Critical behavior of the extended Hubbard model with bond dimerization

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ABSTRACT

Exploiting the matrix-product-state based density-matrix renormalization group (DMRG) technique we study the one-dimensional extended (U-V) Hubbard model with explicit bond dimerization in the half-filled band sector. In particular we investigate the nature of the quantum phase transition, taking place with growing ratio V/U between the symmetry-protected-topological and charge-density-wave insulating states. The (weak-coupling) critical line of continuous Ising transitions with central charge $c = 1/2$ terminates at a tricritical point belonging to the universality class of the dilute Ising model with $c = 7/10$. We demonstrate that our DMRG data perfectly match with (tricritical) Ising exponents, e.g., for the order parameter $\beta = 1/8$ (1/24) and correlation length $\nu = 1$ (5/9). Beyond the tricritical Ising point, in the strong-coupling regime, the quantum phase transition becomes first order.

1. Introduction

Half a century has passed since it was proposed, yet the Hubbard model [1] is still a key Hamiltonian for the investigation of strongly correlated electron systems. Originally designed to describe the ferromagnetism of transition metals, in successive studies the Hubbard model has also been used for heavy fermions and high-temperature superconductors. The physics of the model is governed by the competition between the itinerancy of the charge carriers and their local Coulomb interaction. In one dimension (1D), seen from a theoretical point of view, the Hubbard model is a good starting point to explore, for example, Tomonaga-Luttinger liquid behavior (including spin-charge separation).

While the 1D Hubbard model is exactly solvable by Bethe Ansatz [2], most of its extensions are no longer integrable. This is even true if only the Coulomb interaction between electrons on nearest-neighbor lattice sites is added. The ground-state phase diagram of this so-called extended Hubbard model (EHM) is still a hotly debated issue. At half filling, this relates in particular to the recently discovered bond-order-wave (BOW) state located in between spin-density-wave (SDW) and charge-density-wave (CDW) phases [3,4]. To characterize the BOW state and determine its phase boundaries considerable efforts were undertaken in the last few years, using both analytical [5,6] and numerical [7–9] methods.

At present, quantum phase transitions between topologically trivial and nontrivial states arouse great interest [10–12]. In this context,

extensions of the half-filled EHM also attracted attention, mainly with regard to the formation of symmetry-protected-topological (SPT) states [11]. Including an alternating ferromagnetic spin interaction [13] or an explicit dimerization [14] in the EHM, the SDW and BOW phases are completely replaced by an SPT insulator, whereby a quantum phase transition occurs between the SPT and the CDW, the area of which shrinks. Most interestingly, the SPT-CDW continuous Ising transition with central charge $c = 1/2$ ends at a tricritical point, belonging to the universality class of the tricritical Ising model, a second minimal model with $c = 7/10$ [15,16]. Above this point, the quantum phase transition becomes first order. In Ref. [14] it has been demonstrated that the transition region of the EHM with bond dimerization can be described by the triple sine-Gordon model by extending the former bosonization analysis [17]. The predictions of field theory regarding power-law (exponential) decay of the density-density (spin-spin) and bond-order correlation functions are shown to be in excellent accordance with the numerical data obtained by a matrix-product-states (MPS) based density-matrix renormalization group (DMRG) technique [18,19].

The Ising criticality of the EHM with explicit dimerization was established in early work [17] that also specifies the critical exponents. The critical exponents at the tricritical point should differ from those at the ordinary Ising transition because the tricritical Ising quantum phase transition belongs to a different universality class.

Simulating the neutral gap and the CDW order parameter by DMRG, in this paper we will determine the critical exponents at both Ising and tricritical Ising transitions. The paper is structured as follows.

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2. Model

2.1. Extended Hubbard model

The Hamiltonian of the EHM is defined as

$$
\begin{aligned}
\widehat{H}_{\text{EHM}} = & -t \sum_{j\sigma} (\hat{c}^{\dagger}_{j\sigma} \hat{c}_{j+1\sigma} + \text{H. c. }) \\
& + U \sum_{j} \left(\hat{n}_{j\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{j\downarrow} - \frac{1}{2}\right) \\
& + V \sum_{j} (\hat{n}_j - 1)(\hat{n}_{j+1} - 1),
\end{aligned}
\tag{1}
$$

where $\hat{c}^{\dagger}_{j\sigma}$ ($\hat{c}_{j\sigma}$) creates (annihilates) an electron with spin projection $\sigma = \uparrow, \downarrow$ at Wannier site j, $\hat{n}_{j\sigma} = \hat{c}^{\dagger}_{j\sigma}\hat{c}_{j\sigma}$, and $\hat{n}_j = \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}$. In the Hubbard model limit ($V = 0$), at half-filling, no long-range order exists. Instead the system shows fluctuating SDW order. The spin (charge) excitations are gapless (gapped) $\forall \, U > 0$ [2]. At finite V, for $V/U \lesssim 1/2$, the ground state is still a SDW. When V/U becomes larger than $1/2$ a $2 k_F$-CDW is formed. As pointed out first by Nakamura [3,4] and confirmed later by various analytical and numerical studies [8,9,20,21], the SDW and CDW phases are separated by a narrow BOW phase below the critical end point, $(U^{\text{EHM}}_{\text{ce}}, V^{\text{EHM}}_{\text{ce}}) \approx (9.25t, 4.76t)$. In the BOW phase translational symmetry is spontaneously broken, which implies that the spin gap opens passing the SDW-BOW phase boundary at fixed $U < U^{\text{EHM}}_{\text{ce}}$. Increasing V further, the system enters the CDW phase with finite spin and charge gaps. The BOW-CDW Gaussian transition line with central charge $c = 1$ terminates at the tricritical point, $(U^{\text{EHM}}_{\text{tr}}, V^{\text{EHM}}_{\text{tr}}) \approx (5.89t, 3.10t)$ [9]. For $U^{\text{EHM}}_{\text{tr}} < U < U^{\text{EHM}}_{\text{ce}}$, the BOW-CDW transition becomes first order, characterized by a jump in the spin gap (see, Fig. 3 in Ref. [9]). Fig. 1 summarizes the rich physics of the half-filled EHM.

The criticality at the continuous BOW-CDW transition line can be verified numerically by extracting, e.g., the central charge from the correlation length (ξ_{χ}) and von Neumann entropy (S_{χ}), where ξ_{χ} can be obtained from the second largest eigenvalue of the transfer matrix for some bond dimension χ used in a infinite DMRG (iDMRG) simulation [19,22]. Conformal field theory tells us that the von Neumann entropy for a system between two semi-infinite chains is [23]

$$
S_{\chi} = \frac{c}{6} \ln \xi_{\chi} + s_0
\tag{2}
$$
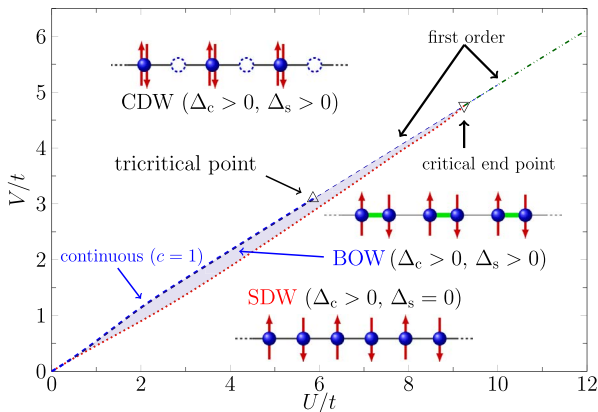
Fig. 1. DMRG ground-state phase diagram of the 1D EHM (1) at half filling [9]. The red dotted line gives the continuous SDW-BOW transition. The bold (thin) blue dashed line marks the continuous (first-order) BOW-CDW transition and the green dashed-dotted line denotes the first-order SDW-CDW transition. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
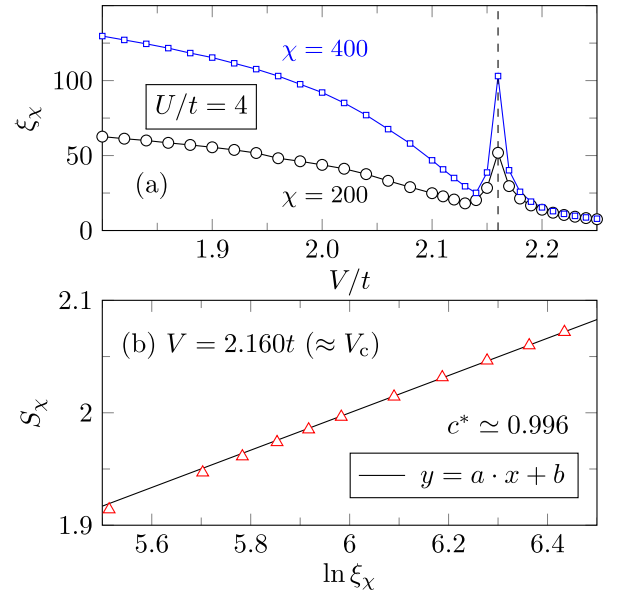
Fig. 2. (a): Correlation length ξ_{χ} of the EHM as a function of V/t for $U/t = 4$ obtained from iDMRG. The dashed line indicates the BOW-CDW transition point. (b): von Neumann entropy S_{χ} as a function of logarithm of ξ_{χ} at $V \approx V_c$ for $U/t = 4$. The iDMRG data for $\ln \xi_{\chi} > 6$ ($\chi \geq 1800$) provide us the numerically obtained central charge $c^* \simeq 0.996$ by fitting to Eq. (2).

with a non-universal constant s_0.

Fig. 2(a) shows iDMRG results of ξ_{χ} as a function of V/t for fixed $U/t = 4$. Since the system is critical in the SDW phase and at the BOW-CDW transition point, we find a rapid increase of ξ_{χ} in the SDW phase and a distinct peak at the BOW-CDW critical point ($V_c/t \approx 2.160$) when we increase χ from 200 to 400. This indicates the divergence of the correlation length $\xi_{\chi} \to \infty$ as $\chi \to \infty$. Now, plotting the von Neumann entropy S_{χ} as a function of $\ln \xi_{\chi}$ and fitting the graph to Eq. (2), the criticality at $V = V_c$ can be proved, as demonstrated by Fig. 2(b). The obtained $c^* \simeq 0.996$ for iDMRG data with $\chi \geq 1800$ corroborates the Gaussian transition resulting from a bosonization analysis [5,6]. Note that for the confirmation of the SDW-BOW transition much larger bond dimensions χ are required in order to make clear the convergence of ξ_{χ} in the BOW phase of Fig. 2.

2.2. EHM with explicit bond dimerization

Let us now add a staggered bond dimerization to the EHM, $\widehat{H} = \widehat{H}_{\text{EHM}} + \widehat{H}_{\delta}$, where

$$
\widehat{H}_{\delta} = -t \sum_{j\sigma} \delta (-1)^j (\hat{c}^{\dagger}_{j\sigma} \hat{c}_{j+1\sigma} + \text{H. c. }).
\tag{3}
$$

Previous studies of this model have shown that the low lying excitations in the large-U limit are chargeless spin-triplet and spin-singlet excitations [24–30], whereby the dynamics is described by an effective spin-Peierls Hamiltonian. Moreover, at finite U, the Tomonaga-Luttinger parameters have been explored at and near commensurate fillings by DMRG [31]. Particularly for half filling, it has been proven by perturbative [32,33] and renormalization group [6,34,35] approaches that the system realizes Peierls insulator (PI) and CDW phases in the weak-coupling regime. According to weak-coupling renormalization-group results [6], any finite bond dimerization δ will change the universality class of the continuous BOW-CDW transition (realized in the pure EHM) from Gaussian to Ising type. Thereby the PI-CDW transition in the weak-to-intermediate coupling regime belongs to the universality class of the two-dimensional (2D) Ising model [6,17].

Even more interesting physics appears analyzing the intermediate-to-strong-coupling regime [14] by analogy with an effective spin-1
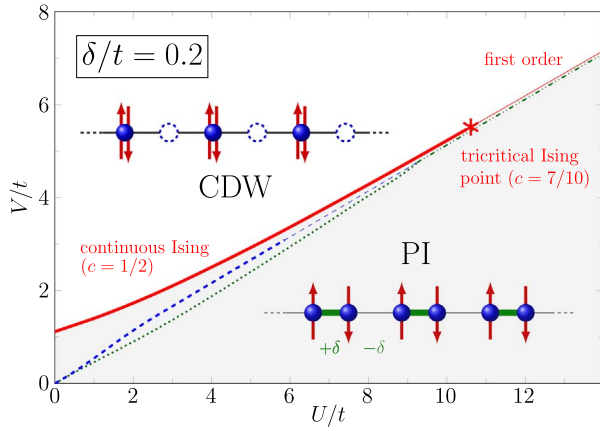
Fig. 3. Ground-state phase diagram of the 1D EHM with bond dimerization in the half-filled band sector [14]. The red solid line marks the PI-CDW phase boundaries for $\delta/t = 0.2$. The tricritical Ising point $[U_{tr}, V_{tr}]$ separates continuous Ising and first-order phase transitions. For comparisons, the phase boundaries of the pure EHM ($\delta = 0$) were included. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

(EHM) system with alternating ferromagnetic spin interaction [13]: Here the continuous PI-CDW Ising transition line with central charge $c = 1/2$ terminates at a tricritical point that belongs to the universality class of the 2D dilute Ising model with $c = 7/10$. Above the tricritical Ising point the quantum phase transition becomes first order. Displaying the ground-state phase diagram, Fig. 3 summarizes these results. A field theoretical description of the tricritical transition region has been performed in terms of a triple sine-Gordon model [14], based on the bosonization analysis in Ref. [17], providing results for the decay of various correlation functions, such as the density-density, bond-order or spin-spin two-points functions. The predictions of field theory are in excellent agreement with iDMRG data.

3. Critical exponents

In the following, we give further evidence for the Ising respectively the tricritical Ising universality classes of the quantum phase transitions in the EHM with bond dimerization by calculating the critical exponents of various physical quantities. When approaching a continuous phase transition by varying a parameter (e.g., a coupling strength) g of the Hamiltonian, the correlation length diverges as

$$\xi \propto |g - g_c|^{-\nu} . \tag{4}$$

Here, g_c denotes the (critical) value of g at the transition point and ν is the corresponding critical exponent. Other quantities such as the order parameters or energy gaps also show power-law behavior. In this way the system is characterized by a set of universal exponents near the continuous phase transitions. The exact values of the most common exponents for the 2D Ising and tricritical Ising universality classes are listed in Table 1.

The exponents satisfy the following scaling relation

$$\frac{\nu}{2}(\eta + d - 2) = \beta, \tag{5}$$

Table 1
Critical exponents belonging to the Ising and tricritical Ising universality classes in 2D [36–38]. The critical exponent η for the pair correlation function has been confirmed in Ref. [14].

Quantity	Exponent	Ising	tricritical Ising
Magnetization	β	1/8	1/24
Correlation length	ν	1	5/9
Pair correlation	η	1/4	3/20

where d is the spatial dimension (in our case d = 2).

For the EHM with bond dimerization, β and ν can be extracted from the CDW order parameter and the neutral gap, respectively. The CDW order parameter is defined as

$$m_{CDW} = \frac{1}{L} \sum_j (-1)^j (\hat{n}_j - 1). \tag{6}$$

The neutral gap is obtained from

$$\Delta_n(L) = E_1(N) - E_0(N), \tag{7}$$

where $E_0(N)$ [$E_1(N)$] denotes the energy of the ground state [first excited state] of a system with L sites, N electrons, and vanishing total spin z component.

3.1. Ising transition

We now show that the critical exponents $\beta = 1/8$ and $\nu = 1$ follow from (i)DMRG simulations by varying V at fixed U and δ, just as the corresponding phase transition line was obtained in Fig. 3. Note that $\beta = 1/8$ and $\nu = 1$ were extracted in Ref. [17] by means of the DMRG method, varying δ for fixed U and V.

Fig. 4 gives the CDW order parameter as a function of V/t, fixing $U/t = 4$ and $\delta/t = 0.2$, calculated by iDMRG technique with bond dimensions $\chi = 800$. Obviously, in the CDW (PI) realized for $V > V_c$ ($V < V_c$), $|m_{CDW}|$ is finite (zero). Using $V_c/t \approx 2.5035$, the iDMRG data are well fitted by $(V - V_c)^\beta$ near the transition, where the critical exponent $\beta = 1/8$ can be easily read off from a log-log plot; see inset of Fig. 4.

Extrapolating the values of the neutral gap Δ_n to the thermodynamic limit, the critical exponent $\nu = 1$ is verified, as demonstrated by Fig. 5. Increasing V at fixed $U/t = 4$, the neutral gap decreases linearly and closes at the Ising transition point. If V grows further, Δ_n opens again with linear slope. This is clearly visible in the log-log plots representation, both for $V > V_c$ and $V < V_c$; see Fig. 5(b).

### 3.2. Perturbed tricritical Ising model

As quoted above and demonstrated in Ref. [14], the tricritical point in the EHM with bond dimerization belongs to the universality class of the 2D tricritical Ising model with the critical exponents given in Table 1. Let us emphasize that it is exceptionally challenging to verify the critical exponents at the tricritical Ising point numerically, not least because one first has to determine the tricritical point itself, with high precision, varying U and V simultaneously [14].

The exponent η characterizes the power-law decay of the CDW order-parameter two-point function at the critical point. As shown in Ref. [14] one has
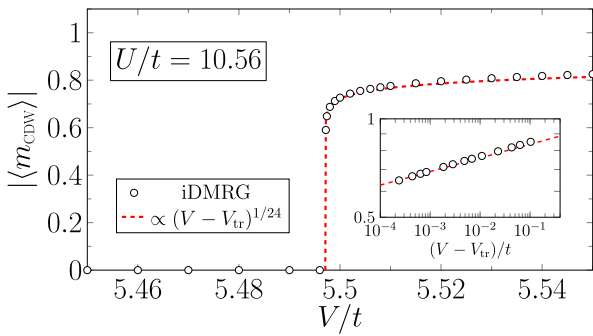
$$\langle (-1)^\ell (\hat{n}_{j+\ell} - 1)(\hat{n}_j - 1) \rangle \propto \ell^{-3/20}, \quad \ell \gg 1. \tag{8}$$
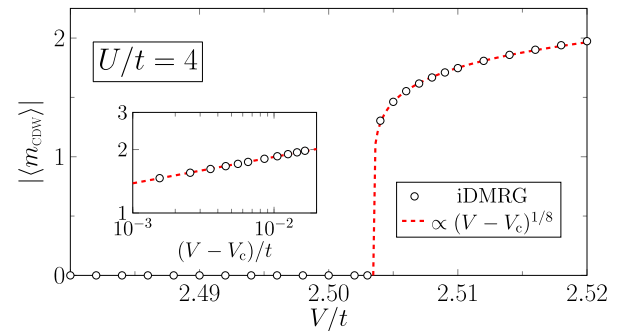
Fig. 4. Absolute value of the CDW order parameter in the vicinity of the Ising transition at fixed $U/t = 4$. Symbols are iDMRG data; the dashed line displays the fitting function $|\langle m_{CDW} \rangle| \propto (V - V_{tr})^\beta$ with critical exponent $\beta = 1/8$ (Ising universality class). Inset: Log-log plot of the order parameter for $V > V_{tr}$ demonstrating the power-law decay with exponent β.
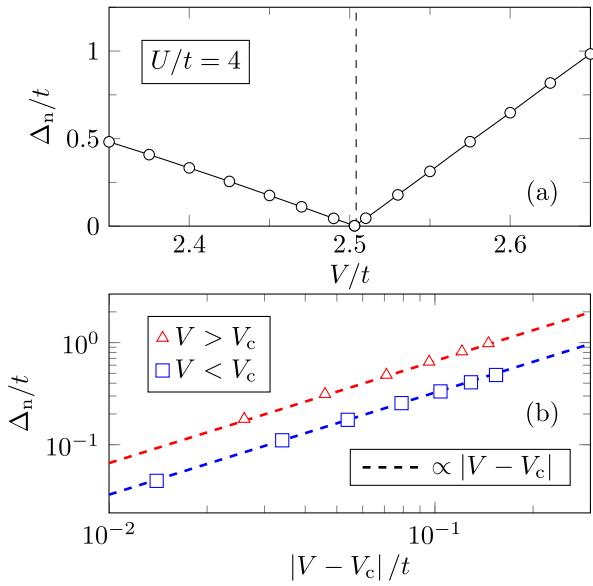
Fig. 5. (a): Neutral gap Δ_n near the Ising transition at fixed $U/t = 4$ (symbols are DMRG data taken from Ref. [14]). (b): Log-log plots of Δ_n as a function of $|V - V_c|$, fitted by $|V - V_c|^\nu$ with $\nu = 1$ (Ising universality class).

Fig. 6. Absolute value of the CDW order parameter in the vicinity of the tricritical Ising point at fixed $U/t = 10.56$. Symbols are iDMRG data; the dashed line displays the fitting function $|\langle m_{CDW} \rangle| \propto (V - V_{tr})^\beta$ with critical exponent $\beta = 1/24$ (tricritical Ising universality class). Inset: Log-log plot of the order parameter for $V > V_{tr}$ demonstrating the power-law decay with exponent β.

This establishes that $\eta = 3/20$. In order to determine the exponents β and ν one needs to consider the off-critical regime. We therefore consider the perturbation of the tricritical Ising conformal field theory by the "energy operator" $\epsilon(x)$, which has conformal dimensions $(\Delta_\epsilon, \overline{\Delta}_\epsilon) = (\frac{1}{10}, \frac{1}{10})$ [36–38]

$$H = H_{CFT} + h \int dx \, \epsilon(x). \tag{9}$$

The perturbing operator has scaling dimension $d = 1/5$ and is therefore relevant in the renormalization group (RG) sense. It generates a spectral gap M that scales as

$$M \sim Ch^{1/(2-d)} = Ch^{5/9}, \tag{10}$$

where C is a constant. This identifies the critical exponent $\nu = 5/9$. The magnetization operator $\sigma(x)$ in the tricritical Ising model has scaling dimension $(\Delta_\sigma, \overline{\Delta}_\sigma) = (\frac{3}{80}, \frac{3}{80})$. In the perturbed theory (9) it acquires a non-zero expectation value that scales as

$$\langle \sigma(x) \rangle \sim Dh^{\Delta_\sigma/(1-\Delta_\epsilon)} = Dh^{1/24}, \tag{11}$$

where D is a constant. This identifies the critical exponent $\beta = 1/24$.

The predictions of perturbed conformal field theory for β and ν can be checked against numerical computations as follows. Fixing $U = 10.56t$ ($\simeq U_{tr}$), we first give the iDMRG results for the CDW order
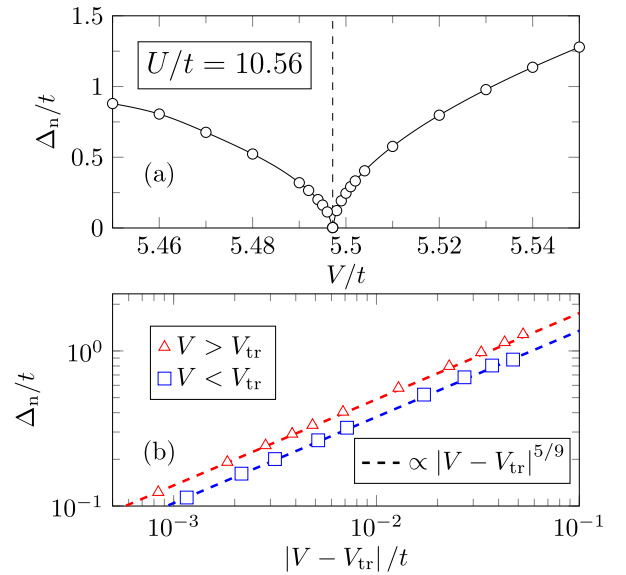
Fig. 7. (a): DMRG data for the neutral gap Δ_n in the vicinity of the tricritical Ising point where $U/t = 10.56$. (b): Log-log plots of Δ_n as a function of $|V - V_{tr}|$, fitted by $|V - V_{tr}|^\nu$ with $\nu = 5/9$ (tricritical Ising universality class).

parameter $|\langle m_{CDW} \rangle|$ as a function of V, cf. Fig. 6. Just as in the case of the Ising universality class, $|\langle m_{CDW} \rangle|$ is finite (zero) for $V > V_{tr}$ ($V < V_{tr}$). The order parameter $|\langle m_{CDW} \rangle|$ now vanishes much more abruptly approaching the quantum phase transition point from above. Fitting the iDMRG data for $V > V_{tr}$ to $(V - V_{tr})^\beta$ with $V_{tr}/t \approx 5.497$ and $\beta = 1/24$ works perfectly, see the log-log representation Fig. 7.

In order to verify the field theory prediction for ν we examine the $L \to \infty$ extrapolated values of the neutral gap Δ_n. Increasing $V(<V_{tr})$ at fixed $U/t = 10.56$, Δ_n is reduced but not linearly as in the Ising case (cf. Fig. 4), and closes at $V \approx V_{tr}$ before it becomes finite again for $V > V_{tr}$. Again the log-log representation can be used to extract the critical exponent for $|V - V_{tr}|^\nu$, $\nu = 5/9$, for both $V < V_{tr}$ and $V > V_{tr}$, in conformity with the tricritical Ising universality class.

4. Summary

To conclude, we have investigated the criticality of the 1D half-filled extended Hubbard model (EHM) with explicit dimerization δ. The BOW-CDW Gaussian transition with central charge $c = 1$ of the pure EHM gives way to an Ising transition with $c = 1/2$ at any finite δ. The Ising transition line terminates at a tricritical point, which belongs to the universality class of the tricritical Ising model in two dimensions. The change of the universality class is verified numerically by (i)DMRG (see also [14]). Furthermore, we demonstrate that not only the Ising but also the tricritical Ising critical exponents β and ν can be obtained with high accuracy by simulating the CDW order parameter and the neutral gap.

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