow\downarrow\rangle\langle 0,\uparrow\downarrow|$ or $|\uparrow\downarrow,0\rangle\langle\uparrow\downarrow,0|$ from equation (13). We have

$$P_{\mathrm{CDW}} = \gamma^2 p_P + 0.5 p_O + \alpha^2 p_G. \tag{15}$$

Figure 13 shows a plot of P_{SDW}, P_{CDW} and the off-diagonal matrix elements z as a function of V. On the two regimes far away from $V = 2$, the largest weight would correspond to SDW and CDW, respectively as expected from previous analysis. However, around $V = 2$, the off-diagonal matrix elements in $\rho_{\tilde{i}\uparrow}$ and $\rho_{\tilde{i}\downarrow}$ are dominating instead. If we just pick this dominating weight to define the order parameter, we have

$$\begin{aligned} O_{\tilde{i}} = {} & \omega_1 |0,\uparrow\rangle\langle\uparrow,0| + \omega_1^* |\uparrow,0\rangle\langle 0,\uparrow| \\ & + \omega_2 |0,\downarrow\rangle\langle\downarrow,0| + \omega_2^* |\downarrow,0\rangle\langle 0,\downarrow|. \end{aligned} \tag{16}$$

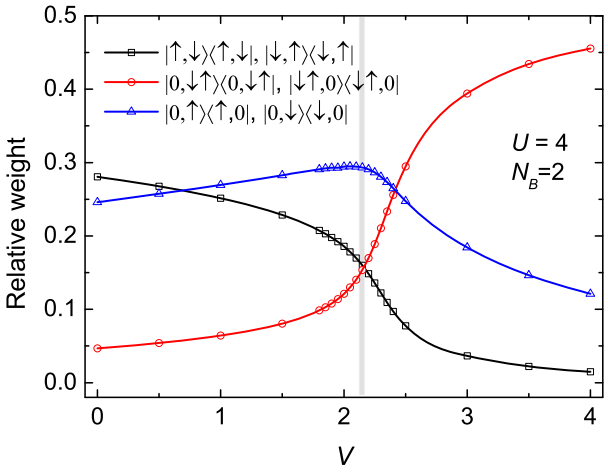

Fig. 13. The relative weight of some of the matrix elements in the single-block reduced density matrix in the 1D extended Hubbard model as a function of V.

As mentioned before, the system possesses up-down spin symmetry. We could take $\omega_1 = \omega_2 = \omega$, and then separate the operator into the real and imaginary parts. We have

$$\begin{aligned} O_{\tilde{i}} = {} & \omega\Big(|0,\uparrow\rangle\langle\uparrow,0| + |0,\downarrow\rangle\langle\downarrow,0| \Big) \\ & + \omega^*\Big(|\uparrow,0\rangle\langle 0,\uparrow| + |\downarrow,0\rangle\langle 0,\downarrow| \Big), \\ = {} & x\Big(|0,\uparrow\rangle\langle\uparrow,0| + |0,\downarrow\rangle\langle\downarrow,0| \\ & + |\uparrow,0\rangle\langle 0,\uparrow| + |\downarrow,0\rangle\langle 0,\downarrow| \Big) \\ & + iy\Big(|0,\uparrow\rangle\langle\uparrow,0| + |0,\downarrow\rangle\langle\downarrow,0| \\ & - |\uparrow,0\rangle\langle 0,\uparrow| - |\downarrow,0\rangle\langle 0,\downarrow| \Big). \end{aligned} \tag{17}$$

Either the first term or the second term in the bracket above, or their linear combination can be taken as the order parameter. Let us take the real part as the order parameter, i.e.

$$\begin{aligned} O_{\tilde{i}} = {} & |0,\uparrow\rangle\langle\uparrow,0| + |0,\downarrow\rangle\langle\downarrow,0| \\ & + |\uparrow,0\rangle\langle 0,\uparrow| + |\downarrow,0\rangle\langle 0,\downarrow|. \end{aligned} \tag{18}$$

In terms of the fermion creation and annihilation operators, we have

$$O_{\tilde{i}} = c_{i,\uparrow}^\dagger c_{i+1,\uparrow} + c_{i+1,\uparrow}^\dagger c_{i,\uparrow} + c_{i,\downarrow}^\dagger c_{i+1,\downarrow} + c_{i+1,\downarrow}^\dagger c_{i,\downarrow}, \tag{19}$$

which is the conventional order parameter that has been used to investigate the BOW in the extended Hubbard model [28].

4 Summary

With our proposed scheme [6], we derived the order parameters which show long-range correlation in the ground state of the 1D EHM without using any empirical

knowledge. Such an application confirmed that the order parameter for a quantum many-body system can be systematically derived even without the knowledge of symmetry in the system. We believe that these can shed new lights on the controversies in bond-order wave in the extended Hubbard model [22–25] and some frustrated antiferromagnet [39].

In recent decades, attention has been paid to study quantum phase transitions using quantum information concepts such as the entanglement [40–42] and the fidelity [43–45]. One could use entanglement or the fidelity to determine the phase boundaries. Then derive the potential order parameters from the reduced density matrix spectrum and calculate the correlation function to study the structure of the quantum phase. This provides an effective way to investigate the phase diagram of new models without a prior knowledge in the system's symmetry.

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