Phase diagram of the triangular extended Hubbard model Supplemental Material

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In this Supplemental Material, we show the accuracy of our wave function, compared with exact diagonalization calculations on a small cluster. We show also how charge-ordered metallic states can be obtained with a uniform wave function that does not break the translational invariance. The presence of long-range charge order is signaled by a divergence in the static structure factor at momentum $Q = (4\pi/3, 0)$; for comparison, the static structure factor is also presented for all the q points in the first quarter of the Brillouin zone. We discuss then how the formula for the charge gap, based on the behavior of the static structure factor, can be derived when the exact ground state is replaced by a variational approximation of it. Finally, we present more details on the quarter-filled case $n = 1/2$ and on the transition between the pinball and the 200 ordered metal phases.

I. ACCURACY OF THE WAVE FUNCTION

We present in Fig. 1 a comparison between our variational energies and the exact ones, on a small 6×3 lattice size, for the most correlated case, i.e. the commensurate filling $n = 2/3$. Variational energies are calculated by considering an unprojected state $|\mathrm{FS}\rangle$ with three different chemical potentials, as well as Jastrow and backflow corrections. Our data show a remarkably good agreement with the exact diagonalization calculations. Indeed, our accuracy is significantly better than the already good estimate of the ground state energy that was found for the Hubbard model on the half-filled triangular lattice [1] and on the square lattice with nearest and next-nearest neighbor hopping [2].

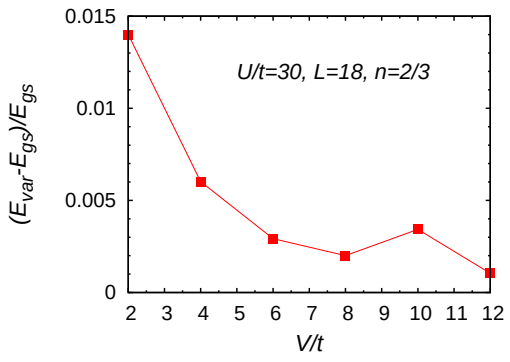

FIG. 1: (Color online) Relative error between the exact energy E_{gs} and the variational estimate E_{var}: $(E_{var} - E_{gs})/E_{gs}$, on a 6×3 lattice size for $U/t = 30$ and $n = 2/3$, as a function of V/t.

II. UNIFORM WAVE FUNCTION

Charge ordered states are a solid feature of the model we consider, since charge order spontaneously appears also when using a uniform chemical potential in the variational wave function. In Fig. 2 we present the phase diagram obtained by using a wave function that does not break the translational invariance, which is in good agreement with the results in the paper, where sublattice dependent chemical potentials were used. The main difference is that the phase transition between ordinary metal and ordered metal requires larger values of the interaction. Our results show that the presence of a (long-range) Jastrow factor $\mathcal{J} = \exp(-1/2 \sum_{ij} v_{ij} n_i n_j)$ in the wave function is sufficient to induce a spontaneous charge order.

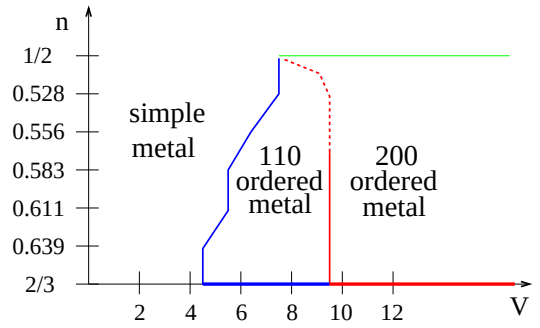

FIG. 2: (Color online) Phase diagram of the Hubbard model for $U = 30t$ as a function of V/t and filling, when using an uniform variational state. The results show a similar phase diagram compared to what has been obtained by using the wave function with three independent chemical potentials. The presence of magnetic order has not been investigated with the uniform variational state.

The presence of long-range charge order is signaled, for instance, by a peak, divergent with the system size L, in the static structure factor $N(q) = \langle n_{-q} n_q \rangle$ at a given momentum Q. In our case, the peak is located at $(4\pi/3, 0)$ thus indicating a tripling of the unit cell, which distinguishes the ordered metal phases from the simple metal one. As shown in Fig. 3 we can clearly observe long range order in the corresponding regions of parameter space, by using a uniform variational state. At commensurate filling the transition to charge order coincides with the metal-insulator transition, as expected.

We would like to remark that the long-range correlations in the Jastrow factor $\mathcal{J} = \exp(-1/2 \sum_{ij} v_{ij} n_i n_j)$ are crucial to describe the 110 charge ordered metal, as

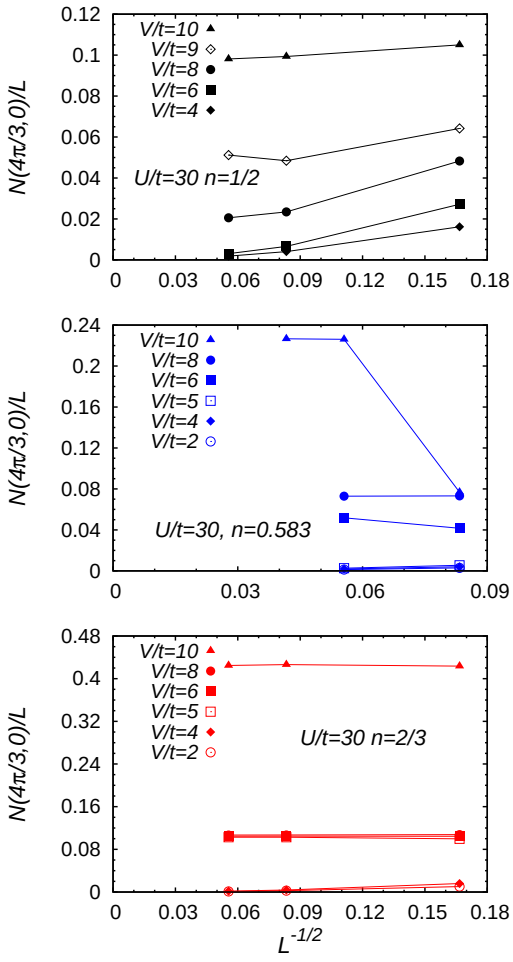

FIG. 3: (Color online) Static structure factor $N(q)$ at the point $(4\pi/3, 0)$, divided by the lattice size L, as a function of $1/\sqrt{L}$ for $U = 30t$ and selected parameters V/t and n.

can be seen by using only a local Gutzwiller term v_{ii} and Jastrow factors up to the third nearest neighbor term. In this case we find that the static structure factor does not exhibit any divergence. This suggests that long-range correlations are crucial to induce a transition from a simple to a charge ordered metal in the model. On the contrary, long-range correlations seem to be not important in the large V/t region, where only the short-range part of the Jastrow factor is sufficient in driving the system into the 200 phase.

III. STATIC STRUCTURE FACTOR

In this section we present the static structure factor $N(q) = \langle n_{-q} n_q \rangle$ for all the q points in the first quarter of the Brillouin zone, within the charge ordered metallic region, see Fig. 4. Analogous results (not shown) can be obtained in the insulating region at commensurate filling. Our data show clearly that there is a peak in

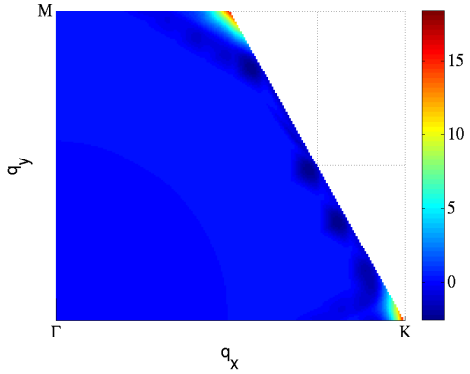

FIG. 4: (Color online) Static structure factor $N(q)$ computed within the charge ordered metallic region at $U/t = 30$, $V/t = 6$, and $n = 0.583$. Results are reported in the first quarter of the Brillouin zone with $\mathbf{\Gamma} = (0, 0)$, $\mathbf{K} = (4\pi/3, 0)$, and $\mathbf{M} = (0, 2\pi/\sqrt{3})$.

the static structure factor located at $\mathbf{K} = (4\pi/3, 0)$, as well as at the equivalent point $\mathbf{K'} = (2\pi/3, 2\pi/\sqrt{3})$. The divergence of the peak with the system size is shown in Fig. 3.

IV. VARIATIONAL CHARGE GAP

A formula for the single-particle charge gap, that is related to the static structure factor $N(q) = \langle n_q n_{-q} \rangle$, has been derived in the Appendix of Ref. [3], by assuming that the exact ground state of the Hubbard model is known. Here we show that the same formula for the charge gap can be obtained when the true ground state is replaced by its optimal variational approximation, as long as the variational state includes a long-range density-density Jastrow factor.

Let us consider the wave function $|\Psi_{\rm FS}\rangle = \mathcal{J}|{\rm FS}\rangle$, where $\mathcal{J} = \exp(-1/2 \sum_{ij} v_{ij} n_i n_j) = \exp(-1/2 \sum_q v_q n_{-q} n_q)$ and $n_q = 1/\sqrt{L} \sum_{r,\sigma} e^{iqr} n_{r,\sigma}$ is the Fourier transform of the particle density, that has been defined in the manuscript. The following condition holds at the variational minimum:

$$\frac{\partial E_{\rm var}}{\partial v_q} = 0 \quad \forall q, \tag{1}$$

where $E_{\rm var} = \frac{\langle \Psi_{\rm FS}|\mathcal{H}|\Psi_{\rm FS}\rangle}{\langle \Psi_{\rm FS}|\Psi_{\rm FS}\rangle}$. From Eq. (1) one derives that

$$\frac{\partial}{\partial v_q} \frac{\langle {\rm FS}|e^{-1/2\sum_q v_q n_{-q} n_q} \mathcal{H} e^{-1/2\sum_q v_q n_{-q} n_q}|{\rm FS}\rangle}{\langle {\rm FS}|e^{-1/2\sum_q v_q n_{-q} n_q} e^{-1/2\sum_q v_q n_{-q} n_q}|{\rm FS}\rangle} = 0$$

$$-\frac{1}{2}\left[\langle \mathrm{FS}|e^{-1/2\sum_q v_q n_{-q} n_q} n_{-q} n_q \mathcal{H} e^{-1/2\sum_q v_q n_{-q} n_q}|\mathrm{FS}\rangle + \langle \mathrm{FS}|e^{-1/2\sum_q v_q n_{-q} n_q} \mathcal{H} n_{-q} n_q e^{-1/2\sum_q v_q n_{-q} n_q}|\mathrm{FS}\rangle\right]\langle \Psi_{\mathrm{FS}}|\Psi_{\mathrm{FS}}\rangle$$
$$+\langle \Psi_{\mathrm{FS}}|\mathcal{H}|\Psi_{\mathrm{FS}}\rangle\langle \Psi_{\mathrm{FS}}|n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle = 0$$

$$\frac{\langle \Psi_{\mathrm{FS}}|\mathcal{H}|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|\Psi_{\mathrm{FS}}\rangle} = \frac{1}{2}\left[\frac{\langle \Psi_{\mathrm{FS}}|n_{-q}n_q\mathcal{H}|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle} + \frac{\langle \Psi_{\mathrm{FS}}|\mathcal{H}n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle}\right]. \quad (2)$$

The variational charge gap E_q between the variational approximation of the ground state $|\Psi_{\mathrm{FS}}\rangle$ and its excited state $|\Psi_q\rangle = n_q|\Psi_{\mathrm{FS}}\rangle$ can then be written as:

$$E_q = \frac{\langle \Psi_q|\mathcal{H}|\Psi_q\rangle}{\langle \Psi_q|\Psi_q\rangle} - \frac{\langle \Psi_{\mathrm{FS}}|\mathcal{H}|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|\Psi_{\mathrm{FS}}\rangle} = \frac{1}{2}\left[\frac{\langle \Psi_{\mathrm{FS}}|n_{-q}[n_q,\mathcal{H}]|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle} + \frac{\langle \Psi_{\mathrm{FS}}|[n_{-q},\mathcal{H}]n_q|\Psi_{\mathrm{FS}}\rangle}{\langle \Psi_{\mathrm{FS}}|n_{-q}n_q|\Psi_{\mathrm{FS}}\rangle}\right],$$

where the result of Eq. (2) has been used.

Then, our calculation shows that Eq. (B1) in Ref. [3], that is at the basis of the derivation of the charge gap, can be obtained also when the exact ground state $|\Psi\rangle$ is replaced by a variational approximation of it, namely $|\Psi_{\mathrm{FS}}\rangle$, as long as the variational state includes a long-range density-density Jastrow factor.

V. $n = 1/2$ CASE

The main feature of the quarter-filled $n = 1/2$ case is the transition around $V/t = 5.5$ between a simple uniform metal and a charge ordered one with higher occupation on sublattice A and reduced occupation on sublattices B and C. However, two different phases with charge order can be further distinguished, as indicated in Fig. 5.

Between $V/t = 5$ and $V/t \approx 10$ the occupation of sublattice A increases as a function of V/t, while sublattices B and C are progressively depleted. However, as confirmed by the fact that the total density of double occupancies $D = \frac{1}{L}\sum_i n_{i,\uparrow}n_{i,\downarrow}$ remains small and almost constant, the sublattice A is only singly occupied and a still large fraction of electrons resides on the sublattices B and C. This phase corresponds to the pinball liquid introduced by Hotta and Furukawa [4, 5].

By increasing the ratio V/t to values larger than 10, there is a sudden increase in the occupation of sublattice A as well as in the density of double occupancies. At $V/t = 15$, the saturation plateau has been substantially reached with almost all the electrons located on sublattice A with $n_A = 1.5$. This phase has not been considered by the spinless model of Hotta and Furukawa and it has been named 3CO in Refs. [6, 7].

Note that all the phases at quarter filling are always metallic, as indicated in Fig. 6. Indeed, even at $V/t = 15$, the tiny fraction of electrons on sublattices B and C leads to a metallic behavior.

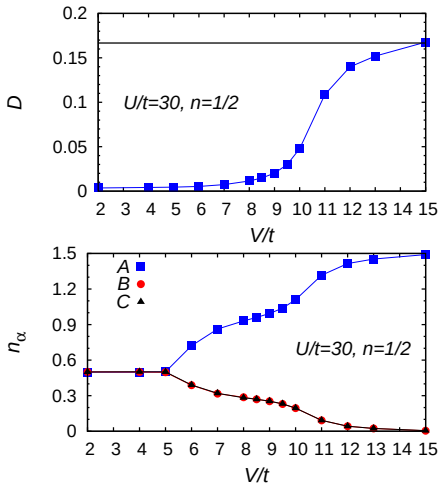

FIG. 5: (Color online) Lower panel: Electronic density n_α in each of the three sublattices A, B, and C as a function of V/t at quarter filling $n = 1/2$. Upper panel: Density of double occupancies D as a function of V/t at quarter filling $n = 1/2$. The black horizontal line represents the density of double occupancies when exactly half of the sites on sublattice A is doubly occupied. In both panels, the on-site Coulomb repulsion is $U = 30t$ and the lattice size is $L = 324$.

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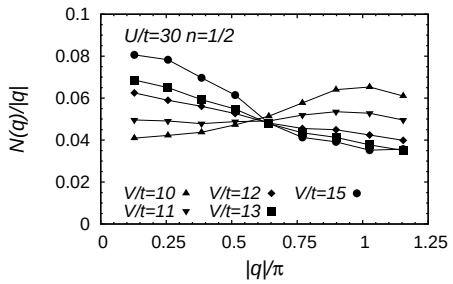

FIG. 6: (Color online) $N(q)/q$ as a function of $|q|/\pi$ between $V/t = 10$ and $V/t = 15$ at quarter filling $n = 1/2$. Data are shown along the path in the Brillouin zone connecting the point $\mathbf{M} = (0, 2\pi/\sqrt{3})$ to the point $\mathbf{\Gamma} = (0, 0)$. The on-site Coulomb repulsion is $U = 30t$ and data refer to the $L = 342$ case.

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