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An infinite projected entangled-pair state (iPEPS) is a variational tensor network ansatz for two-dimensional wave functions in the thermodynamic limit where the accuracy can be systematically controlled by the bond dimension D. We show that for the doped Hubbard model in the strongly correlated regime ($U/t = 8, n = 0.875$) the iPEPS yields lower variational energies than state-of-the-art variational methods in the large two-dimensional limit, which demonstrates the competitiveness of the method. In order to obtain an accurate estimate of the energy in the exact infinite-D limit we introduce and test an extrapolation technique based on a truncation error computed in the iPEPS imaginary time evolution algorithm. The extrapolated energies are compared with accurate quantum Monte Carlo results at half-filling and with various other methods in the doped, strongly correlated regime.

I. INTRODUCTION

The accurate study of strongly correlated systems is one of the biggest challenges in condensed matter physics. A well-known example is the two-dimensional (2D) Hubbard model [1], which potentially captures the relevant physics of the cuprate high-T_c superconductors. Despite its simplicity and the enormous effort made to try to solve the model, the phase diagram of the Hubbard model is still controversial. Still, in recent years substantial progress has been achieved with a variety of different numerical methods (see, e.g., Refs. [2–9]), so that there is hope that the full solution of the Hubbard model may be within reach in the near-future. For recent state-of-the-art benchmark results from various methods, see Ref. [9].

Solving systems in one dimension is under far better control than solving in two dimensions, mostly thanks to the well-known density-matrix renormalization-group (DMRG) method [10]. DMRG has an underlying variational tensor network ansatz, called the matrix product state, in which the wave function is efficiently represented by a trace over the product of tensors. The accuracy of the ansatz can be systematically controlled by the bond dimension D of the tensors, and one typically reaches extremely accurate results in one dimension (and quasi–one dimension). DMRG can also be used to study 2D systems (typically on cylinders) by mapping the system onto a 1D problem with long-ranged interactions [11]. However, the computational cost scales exponentially with the width of the cylinder such that the approach is not scalable to large 2D systems [12].

In order to overcome this exponential scaling 2D tensor network ansatzes have been developed, such as projected entangled-pair states (PEPS [13–16]; also called tensor product states [17,18]) and the 2D multiscale entanglement renormalization ansatz [19,20]. These networks are designed in such a way that they reproduce an area-law scaling of the entanglement entropy which a large class of relevant 2D ground states fulfills [21]. The involved methods are technically more complicated than matrix-product-state-based

approaches, which is one of the main reasons why it took several years to develop these methods. However, recently there have been substantial breakthroughs which clearly demonstrate the enormous potential of 2D tensor networks. For example, it was shown for the t-J model [22] that infinite PEPS (iPEPS)—an ansatz for a state in the thermodynamic limit—yield lower variational energies than the state-of-the-art results from the fixed-node Monte Carlo (FNMC) method [23]. Another example is the Shastry-Sutherland model in a magnetic field [24], where iPEPS helped us to gain a new understanding of the magnetization process, thanks to largely unbiased simulations.

Thus, already current (i) PEPS algorithms can outperform (or compete with) the best variational methods for strongly correlated fermionic models like the t-J model and also for frustrated spin systems (see, e.g., Refs. [25–27]). In this paper we show that the same is true also in the strongly correlated regime of the 2D Hubbard model, where we find variational energies lower than the best variational Monte Carlo results for large 2D systems [9].

One major difficulty in iPEPS simulations so far has been to obtain an accurate estimate of the energy in the exact, infinite-D limit. Typically the energy does not smoothly depend on the bond dimension D, which makes extrapolating the finite-D data to the infinite-D limit problematic. Accurate extrapolations become particularly important if several states at finite D are strongly competing, as, e.g., in the t-J model [22], where uniform and stripe states exhibit almost the same energy at finite D. A precise estimate of the energy is crucial to identifying the true ground state among these competing states.

In this paper we propose and test an approach to extrapolating the energy based on a truncation error w which quantifies the degree of approximation in the iPEPS imaginary time evolution algorithm. This quantity plays a role similar to that of the truncation error in conventional DMRG simulations, which is typically used to extrapolate energies. Empirically we find here that the energy varies in a much smoother way with w than with $1/D$ such that an extrapolation in $w \to 0$ yields an improved estimate of the exact ground-state energy.

We benchmark this extrapolation technique for the 2D Hubbard model, first in the exactly solvable $U/t = 0$ limit

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(which is particularly challenging for iPEPS since the ground state is strongly entangled), then at finite U/t at half-filling, where we compare our results with accurate quantum Monte Carlo results [9]. Finally, we also provide an estimate of the energy in the doped, strongly correlated regime ($U/t = 8$, $n = 0.875$) and a comparison with various other methods from Ref. [9].

This paper is organized as follows. In the next section we give a short introduction to the iPEPS ansatz and the ground-state algorithm based on imaginary time evolution. In Sec. III we discuss ways to perform energy extrapolations with iPEPS; in particular, we explain how to compute a truncation error and use this quantity as an extrapolation parameter. In Sec. IV we present our finite D and extrapolated energies for the 2D Hubbard model and a comparison with other methods. Finally, in Sec. V we summarize our findings and give prospects for solving the Hubbard model. In the Appendix we present additional results for the 2D Heisenberg model and a model of noninteracting spinful fermions with a pairing potential, to provide further evidence for the usefulness of the extrapolation technique based on the truncation error.

II. iPEPS ANSATZ AND METHOD

An iPEPS [13,15,16] is an efficient variational tensor network ansatz for 2D states in the thermodynamic limit which obey an area law of the entanglement entropy (typically ground states of local Hamiltonians). The ansatz consists of a supercell of tensors which is periodically repeated on a lattice, with one tensor per lattice site [28]. On the square lattice, each tensor has a physical index and four auxiliary indices which connect to the nearest-neighboring tensors. The accuracy of the ansatz can be systematically controlled by the bond dimension D of the auxiliary indices (i.e., each tensor contains dD^4 variational parameters, where d is the local dimension of a lattice site). An iPEPS with $D = 1$ corresponds to a product state, and by increasing D entanglement can be added in a systematic way.

For translational invariant states a supercell with only one single tensor can be used. If the translational symmetry is spontaneously broken, a supercell compatible with the symmetry-breaking pattern is needed (e.g., for an antiferromagnetic state two different tensors for the two sublattices are required). Since in practice the structure of the ground state is not known in advance, we run simulations using different supercell sizes to check which supercell yields the lowest variational energy. This approach also provides a way to determine several competing low-energy states, as, for example, done in the t-J model [22], in which uniform and different stripe states have been found using different supercell sizes. In order to find the true ground state among these competing states, one needs to have an accurate estimate of the energy of each state in the infinite-D limit. However, a simple extrapolation in D often fails to give an accurate estimate, due to the nonsmooth dependence of the energy on D, and this is why it is important to find alternative ways to perform such extrapolations. Such an improved extrapolation technique is presented in the next section.

The iPEPS wave function is evaluated by contracting the 2D tensor network in a controlled approximate way. In the present work we use a variant [22] of the corner-transfer matrix

(CTM) method [29,30]. The accuracy of the contraction is controlled by the "boundary" dimension χ, which we choose large enough (up to several hundreds) so that the resulting error is negligible (compared to the effect of the finite D). To increase the efficiency we make use of Abelian symmetries [31,32]. For an introduction to iPEPS, see, e.g., Refs. [33] and [34]. We note that 2D tensor networks were first introduced for spin systems and later extended to fermionic systems (see Refs. [33] and [35–42]).

In order to obtain an approximate representation of the ground state for a given Hamiltonian $\hat{H}$, the tensors need to be *optimized*; i.e., the best variational parameters have to be found. For iPEPS this is typically done by performing an imaginary time evolution of an initial (e.g., random) iPEPS. The evolution operator is split into a product of two-site operators via a Trotter-Suzuki decomposition (assuming nearest-neighbor interactions),

$$\exp(-\beta\hat{H}) \approx \left(\prod_b \hat{U}_b\right)^n, \quad \hat{U}_b = \exp(-\tau\hat{H}_b), \quad (1)$$

where the product goes over all nearest-neighbor bonds b in the supercell, $\hat{H}_b$ is the Hamiltonian term on bond b, and $\tau = \beta/n$ is a small imaginary time step. The imaginary time evolution is performed by sequentially multiplying the two-site operators $\hat{U}_b$ to the iPEPS and representing the resulting wave function again as an iPEPS, until convergence is reached [43].

Let us consider the application of such a two-site operator $\hat{U}_b$ to two tensors A and B which are connected by the bond b. The resulting state $|\Psi'_{A'B'}\rangle = \hat{U}_b|\Psi_{AB}\rangle$ can be represented by two new tensors A' and B', where the bond dimension on bond b has increased from D to $D' \leqslant d^2 D$. For an efficient evolution the corresponding bond needs to be truncated back to the original bond dimension D, resulting in a truncated wave function $|\tilde{\Psi}_{\tilde{A}\tilde{B}}\rangle$. In the so-called full update [33] (or fast full update [34]) this truncation is done by finding the new tensors $\tilde{A}$ and $\tilde{B}$ which minimize the cost function,

$$C = \min_{\tilde{A},\tilde{B}} |\,|\Psi'_{A'B'}\rangle - |\tilde{\Psi}_{\tilde{A}\tilde{B}}\rangle| = \min_{\tilde{A},\tilde{B}} \sqrt{d(\tilde{A},\tilde{B})}, \quad (2)$$

with

$$d(\tilde{A},\tilde{B}) = \langle\Psi'_{A'B'}|\Psi'_{A'B'}\rangle + \langle\tilde{\Psi}_{\tilde{A}\tilde{B}}|\tilde{\Psi}_{\tilde{A}\tilde{B}}\rangle$$
$$- \langle\Psi'_{A'B'}|\tilde{\Psi}_{\tilde{A}\tilde{B}}\rangle - \langle\tilde{\Psi}_{\tilde{A}\tilde{B}}|\Psi'_{A'B'}\rangle. \quad (3)$$

Finding the new tensors can be solved in an iterative way, as explained, e.g., in Refs. [33] and [34] (see also [44]).

III. ENERGY EXTRAPOLATION WITH iPEPS

Typically, for challenging problems, one does not reach convergence as a function of D and one needs to perform an extrapolation to the infinite-D limit to obtain an estimate of the true ground-state energy. One possibility is to plot the energy as a function of $1/D$ and then try to extrapolate the data to $1/D \to 0$. However, in practice the energy does not depend on $1/D$ in a smooth way, which makes an accurate extrapolation difficult (for examples see, e.g., Refs. [24,25,45], and [46]).

Empirically one finds that the overall convergence of the energy goes more rapidly than linear at $1/D$, such that a

linear extrapolation at $1/D$ (using the largest few values of D) provides a lower bound E_l of the true ground-state energy. Since the method is variational, the energy for the largest value of D corresponds to an upper bound E_u. In practice a crude estimate of the energy can be obtained from the mean value $E_m = (E_u + E_l)/2$ with an error bar of $\Delta = (E_u - E_l)/2$. Examples of these estimates are given in the next section. While this approach can provide a reasonable guess of the exact energy, a more accurate and controlled extrapolation would be highly desirable.

In DMRG simulations energy extrapolations are typically much more accurate with extrapolation in the truncation error ϵ, corresponding to the sum of the discarded squared singular values in the two-site variational optimization [47]. In simple words, the truncation error measures how far away the state is from the true ground state, which is reached if ϵ goes to 0. The question is now whether a similar quantity could also be used in iPEPS simulations to improve energy extrapolations. The most natural way would be to implement a similar two-site variational optimization algorithm in iPEPS. However, the imaginary time evolution algorithm is more commonly used and more easy to implement, and we therefore aim to define a similar quantity within this approach [48].

Let us consider the cost function C in Eq. (2). For the true ground state, which is reached for sufficiently large D and β, the cost function C is 0. However, if the true ground state is not reached because D is too small, then the cost function will reach a certain nonzero value $C(D, \beta \to \infty)$ for large β. For small τ the cost function depends linearly on the time step (to lowest order). We now define the quantity $w(D) = C(D, \beta \to \infty)/\tau$, which is independent of τ (for small τ) and decreases monotonously with D. This quantity w measures the truncation error when approximating an iPEPS with an enlarged bond dimension D' on a bond, $|\Psi'_{A'B'}\rangle$, with a new iPEPS with a smaller bond dimension D, $|\tilde\Psi_{\tilde A \tilde B}\rangle$. Thus, w plays a role similar to that of the truncation error ϵ in DMRG simulations.

A priori we do not know how the energy depends on w, in contrast to DMRG simulations, where the energy converges linearly in the truncation error for sufficiently large bond dimensions (after a suitable number of finite-system sweeps). Nevertheless, we find here that the energy depends on w in a much more regular way than on $1/D$, such that an extrapolation in w using a polynomial fit to the data provides an improved estimate of the exact energy in the $w \to 0$ limit. This is illustrated with several examples for the Hubbard model in the next section.

IV. BENCHMARKS: 2D HUBBARD MODEL

As a benchmark we consider the single-band 2D Hubbard model with only nearest-neighbor hoppings,

$$\hat{H} = -t \sum_{\langle i,j,\sigma\rangle} (\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \text{H.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \quad (4)$$

where $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) creates (annihilates) an electron with spin $\sigma = \{\uparrow, \downarrow\}$ at site i, $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$ is the number operator, U is the on-site repulsion, and t is the hopping amplitude.

In the following we first present the iPEPS results in the noninteracting case $U/t = 0$ at half-filling ($n = 1$), which can be exactly solved. For the interacting case $U/t > 0$ we make a comparison with several other methods from the recent state-of-the-art benchmark paper by LeBlanc *et al.* [9], including auxiliary-field quantum Monte Carlo (AFQMC), density-matrix embedding theory (DMET), DMRG, and FNMC. We first consider the half-filled case for $U/t = 4$ and $U/t = 8$, which can be accurately solved by AFQMC simulations since there is no sign problem at half-filling. Finally, results for the doped case $n = 0.875$ in the strongly correlated regime $U/t = 8$ are presented and compared to the best available data. All energies are given in units of t.

A. $U/t = 0$ at half-filling

It is known that 2D free fermionic systems with a 1D Fermi surface have a multiplicative logarithmic correction to the area law of the entanglement entropy [21]. Since an iPEPS can only reproduce an area law this case poses a particular challenge and we do not expect to obtain the exact result for finite D (on an infinite lattice). Nevertheless, since the area law is only weakly violated (in contrast to a volume law), one can still obtain an approximation to the ground state and a variational estimate of the ground-state energy. For example, for $D = 16$ iPEPS yields an energy per site of $E = -1.597$. Compared to the exact result $-1.6211\ldots$, this corresponds to a relative error of $\approx 1.5\%$.

The iPEPS energies as a function of $1/D$ are shown in Fig. 1 (squares). One can clearly see how the variational energy improves upon increasing D. However, the dependence on $1/D$ is not very regular, which makes an extrapolation in $1/D$ somewhat difficult. As discussed in the previous section we can obtain a lower bound, E_l, of the ground-state energy by a linear extrapolation of the data in $1/D$, whereas the value at the largest D corresponds to a variational upper bound, E_u. The range of energies estimated in this way is $[-1.597, -1.636]$,
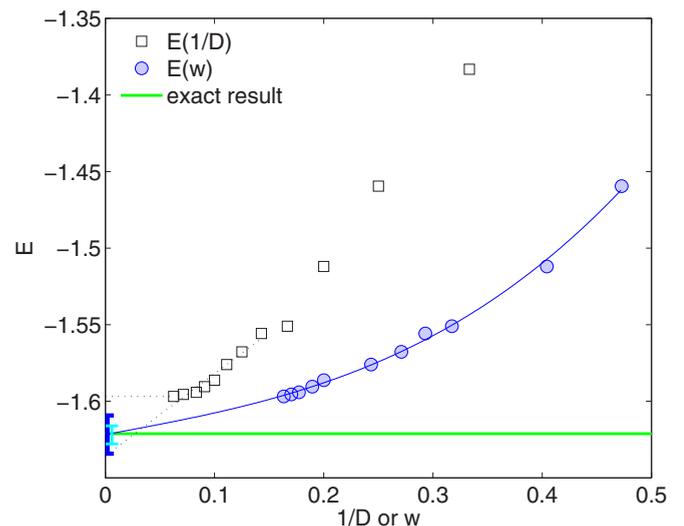

FIG. 1. iPEPS energies as a function of the inverse bond dimension (squares) and as a function of the truncation error w (circles) for the noninteracting case $U/t = 0$.

which includes the exact value. Based on these data we obtain the estimate $E_m = -1.616 \pm 0.019$.

We next consider the iPEPS data plotted as a function of the average truncation error w (circles in Fig. 1). One can clearly observe a smoother dependence in the $E(w)$ than in the $E(1/D)$ data. Fitting the data with a third-order polynomial yields an energy $E_w = -1.6217$ in the limit $w \to 0$, which is close to the exact energy. As an estimate of the error we take half the difference between the lowest variational energy and the extrapolated value, $\Delta = (E_u - E_w)/2 = 0.012$, shown by the dark-blue error bar in Fig. 1. As an alternative estimate we average over several fits using different ranges of data points, which yields $\tilde{E}_w = -1.6219$, with a standard deviation of 0.006, shown by the light-blue error bar in Fig. 1.

Thus, even in the "worst case" for iPEPS (i.e., free fermionic systems) we can obtain quite an accurate estimate of the ground-state energy based on an extrapolation in the truncation error w.

B. $U/t = 4$ at half-filling

Next we consider the case $U/t = 4$ at half-filling, where the ground state is insulating and exhibits antiferromagnetic long-range order. Since there is no 1D Fermi surface as in the $U/t = 0$ case, we expect the ground state to be less entangled (obeying an area law). This is reflected in the higher accuracy of the ground-state energy obtained with iPEPS and in the smaller truncation error w compared to that in the $U/t = 0$ case. For example, taking $D = 16$ the relative error (compared to the extrapolated AFQMC result [9], -0.8603 ± 0.0002) is of the order of 0.14%, i.e., an order of magnitude better than the $U/t = 0$ result. The truncation error is $w(D = 16) \sim 0.05$, compared to $w(D = 16) \sim 0.16$ in the $U/t = 0$ case.

The iPEPS energies exhibit a rather irregular behavior as a function of $1/D$, shown by the squares in Fig. 2. A linear fit using the five largest D values yields the lower bound $E_l = -0.8610$. Computing an estimate based on the $1/D$ extrapolation as in the $U/t = 0$ case yields -0.8602 ± 0.0008, in agreement with the AFQMC result.

The energies as a function of w (circles) exhibit a more regular behavior, as previously observed in the $U/t = 0$ case. A third-order polynomial fit including all data points yields $E_w = -0.8603 \pm 0.0005$. If we average again over several fits using different ranges of data points, we obtain $\tilde{E}_w = -0.8604 \pm 0.0005$, in agreement with the AFQMC result.

Our data are also in agreement with the extrapolated DMET and DMRG results, shown in Fig. 2, with a comparable error bar.

C. $U/t = 8$ at half-filling

As we move away from the noninteracting limit, iPEPS becomes more accurate (in contrast to weak-coupling approaches). For $U/t = 8$, $D = 16$ the energy is -0.52415. The relative error compared to the AFQMC result (-0.5247 ± 0.0002) is small, only 0.1%. Thus, even without using any extrapolation we already obtain a remarkably accurate result in the thermodynamic limit.

The iPEPS estimate in the infinite-D limit based on the $1/D$ extrapolation is -0.5246 ± 0.0005 (using the four largest
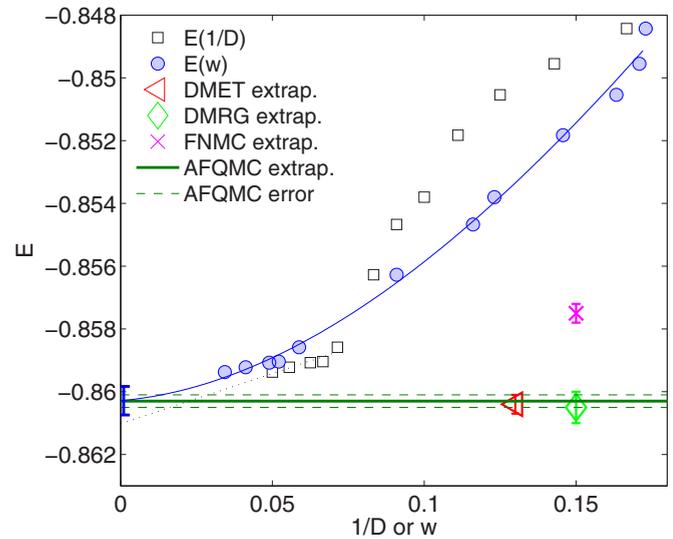

FIG. 2. iPEPS results for the energy for $U/t = 4$ at half-filling ($n = 1$) as a function of $1/D$ (squares) and w (circles), in comparison with the results from other methods (extrapolated to the thermodynamic limit). The reference value obtained from AFQMC is shown by the thick solid (green) line, with the error bar indicated by the dashed lines.

D values) and -0.5250 ± 0.0008 (using the five largest D values), in agreement with the AFQMC result.

Also here, the $E(w)$ curve is much smoother than the $E(1/D)$ data, shown in Fig. 3. A third-order polynomial fit yields $E_w = -0.5244 \pm 0.0001$, which is slightly higher but still compatible with the AFQMC result. (A similar result is obtained by taking the average over several fits.) Compared to the other methods iPEPS shows the best agreement with the AFQMC data: DMRG is slightly too high (-0.5241 ± 0.0001), DMET has a large error bar (-0.5234 ± 0.001), and the FNMC estimate is too high (-0.52315 ± 0.00005).
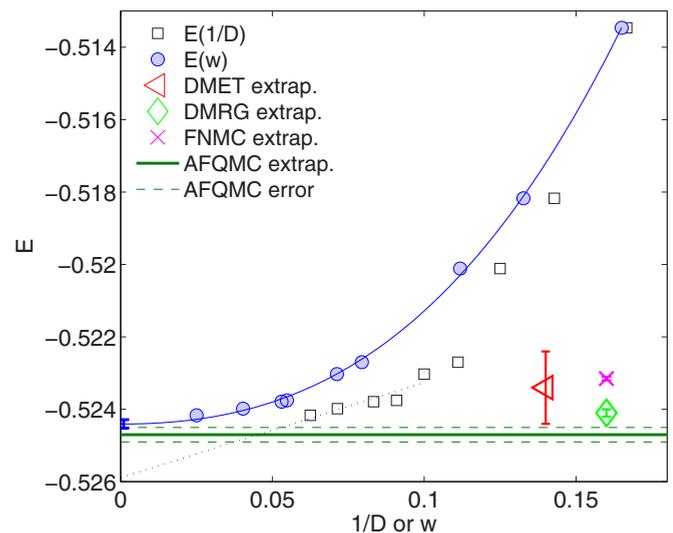

FIG. 3. iPEPS results for the energy for $U/t = 8$ at half-filling ($n = 1$) in comparison with results of other methods.
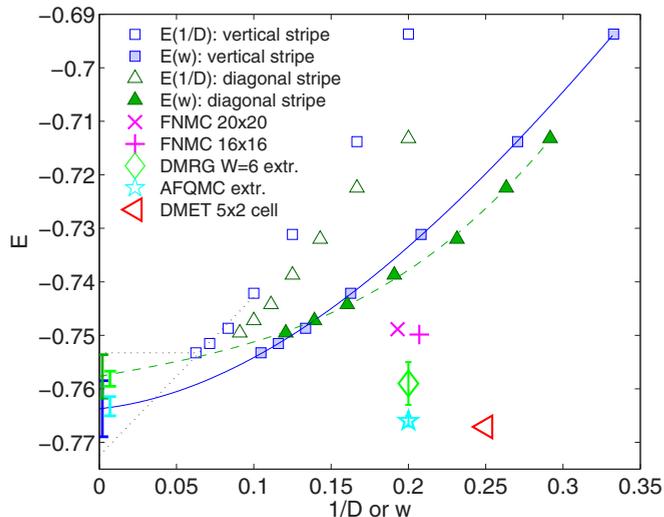
FIG. 4. iPEPS energy of a vertical stripe with period 5 and a diagonal stripe with period 16 for the doped Hubbard model in the strongly correlated regime ($U/t = 8, n = 0.875$) in comparison with those found using other methods.

D. Doped case for $U/t = 8$

Finally, in Fig. 4 we present results in the doped, strongly correlated regime for $U/t = 8$ and $n = 0.875$, for which AFQMC is no longer exact due to a strong sign problem. Determining the ground state in this regime is one of the fundamental open problems in the field of strongly correlated systems. The main reason why this is so challenging is that there are many different states which are energetically very strongly competing (e.g., uniform superconducting states or different types of stripe states), which explains why different state-of-the-art methods yield different answers for the physics in this regime (see, e.g., Ref. [9]).

One of the main advantages of iPEPS is that the different competing states can be obtained by using different supercell sizes, and the properties of these states (e.g., order parameters) can then be studied individually for each low-energy state. This was done, for example, in Ref. [22] for the t-J model (an effective model of the Hubbard model in the strongly interacting limit), where, e.g., a uniform d-wave superconducting state with coexisting antiferromagnetic order is found by using a two-site supercell or a period-5 stripe in a 5×2 supercell. In order to identify the true ground state among these competing states, one needs to compare their extrapolated energies, and this why an accurate extrapolation of the energy is important.

A systematic study of all possible supercell sizes and a discussion of the physics of all the competing states are beyond the scope of this paper and left for future work. Instead we illustrate here the advantage of the improved extrapolation technique by comparing the energies of two competing states: a vertical-stripe state with period 5, with charge and spin orders coexisting with superconductivity, and a (nonsuperconducting) diagonal-stripe state with period 16, with one hole per unit length per stripe.

If we consider the energies plotted as a function of $1/D$, shown in Fig. 4, we can observe that for a given D the diagonal stripe state has a lower variational energy than the vertical

stripe state. However, since the energies of both states are still rapidly decreasing with increasing D it is hard to predict which state is lower in energy in the large-D limit based on a $1/D$ extrapolation, which yields $E_m = -0.763 \pm 0.010$ and $E_m = -0.764 \pm 0.015$ for the vertical and diagonal stripe, respectively. These values lie very close and have a large overlapping error bar.

If, however, we use the truncation error w as an extrapolation parameter, we can obtain a much clearer distinction between the two states. The extrapolation in w yields $E_w = -0.7637 \pm 0.005$ ($E_w = -0.7577 \pm 0.004$) for the vertical (diagonal) stripe; averaging over several fits using different ranges yields $\tilde{E}_w = -0.7633 \pm 0.002$ ($\tilde{E}_w = -0.7581 \pm 0.0014$). Thus, in the large-$D$ limit the vertical-stripe state is favored over the diagonal-stripe state.

We next compare our results for the vertical-stripe states with other methods from Ref. [9]. Our best iPEPS variational energy for $D = 16$ is $E = -0.75325$. This is lower than the best variational result, -0.74884, from FNMC for a 20×20 system where the FNMC energies are increasing with system size. Thus, the iPEPS clearly provides a lower variational energy in the thermodynamic limit than FNMC, which demonstrates the competitiveness of iPEPS in the doped, strongly correlated regime.

The extrapolated iPEPS energy is comparable to the result obtained with the (approximate) constrained path AFQMC (-0.766 ± 0.001), the DMRG result (extrapolated in the truncation error) for a finite cylinder of width 6 (-0.759 ± 0.004), and the DMET result in a 5×2 cell (-0.7671) [49].

V. SUMMARY AND PROSPECTS

We have presented iPEPS results for the energy of the 2D Hubbard model at half-filling for $U/t = 0$, 4, and 8 and away from half-filling for $U/t = 8$, $n = 0.875$. In the doped case the variational energies at large bond dimensions are lower than the best available variational Monte Carlo results, which demonstrates that iPEPS is a very competitive variational method in the strongly correlated regime. It is in this challenging and physically relevant region where iPEPS (or 2D tensor networks in general) have the largest potential to go substantially beyond the present state of the art.

In order to obtain an estimate of the exact ground-state energies we propose performing an extrapolation in the truncation error w, complementary to the (more crude) extrapolations in $1/D$, allowing us to compute the ground-state energies with a higher accuracy. At half-filling the extrapolated results agree with the exact value in the noninteracting case and with the accurate AFQMC results for $U/t = 4$ and $U/t = 8$. These extrapolations will play a key role in identifying the true ground state among several competing states (e.g., stripe and uniform states [22]) which lie very close in energy. As an example we have provided an estimate of the energy of a (vertical) period-5 stripe for $U/t = 8$, $n = 0.875$ and shown that the extrapolated energy is lower than that of a period-16 diagonal stripe.

The present iPEPS data have been obtained using modest computational resources. We believe that with large-scale parallel simulations using bond dimensions up to $D \sim 20 \ldots 24$, in combination with the present extrapolation technique,

the ground-state phase diagram in the strongly correlated regime ($U/t \geqslant 6$) is accessible. Combined with approaches which work best in the weakly correlated regime [8,9] and with supporting results from other methods in the strongly correlated regime, the full solution of the 2D Hubbard model seems to be within reach.

APPENDIX: ADDITIONAL RESULTS

In order to further demonstrate the usefulness of the energy extrapolation technique based on the truncation error w we present additional results for the 2D Heisenberg model and for an exactly solvable model of noninteracting spinful fermions with a pairing potential in this appendix.

1. 2D Heisenberg model

We consider the 2D $S = 1/2$ Heisenberg model on a square lattice with Hamiltonian

$$\hat{H} = J \sum_{\langle i,j \rangle} \mathbf{S_i} \mathbf{S_j}, \tag{A1}$$

where $\mathbf{S_i}$ is a spin-1/2 operator on site i. We set the coupling $J = 1$. Since there is no negative sign problem this model can be solved by quantum Monte Carlo, and accurate estimates of the energy can by obtained by an extrapolation of the finite-size data to the thermodynamic limit. The Monte Carlo estimate from Ref. [50] is $E = -0.669437(5)$, obtained with linear system sizes up to $L = 16$. A more precise estimate was presented in Ref. [51], $E = -0.6694421(4)$, using larger system sizes.

Also in this example the iPEPS energies as a function of $1/D$ show rather irregular behavior, as shown in Fig. 5. Using an $1/D$ extrapolation yields $-0.66943(6)$ (using the four largest values of D), in agreement with the extrapolated QMC result.

The truncation errors in this example are considerably smaller than for the Hubbard model, indicating that the ground state is less entangled. Also in this case the dependence on w is much smoother than that on $1/D$. A second-order polynomial fit including all data points yields $E_w = -0.66945(4)$. A similar result is obtained by averaging over several fits including different ranges of data points.

2. Noninteracting spinful fermions with a pairing potential

In this section we consider an exactly solvable model of spinful fermions with a nearest-neighbor hopping and a pairing potential term,

$$\hat{H} = -t \sum_{\langle i,j,\sigma \rangle} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \text{H.c.}) + \sum_{\langle i,j \rangle} \gamma_{ij} (\hat{c}_{i\uparrow}^{\dagger} \hat{c}_{j\downarrow}^{\dagger} - \hat{c}_{i\downarrow}^{\dagger} \hat{c}_{j\uparrow}^{\dagger} + \text{H.c.}),$$
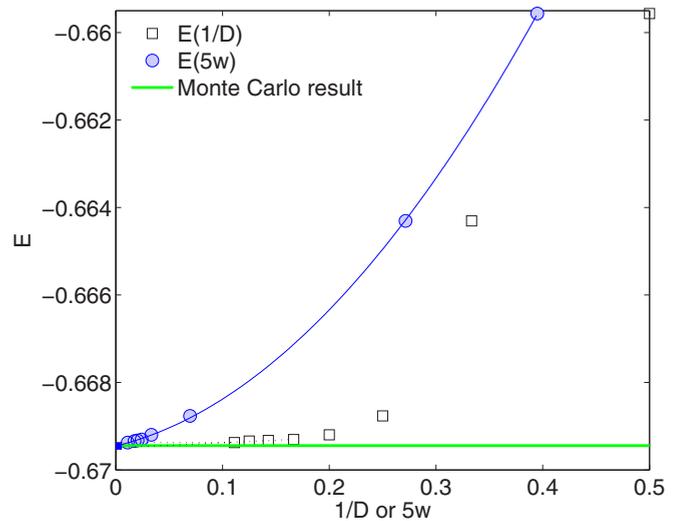
$$\tag{A2}$$

FIG. 5. iPEPS energy per site of the 2D Heisenberg model compared to the quantum Monte Carlo result. Note that the truncation error on the x axis has been rescaled by a factor of 5 for better visibility.

with γ_{ij} the amplitude of the pairing potential. In the present example we set $t = 1$, and $\gamma_{ij} = \pm 1$ for bonds oriented along the x and y directions, respectively. The exact energy in the thermodynamic limit is $-1.35494 \ldots$.

The iPEPS energies shown in Fig. 6 decrease rapidly with increasing D. As a consequence, the linear extrapolation in $1/D$ leads to an estimate with a very large error range, -1.36 ± 0.01. In contrast, performing an extrapolation in the truncation error yields a much better estimate, $E_w = -1.3547 \pm 0.002$, or, when taking the average over several fits, $\tilde{E}_w = -1.3547 \pm 0.001$.

This example illustrates that estimating the correct energy based on a $1/D$ extrapolation can be hard, even though the exact value lies not far from the energy at the largest bond dimension. Thanks to the much smoother behavior of the $E(w)$ curve one can obtain a much more accurate estimate using an extrapolation in w.
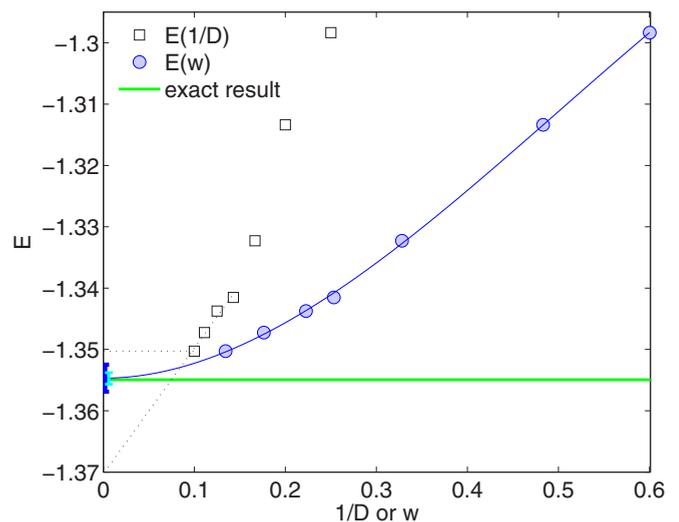

FIG. 6. iPEPS energy per site of an exactly solvable model of spinful fermions compared to the exact result.

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