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EPL, **84** (2008) 57001

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December 2008

EPL, **84** (2008) 57001 www.epljournal.org
doi: 10.1209/0295-5075/84/57001

Metallicity in the half-filled Holstein-Hubbard model

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received 6 August 2008; accepted in final form 21 October 2008
published online 24 November 2008

PACS 71.30.+h – Metal-insulator transitions and other electronic transitions
PACS 71.10.Hf – Non-Fermi-liquid ground states, electron phase diagrams and phase transitions in model systems
PACS 71.38.-k – Polarons and electron-phonon interactions

Abstract – We re-examine the Peierls insulator to Mott insulator transition scenario in the one-dimensional Holstein-Hubbard model where, at half-filling, electron-phonon and electron-electron interactions compete for establishing charge- and spin-density-wave states, respectively. By means of large-scale density-matrix renormalization group calculations we determine the spin, single-particle and two-particle excitation gaps and prove —in the course of a careful finite-size scaling analysis— recent claims for an intervening metallic phase in the weak-coupling regime. We show that for large phonon frequencies the metallic region is even more extended than previously expected, and subdivided into ordinary Luttinger-liquid and bipolaronic-liquid phases.

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The challenge of understanding the subtle interplay of electron-electron and electron-phonon interaction effects in low-dimensional condensed-matter systems, such as conjugated polymers, charge transfer salts, inorganic spin-Peierls compounds, halogen-bridged transition metal complexes, ferroelectric perovskites, or organic superconductors [1–4], has stimulated intense work on generic fermion/spin-boson models. In this respect the one-dimensional (1D) Holstein[1]-Hubbard[2] model (HHM) is particularly rewarding to study [5–14]. It accounts for a tight-binding electron band, an intra-site Coulomb repulsion between electrons of opposite spin, a local coupling of the charge carriers to optical phonons, and the energy of the phonon subsystem in harmonic approximation:

$$H = -t\sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} - \sqrt{\varepsilon_{\rm p}\omega_0}\sum_{i\sigma}(b^\dagger_i + b_i)n_{i\sigma} + \omega_0\sum_i b^\dagger_i b_i\,. \qquad (1)$$

In eq. (1), $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$, where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) a spin-σ electron at the Wannier site i of a 1D lattice with N sites, and $b^\dagger_i$ (b_i) are the corresponding bosonic operators for a dispersionless phonon with frequency ω_0.

The physics of the HHM is governed by three competing effects: the itinerancy of the electrons ($\propto t$), their on-site Coulomb repulsion ($\propto U$), and the local electron-phonon (EP) coupling ($\propto \varepsilon_{\rm p}$). Since the EP interaction is retarded, the phonon frequency (ω_0) defines a further relevant energy scale. Hence one is advised to introduce besides the adiabaticity ratio,

$$\alpha = \omega_0/t\,, \qquad (2)$$

two dimensionless coupling constants:

$$u = U/4t, \quad \text{and} \quad g^2 = \varepsilon_{\rm p}/\omega_0 \quad \text{or} \quad \lambda = \varepsilon_{\rm p}/2t\,. \qquad (3)$$

Both Holstein and Hubbard interactions tend to immobilize the charge carriers, and even may drive a metal-insulator transition at commensurate band fillings. For the half-filled band case (one electron per lattice site), most previous analytical and numerical studies of the HHM reveal that Peierls insulator (PI) or Mott insulator (MI) states are favored over the metallic state at zero temperature. Whereas the PI is characterized by a distortion of the underlying lattice accompanied by dominant charge-density-wave (CDW) correlations, the Mott insulator is basically a spin-density-wave (SDW) state without

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[1] The Holstein model (cf. Holstein T., *Ann. Phys. (N.Y.)*, **8** (1959) 325; 343) has been studied extensively as a paradigmatic model for polaron formation in the low-density limit. For commensurate band fillings the coupling to the lattice supports charge ordering.

[2] The Hubbard model (cf. Hubbard J., *Proc. R. Soc. London, Ser. A*, **276** (1963) 238), originally designed to describe ferromagnetism of transition metals, has more recently been used as the probably most simple model to account for strong Coulomb correlation effects in a great variety of materials.

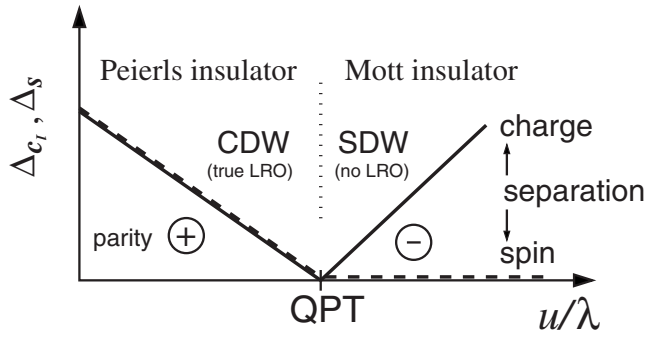

Fig. 1: Schematic representation of the Peierls insulator to Mott insulator quantum phase transition at fixed λ and α in the strong-coupling small-to-intermediate phonon-frequency regime of the 1D half-filled Holstein-Hubbard model. The PI exhibits long-range order (LRO) because a discrete symmetry is broken; the SDW MI has continuous symmetry, *i.e.* there is no LRO in 1D. Δ_s (dashed line) and Δ_{c_1} (solid line) denote the spin and charge excitation gap, respectively. For finite periodic chains with $N=4n$, the transition could be identified by a ground-state level crossing associated with a change in the parity eigenvalue $P=\pm 1$, where the site inversion symmetry operator P is defined by $Pc^\dagger_{i\sigma}P^\dagger = c^\dagger_{N-i+1\sigma}$ (cf. refs. [5,15]).

any lattice dimerization. The physical excitations differ accordingly: while "normal" electron-hole excitations are expected in the PI phase, charge (spin) excitations are known to be massive (gapless) in the MI state, at least for the 1D Hubbard-only model. Thus, varying the control parameter u/λ, a cross-over from standard quasi-particle behavior to spin-charge separation might be observed in the more general HHM (see fig. 1). This scenario has been corroborated by extensive Lanczos diagonalization and density-matrix renormalization group (DMRG) studies [5, 7,16]. In particular the existence of a single quantum critical point, separating Peierls- and Mott-insulating phases at $u/\lambda \simeq 1$, has been confirmed by up-to-date stochastic series expansion (SSE) quantum Monte Carlo (QMC) calculations [12]. But this only holds in the *strong-coupling* and *adiabatic-to-intermediate phonon-frequency* regime.

For the pure (spinless and spinful) Holstein model it is well known that quantum phonon fluctuations may destroy the Peierls phase, provided the EP interaction is not too strong [17–22]. In this case, a Luttinger liquid phase exists below a critical coupling g_c, where $\lambda_c \to 0$ as $\alpha \to 0$ (see footnote [3]). For this reason, it is natural to examine the stability of such a metallic state as the Coulomb interaction is turned on. (We call metal any phase with gapless charge excitations.) An intervening metallic phase would of course prevent a direct insulator-to-insulator transition. Recent numerical investigations of the 1D HHM, based on variable-displacement Lang-Firsov [6], DMRG [9,11], and SSE QMC [8,12] approaches, give strong evidence that the CDW-SDW transition does indeed split into two subsequent CDW-metal and metal-SDW transitions in the *weak-coupling intermediate-to-large phonon-frequency* regime[4]. To map out the phase diagram is technically challenging, however, since the energy scales are not well separated in this region. Furthermore, it is not obvious which physical quantities are most suitable to distinguish the various phases. In this respect, local magnetic moment and effective electronic hopping integral [6], charge-, spin- and (superconducting) pairing-correlation functions [9], or Luttinger liquid parameter [8] and charge/spin susceptibilities [12] have been proposed.

In this work our analysis of the weak-to-intermediate coupling regime of the 1D HHM is based on the behavior of various spin and charge excitation gaps. These many-body gaps can be calculated by DMRG with high precision on a sequence of sufficiently large lattices. This allows for a reliable finite-size scaling of the gap data using their expected asymptotic behavior $\Delta(N) = \Delta(\infty) + b/N + c/N^2$ for $N \gg 1$. A detailed description of our fermion-boson DMRG pseudo-site method (which treats electron and phonon degrees of freedom on an equal footing in the whole parameter regime) can be found in ref. [26]. In the numerical work we use typically 3–5 bosonic pseudosites and employ open boundary conditions (OBC).

The charge and spin excitation gaps are determined from

$$\Delta_{c_1} = E_0^+(1/2) + E_0^-(-1/2) - 2E_0(0) \tag{4}$$

and

$$\Delta_s = E_0(1) - E_0(0)\,, \tag{5}$$

respectively, where $E_0^{(\pm)}(S^z)$ is the ground-state energy at (away from) half-filling with $N_e = N$ ($N_e = N \pm 1$) particles in the sector with total spin-z component S^z. In the various phases expected to occur in the 1D HHM Δ_s corresponds to the energy of the lowest spin excitation (spin gap). The one-particle gap Δ_{c_1} yields the energy of the lowest charge excitation (charge gap) in the Peierls band insulator, Luttinger liquid, and Mott insulator phases and is an upper limit for this charge gap in any other phase. Note that since we compare ground-state energies when calculating the charge and spin gaps, lattice relaxation effects arising from different particle numbers are included.

Searching for metallicity in the HHM, we first consider the *anti-adiabatic regime* ($\alpha = 5$), because large phonon frequencies will clearly act against any static Peierls ordering. Figure 2 shows the scaling of Δ_{c_1} and Δ_s with system size N as the EP coupling λ is lowered at fixed Coulomb interaction $u = 0.25$. For large λ there is a CDW made up of "singlet bipolarons", *i.e.* a bipolaronic superlattice. Since the bipolarons that emerge are rather small objects, the finite-size dependencies of Δ_{c_1} and Δ_s are weak. This is just as in the strong-coupling non-too-anti-adiabatic regime [27] (cf. also fig. 11 in ref. [16]).

[3] The metal-insulator transition at g_c is expected to be of Kosterlitz-Thouless type, at least for $\omega_0 \to \infty$ (cf. refs. [23], and [24]).

[4] A intermediate metallic phase has been shown to exist also for the $D = \infty$ HHM (see, *e.g.*, ref. [25] and references therein).

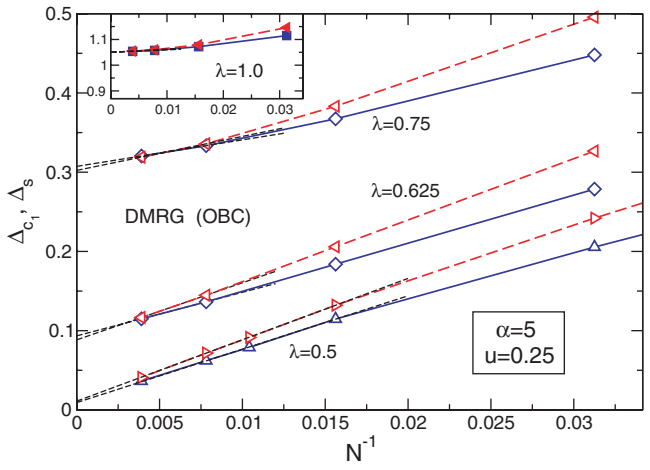

Fig. 2: (Color online) Finite-size scaling of spin (left and right triangles; red dashed lines) and charge (diamonds, triangles up, circles; blue solid lines) excitation gaps in the 1D HHM with OBC. Filled (open) symbols belong to insulating (metallic) states, see fig. 4.

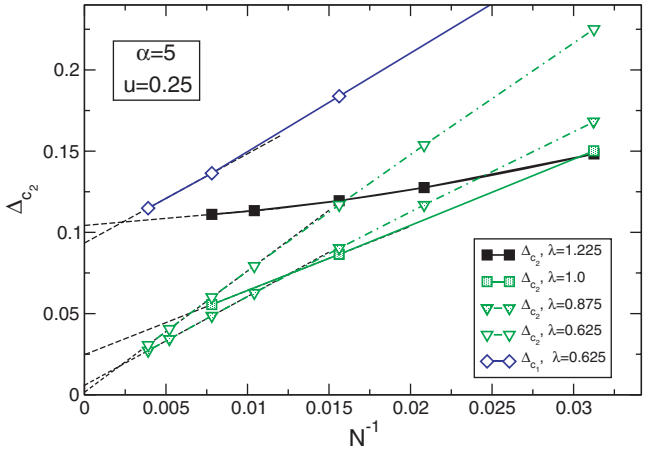

Fig. 3: (Color online) Finite-size scaling of the two-particle excitation gap Δ_{c_2} in the HHM. For comparison we include Δ_{c_1} in the bipolaron liquid phase. For further explanation see text.

With decreasing EP coupling, *i.e.* increasing ratio u/λ, both Δ_{c_1} and Δ_s become smaller, acquire a notable finite-size dependency, and finally both scale to zero, indicating Luttinger-liquid metallic behavior. Since Δ_{c_1} and Δ_s converge to the same value as $N \to \infty$, spin and charge degrees of freedom "stick together". Above a critical ratio u/λ, however, a SDW (Mott-insulating) phase is realized. In the MI we found a finite charge excitation gap, which in the limit $\lambda/u \ll 1$ scales to the charge gap of the Hubbard model, whereas the extrapolated spin gap remains zero (cf. the data for $\lambda = 0.05$). This is in agreement with spin-charge separation.

In order to gain deeper insight into the nature of the intermediate phase between PI and MI we determine, besides Δ_{c_1}, the two-particle excitation gap

$$\Delta_{c_2} = E_0^{2+}(0) + E_0^{2-}(0) - 2E_0(0)\,. \qquad (6)$$

This gap corresponds to the charge gap in a bipolaronic insulator and is an upper limit for it in any other phase. Of course, one- and two-particle excitation gaps should simultaneously open if we enter the PI and MI phases. If the PI phase is a bipolaronic insulator (superlattice) rather than a traditional Peierls band insulator, mobile bipolarons may occur first in the dissolving process of the PI, as the λ/u ratio is lowered. Such a bipolaronic metal/liquid phase will then be characterized by $\Delta_{c_2} = 0$ but finite Δ_{c_1} (and Δ_s). Adding/removing a single particle from the metallic bipolaron phase is energetically costly because the bipolarons are (tightly) bound. A bipolaron as a whole, however, can be added or removed without effort.

Figure 3 illustrates that this scenario holds in the anti-adiabatic weak-coupling regime. As the EP coupling gets weaker, we enter a region where $\Delta_{c_1} > 0$ but $\Delta_{c_2} \to 0$ (see, *e.g.*, the data for $\lambda = 0.625$). Δ_{c_2} stays zero as Δ_{c_1} vanishes at still smaller λ (u fixed), until we enter the MI state.

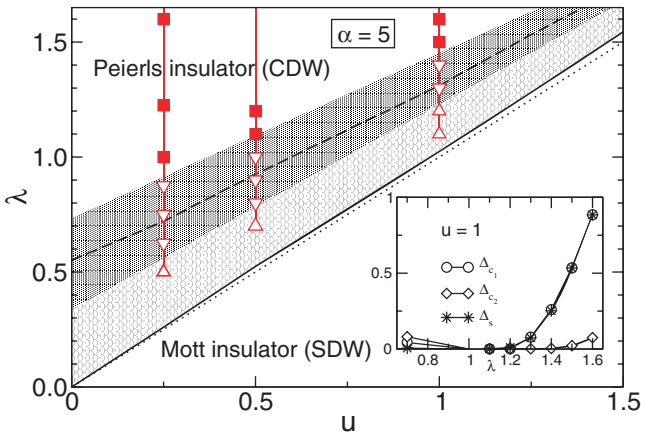

Fig. 4: (Color online) Phase diagram of the half-filled Holstein-Hubbard model in the weak-coupling anti-adiabatic ($\alpha = 5$) regime. Here filled squares, open triangles down, and open triangles up, denote the PI, bipolaronic metal, and Luttinger-liquid metal phases, respectively. The extension of the two latter phases is marked by the intensely (weakly) shaded regions. Dashed (solid) lines designate the Peierls–intermediate state (intermediate phase–Mott) phase boundaries obtained by ref. [8]. The dotted line indicates $u = \lambda$. The inset gives the ($N \to \infty$) extrapolated values of the one-particle, two-particle, and spin excitation gaps at $u = 1$. Note that Δ_{c_2} is twice as large as Δ_{c_1} in the MI phase.

Figure 4 combines the findings of our scaling analysis for Δ_s, Δ_{c_1} and Δ_{c_2} with the results of previous studies of the half-filled HHM based on susceptibility and Luttinger liquid parameter data [8,12]. First, we note that the PI-metal phase boundary is shifted compared to the results of ref. [8], while the metal-MI transition line is the very same. That is, taking $\Delta_{c_2} = 0$ as a criterion for the instability of the PI phase, we find an even larger region for the PI-MI

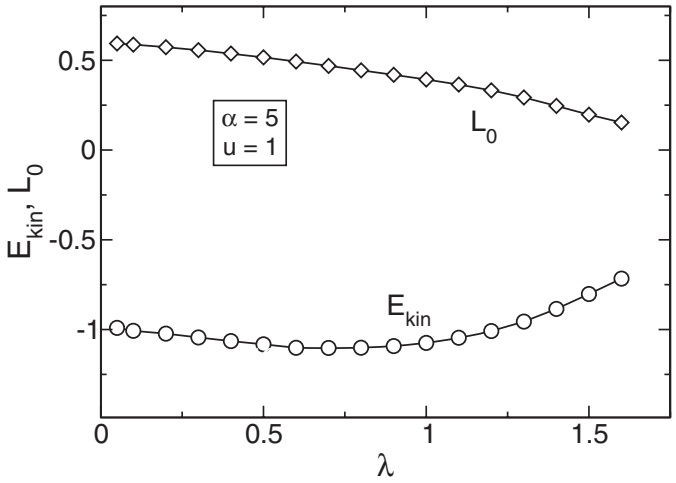

Fig. 5: Kinetic energy E_{kin} and local magnetic moment L_0 at $u=1$, $\alpha=5$.

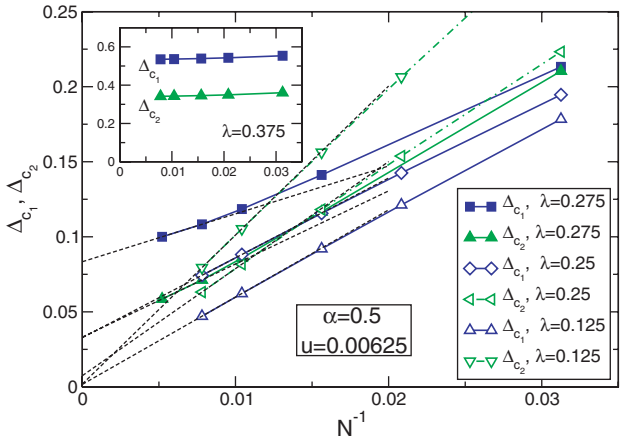

Fig. 6: (Color online) Finite-size scaling of the one- and two-particle excitation gaps in the adiabatic ($\alpha=0.5$) regime of the HHM. The inset gives the results in the PI phase $\lambda=0.375$.

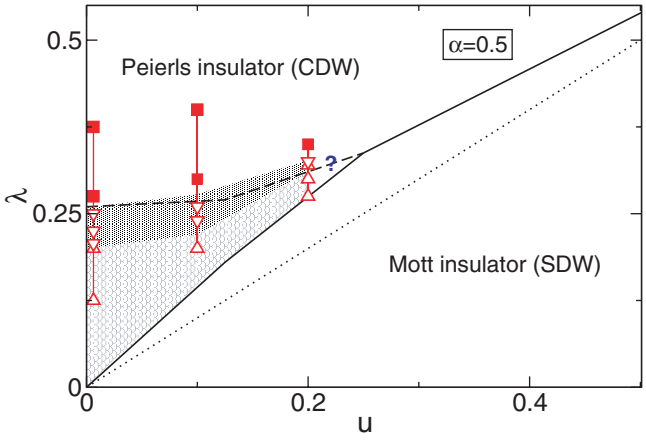

Fig. 7: (Color online) Phase diagram of the HHM in the adiabatic weak-coupling regime. Again filled squares, open triangles down, and open triangles up, denote the PI, bipolaronic metal, and Luttinger-liquid metal phases, respectively. Dashed (solid) lines are taken from ref. [8]; the dotted line gives $u=\lambda$. Since the finite-size scaling becomes exceedingly costly in the vicinity of the tricritical point $u\simeq 0.25, \lambda=0.3375$ given by Clay *et al.* [8], we cannot reliably resolve the phase structure there.

intervening state. Second, within the metallic state, our data suggests a cross-over between a bipolaronic liquid ($\Delta_{c_2}=0$; Δ_{c_1}, $\Delta_s>0$) and a Luttinger liquid ($\Delta_{c_2}=\Delta_{c_1}=\Delta_s=0$) (see footnote [5]).

The mean kinetic energy,

$$E_{kin}=-t\sum_{\langle i,j\rangle\sigma}\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle\,, \tag{7}$$

shown in fig. 5 for $u=1$, exhibits a pronounced minimum in the intermediate metallic phase [6]. The local magnetic moment,

$$L_0=\frac{3}{4N}\sum_i\langle(n_{i,\uparrow}-n_{i,\downarrow})^2\rangle\,, \tag{8}$$

can be taken as a measure for the "localization" of the electron spin. For the pure half-filled Hubbard model it varies between 3/8 (band limit) and 3/4 (atomic limit). As can be seen from fig. 5, L_0 is suppressed in the PI CDW phase because of the alternating arrangement of (almost) empty and double occupied sites. Entering the metallic phase L_0 is enhanced and reaches its maximum in the MI phase. Both E_{kin} and L_0 are however not very suitable for fixing the phase boundaries.

The corresponding results for the *adiabatic regime* ($\alpha=0.5$) are given in figs. 6 and 7. Again we have strong evidence for an intermediate metallic state. The region where bound mobile charge carriers (bipolarons) exist, however, now is a small strip between the PI and metal phases only, and expected to vanish if the adiabaticity ratio α goes to zero[6]. If all energy scales —set by λ, u, α— become small, the finite-size scaling is extremely delicate and it is difficult to resolve the different metallic phases. The main differences in comparison to the anti-adiabatic regime pertain to i) the nature of the Peierls phase, which is a traditional band insulator in the adiabatic case, and ii) the existence of a tri-critical point at moderate coupling strengths.

To summarize, we complemented previous numerical investigations of the half-filled Holstein-Hubbard model [6–9,11,12] by a large-scale DMRG analysis of the weak electron-phonon and electron-electron interaction regime. By calculating spin and charge excitation gaps we confirmed the existence of an intermediate metallic phase in the cross-over region of the Peierls-insulator Mott-insulator transition. This phase is shown to be most extended in the anti-adiabatic limit of large phonon

[5] There is an ongoing discussion, whether superconducting pairing correlations may become dominant in the HHM between the CDW and SDW phases (cf., *e.g.*, ref. [9]). Here, we will not address the highly controversial issue of existence of superconducting ground states (off-diagonal long-range order) in a stricly 1D electron-phonon model.

[6] For the so-called adiabatic HHM with frozen phonons an additional bond-order-wave might occur within the intermediate phase [28].

frequencies. If the PI typifies a bipolaronic superlattice, it gives way to a bipolaronic liquid composed of bound mobile (singlet) charge carriers as the EP coupling weakens. Reducing the EP-to-Coulomb interaction ratio further, a cross-over to a metallic state with unbound (weakly phonon-dressed) electrons (Luttinger liquid) takes place, until the MI state is finally reached at $\lambda \lesssim u$. If the PI typifies a rather standard band insulator in the adiabatic, small phonon-frequency limit, the bipolaron liquid phase narrows substantially, but still a metallic phase exists in between CDW and SDW states. Putting these findings together with the results previously obtained for the strong-coupling case, where a direct first-order PI-MI transition takes place, a rather complete picture of the physical properties of the 1D HHM emerges.

* * *

We would like to thank A. Alvermann, F. F. Assaad, K. W. Becker, S. Ejima, M. Hohenadler, and G. Wellein for valuable discussions. This work was supported by DFG through SFB 652 and KONWIHR Bavaria project HQS@HPC. Furthermore, we acknowledge generous computer time grants by LRZ Munich and HLRN Berlin.

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