Entanglement of Interacting Fermions in Quantum Monte Carlo Calculations

Tarun Grover

Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

(Received 28 July 2013; revised manuscript received 30 August 2013; published 24 September 2013; corrected 27 September 2013)

Given a specific interacting quantum Hamiltonian in a general spatial dimension, can one access its entanglement properties, such as the entanglement entropy corresponding to the ground state wave function? Even though progress has been made in addressing this question for interacting bosons and quantum spins, as yet there exist no corresponding methods for interacting fermions. Here we show that the entanglement structure of interacting fermionic Hamiltonians has a particularly simple form—the interacting reduced density matrix can be written as a sum of operators that describe free fermions. This decomposition allows one to calculate the Renyi entropies for Hamiltonians which can be simulated via determinantal quantum Monte Carlo calculations, while employing the efficient techniques hitherto available only for free fermions. The method presented works for the ground state, as well as for the thermally averaged reduced density matrix.

DOI: 10.1103/PhysRevLett.111.130402 PACS numbers: 05.30.−d, 02.70.Ss, 03.65.Ud, 03.67.Mn

Quantum entanglement plays a crucial role in exposing a variety of many-body quantum phenomena, such as topological order [1,2], surface states in quantum Hall systems and topological insulators [3,4], and the universal features of critical quantum systems [5–8]. Despite its theoretical appeal, the nonlocal nature of the entanglement makes it a rather difficult quantity to measure in experiments, or to even evaluate numerically. In recent years, new numerical methods have been developed to calculate entanglement measures, such as the Renyi entanglement entropy, for Hamiltonians of interacting bosons and quantum spin systems [9,10]. There is no obvious generalization of these techniques to fermionic systems, which differ fundamentally from bosons in the sign structure of their wave functions. In fact, the only known techniques for fermions are either variational in nature [10,11], or they are restricted to one-dimensional systems [12] and do not address the following basic question: *given a specific Hamiltonian of interacting fermions in a general spatial dimension, how does one calculate any entanglement measure in an unbiased manner?* In this paper we provide an answer to this question for all Hamiltonians that can be simulated without the fermionic sign problem in the standard determinantal quantum Monte Carlo (DQMC) technique [13–15].

Our main result is, in fact, more general. We show that the reduced density matrix ρ_A for an interacting fermionic system, corresponding to a subregion A, can be decomposed into a sum of operators that describe *free fermions*. Specifically, $\rho_A = \sum_{\{s\}} P_s e^{-c^\dagger h_s c}$, where $\{s\}$ denotes the configuration space of certain classical variables "s" to be introduced below, while the numbers P_s and the matrices h_s are fully determined by the underlying Hamiltonian, and we provide their general form below. This decomposition works for the ground state, as well as for the thermally averaged reduced density matrix at finite temperatures. Perhaps most interestingly, it allows one to calculate highly nonlocal quantities, such as the Renyi entanglement entropies, in an efficient manner with the DQMC, while employing the analytical techniques which were available only for the free fermions [16–18]. We demonstrate the method by numerically calculating the Renyi entropy S_2 for a one-dimensional chain of Hubbard model and by benchmarking it against the results from the exact diagonalization. Finally, we also develop a systematic expansion for the entanglement Hamiltonian of interacting fermions, which is again calculable within Monte Carlo simulations.

Since the notion of a fermionic sign problem enters in our discussion below, we briefly mention the relevant basics [19,20]. Specifically, in the DQMC technique [13–15], the interparticle interactions of the fermions are reexpressed as space-time fluctuating classical fields coupled to fermion bilinears. This allows one to integrate out the fermions to obtain a partition function written solely in terms of the classical fields. For a class of problems, this partition function is always positive, thereby allowing one to simulate the original interacting fermionic system using the classical Monte Carlo techniques. Such problems are said to be free of the "fermion sign problem," and our results will be most useful for this same set of problems. Some of the problems that fall in this class are the half-filled Hubbard model on bipartite lattices [13,14,21], certain multi-orbital Hubbard models at any chemical potential [20,22], regularized interacting Dirac fermions with even flavors of fermions in the presence of time-reversal symmetry [19,23–25], $SU(2)$ gauge theory with fundamental fermions at any chemical potential [19,24,25], and $SU(N_c)$ QCD with fermions in the adjoint for any N_c, again at any chemical potential [25,26].

Reduced density matrix in determinantal quantum Monte Carlo calculations.—Let us recall that the full density matrix ρ for a quantum Hamiltonian H at a temperature β^{-1} is given by

$$\rho = \frac{e^{-\beta H}}{\mathrm{tr}\,(e^{-\beta H})} = \frac{\sum_i e^{-\beta E_i} |\psi_i\rangle\langle\psi_i|}{\sum_i e^{-\beta E_i}}, \quad (1)$$

where $|\psi_i\rangle$ and E_i are the eigenfunctions and eigenvalues of H. From this, one can define a reduced density matrix ρ_A by spatially partitioning the total system into subregions A and $\bar{A}$ and subsequently tracing over the Hilbert space of the subregion $\bar{A}$: $\rho_A = \mathrm{tr}_{\bar{A}}\rho$. Furthermore, one can define entanglement measures such as the von Neumann entropy $S_{vN} = -\mathrm{tr}(\rho_A \log \rho_A)$ and the Renyi entropies $S_n = -[1/(n-1)] \log \mathrm{tr}(\rho_A^n)$. Our main interest lies in finding a numerically tractable expression for the reduced density matrix ρ_A, and the associated Renyi entropies S_n, for interacting fermion Hamiltonians. We find that the technique of DQMC provides a very fruitful conceptual framework to address this problem.

As already mentioned above, DQMC transforms the problem of interacting fermions into one of free fermions coupled to a fluctuating classical field [13–15]. There are two different versions of this method: a zero temperature method, which is used for calculating the ground state properties, and a finite temperature method for the thermally averaged properties. For completeness, we provide an overview of these two methods in the Supplemental Material [27]. In brief, both of these schemes involve Trotter decomposition of the Hamiltonian H of interest into L_τ "time slices" and then introduction of auxiliary classical degrees of freedom "s" to decouple the interacting (i.e., nonquadratic) part of the Hamiltonian. The main result of this analysis is that one can integrate out the fermions in favor of the classical fields s, which are now governed by a known partition function. Returning to the original fermion problem, the expectation value of any operator O, with respect to either the ground state or the thermally averaged one, may be written as [13–15]

$$\langle O \rangle = \sum_{\{s\}} P_s \langle O \rangle_s. \quad (2)$$

For Hamiltonians without a sign problem, P_s are positive numbers and have the interpretation of the probability distribution for the instantaneous configuration s of the classical variables, while $\langle O \rangle_s$ may be thought of as the expectation value of O with respect to a free fermion Hamiltonian determined also by the instantaneous configuration "s." The exact form of P_s and $\langle O \rangle_s$ depends on the original Hamiltonian H [13–15], and the interested reader may find explicit expressions corresponding to the Hubbard model in the Supplemental Material [27].

Perhaps most crucially, owing to the aforementioned relation to the free fermions, the expectation values $\langle O \rangle_s$ can be shown to follow the Wick's theorem [13,14]. For example, $\langle c_1^\dagger c_2 c_3^\dagger c_4 \rangle_s = \langle c_1^\dagger c_2 \rangle_s \langle c_3^\dagger c_4 \rangle_s - \langle c_1^\dagger c_4 \rangle_s \langle c_3^\dagger c_2 \rangle_s$. As one might expect, this implies that the single particle Green's function G_s, with respect to a fixed configuration s, defined as $G_s^{ij} = \langle c_j^\dagger c_i \rangle_s$, is sufficient to determine the expectation value $\langle O \rangle_s$ of *all* operators at a fixed s.

We claim that within DQMC, ρ_A is given by the following simple expression:

$$\rho_A = \sum_{\{s\}} P_s \rho_{A,s}, \quad (3)$$

where

$$\rho_{A,s} = C_{s,A} e^{-c^\dagger \log(G_{s,A}^{-1} - \mathbb{I}) c}. \quad (4)$$

Here, the fermionic creation and annihilation operators c, $c^\dagger$ are restricted to region A, and $G_{s,A}$ is the projection of the Green's function G_s to the region A. That is, $G_{s,A}^{ij} = G_s^{ij}$ for $i, j \in A$. $C_{s,A} = \mathrm{Det}(\mathbb{I} - G_{s,A})$ is a normalizing coefficient that ensures $\mathrm{tr}\rho_{A,s} = 1$.

Proof.—$\rho_{A,s}$ in Eq. (4) reproduces the single particle Green's function G_s^{ij}: $\mathrm{tr}(\rho_{A,s} c_j^\dagger c_i) = G_s^{ij}$ for $i, j \in A$. This is a consequence of the fact that the reduced density matrix for a free fermionic system [16–18] is given by an expression identical to Eq. (4), with $G_{s,A}$ replaced by the actual Green's function for the free problem [28]. Now, since the Wick's theorem holds for a fixed configuration s, it follows that $\langle O \rangle_s = \mathrm{tr}(\rho_{A,s} O)$ for *all* operators O whose support lies in the subregion A. Therefore,

$$\mathrm{tr}(\rho_A O) = \sum_s P_s \,\mathrm{tr}(\rho_{A,s} O) = \langle O \rangle, \quad (5)$$

where we have used Eq. (2). The operator ρ_A in Eq. (3) thus reproduces the expectation value of all operators O with support in A, and therefore indeed corresponds to the reduced density matrix for A [29].

Equations (3) and (4) are our main result. They express the reduced density-matrix of an interacting fermionic system for arbitrary regions A, as a sum of appropriately weighted operators that describe auxiliary free fermion systems. We emphasize that the form of ρ_A in Eq. (3) holds even for systems that have a fermion sign problem, though in that case, not all P_s will be positive, making the Monte Carlo sampling unfeasible at low temperatures.

Renyi entropies S_n—As a concrete application of the decomposition in Eq. (3), consider the Renyi entanglement entropy $S_n = -[1/(n-1)] \log \mathrm{tr}(\rho_A^n)$ for $n = 2$,

$$S_2 = -\log\Big[\sum_{\{s\},\{s'\}} P_s P_{s'} \{ \mathrm{Det}(G_{s,A} G_{s',A} + (\mathbb{I} - G_{s,A})(\mathbb{I} - G_{s',A})) \} \Big], \quad (6)$$

where Det denotes matrix determinant. The above expression can be readily evaluated in the Monte Carlo simulations by sampling the expression inside the {} brackets over two copies of the system, with the joint probability distribution function $P_s P_{s'}$. As is evident from the above expression, just the knowledge of the single particle's Green's function G_s in the DQMC is sufficient to determine the

Renyi entropy S_2 (or, for that matter, any Renyi entropy S_n by a straightforward generalization [30]). This is rather different than the calculation of the Renyi entropies in the bosonic Monte Carlo simulations [9], or in the variational Monte Carlo simulations [10], where one is required to sample a highly nonlocal quantity (''swap operator'') to calculate the Renyi entropy.

Implementation.—One of the attractive features of our algorithm is that it does not require any technical ingredients beyond the DQMC, because the probability distribution P_s, and the Green's function G_s are exactly the same as the ones that enter the conventional DQMC algorithm. The cost of our algorithm to calculate Renyi entropies S_n scales as $N^3 L_\tau$, where N is the number of particles and L_τ is the number of time slices, akin to the calculation of ground state energy or correlation functions in the DQMC [13–15].

We benchmarked the algorithm by calculating S_2 for the ground state of a one-dimensional chain of ten sites with the Hamiltonian $H = -t\sum_{\sigma,ij}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}$. Figure 1 shows the comparison of S_2 obtained from a projector Monte Carlo scheme with the results from exact diagonalization for three different values of the Hubbard U. Clearly, the algorithm reproduces the correct result rather accurately. This example and other test runs (see the Supplemental Material [27]) suggest that S_2 should be calculable to an accuracy of a few percent with 10^7 Monte Carlo sweeps for subsystems of linear length around ten lattice spacings in two dimensions.

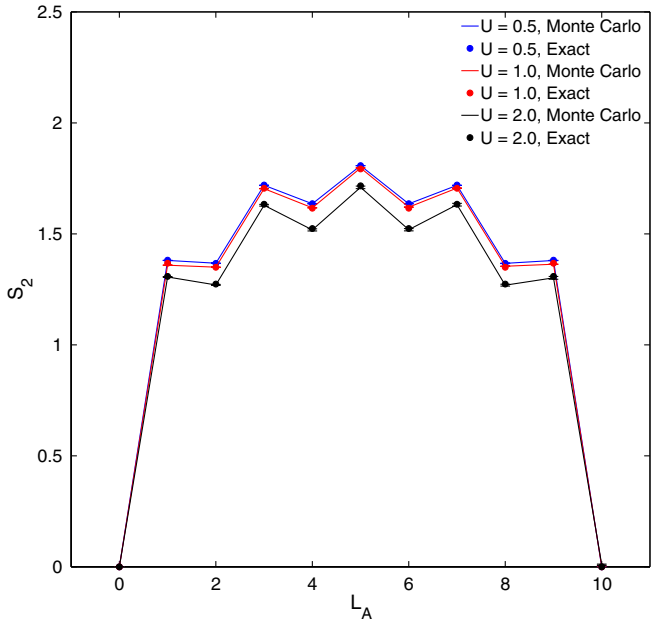

FIG. 1 (color online). Renyi entropy S_2 for the ground state of a ten-site single-band Hubbard model with periodic boundary conditions, as a function of subsystem size L_A. The three different plots correspond to three different values of the Hubbard U (with $t = 1$).

Entanglement Hamiltonian.—The method presented allows one to also obtain an expression for the interacting entanglement Hamiltonian [3]. The entanglement Hamiltonian is defined as $\rho_A = e^{-\mathcal{H}_A}$. For a generic interacting system, it is rather difficult to obtain a closed form expression for $\mathcal{H}_A$ as a second-quantized operator. Bosonic Monte Carlo techniques [9] can only access Renyi entropies, while purely analytical techniques are as yet limited to free bosons or fermions [16–18], in which case $\mathcal{H}_A$ is quadratic, or they include the effect of interactions via the renormalization of $\mathcal{H}_A$ that is still quadratic [31]. We now show that for models that can be simulated via DQMC, a systematic expansion for $\mathcal{H}_A$ can be obtained, which includes all interactions and is calculable within the Monte Carlo simulation. Let us rewrite the expression for the interacting density matrix as

$$\rho_A = \sum_{\{s\}} P_s e^{-c^\dagger h_s c}, \tag{7}$$

where h_s is a matrix with components $h_s^{ij} = (\log(G_s^{-1} - \mathbb{I}))^{ij}$, and we have dropped a constant shift to h_s. A cumulant expansion on ρ_A yields $\mathcal{H}_A$,

$$\mathcal{H}_A = \sum_{ij} h^{ij} c_i^\dagger c_j + \sum_{ijkl} k^{ijkl} c_i^\dagger c_j c_k^\dagger c_l + \cdots, \tag{8}$$

where $h^{ij} = \sum_{\{s\}} P_s h_s^{ij}$ and $k^{ijkl} = (1/2)[\sum_{\{s\},\{s'\}} P_s P_{s'} \times h_s^{ij} h_{s'}^{kl} - \sum_{\{s\}} P_s h_s^{ij} h_s^{kl}]$. One can similarly write down the higher-order terms. As the above expressions show, the numbers h^{ij} and k^{ijkl} can be sampled within the Monte Carlo simulation in an efficient manner, and thus we have obtained a systematically calculable expression for the interacting entanglement Hamiltonian.

Discussion.—Leaving aside interactions, even the free fermions have a rather peculiar ground state entanglement, $S \sim L_A^{d-1} \log L_A$, where L_A is the linear extent of the entangling surface [32,33], and the prefactor is a *universal* number that only depends on the shape of the Fermi surface and the entangling region. This is in contrast to almost all other known systems, where the entanglement scales as $S \sim L_A^{d-1}$, the so-called area law [34,35]. Does a similar violation of area law hold for strongly interacting systems that do not have electronlike quasiparticles [10,36]? Such questions are potentially addressable in the sign-free models, such as the one studied in Ref. [37] using the algorithm presented here. On this note, it is worth mentioning that there is a large class of problems that do not have a fermion sign problem even at a finite density of fermions, including multiorbital Hubbard models [19,20,22]. These models provide a platform to test Widom's conjecture [32,33,38] in Fermi liquids [11,39]. Furthermore, for a single-orbital Hubbard model at half-filling on bipartite lattices, one can study the effect of more generic interactions, for example, spin-orbit coupling [40,41] or the nearest neighbor interactions [21].

Another direction of interest might be to explore the entanglement structure of fermionic systems close to the Mott transition [42]. Such systems can exhibit rich physics including quantum criticality and/or exotic phases [43,44]. A sign-problem-free example is the honeycomb Hubbard model [45–47]. It has been shown recently [46,47] that this model exhibits a second-order Mott transition from a semimetal to an antiferromagnet. The behavior of the Renyi entropy can potentially serve to further characterize the critical point. Indeed, the universal entanglement footprints of a quantum critical point are rather distinctive—for a subsystem of size L_A and a fixed shape, the Renyi entropy at a $2+1$-dimensional relativistic critical point scales as $S_2 = \alpha L_A - C + O(1/L_A)$, where C is a shape-dependent universal number [7,8]; this is in contrast to topological ordered systems [1,2], where the analog of C (topological entanglement entropy) is shape independent. Similar considerations apply to the sign-problem-free multiorbital Hubbard model studied in Ref. [48], where evidence was provided for an exotic algebraic spin-liquid phase [49,50]. Another as yet unexplored territory is the quantum entanglement in heavy fermionic systems [51,52], where the Kondo screening competes with the magnetic interactions. The method is also directly applicable to several lattice matter-gauge theories [19,24,25] and could be useful, for example, in exploring the possibility of topological superconductivity in $SU(2)$ matter-gauge theory [24,25,53]. One can also study entanglement in sign-problem-free spin systems, such as the spin-$1/2$ Heisenberg model on the square lattice, by studying the large U limit of the Hubbard model at half-filling. This will provide an alternate viewpoint as compared to the bosonic Monte Carlo simulation [9].

Finally, we note that the expansion in Eq. (8) for $\mathcal{H}_A$ might help in understanding which specific interacting systems have a (non) local entanglement Hamiltonian. The problem of determining the locality of $\mathcal{H}_A$ for a given problem has been essentially reduced to understanding the locality of the average $\langle h_s \rangle$ with respect to the probability distribution P_s. The expansion for $\mathcal{H}_A$ is also suggestive of an area law scaling for the entanglement entropy $S \sim L_A^{d-1}$, up to multiplicative logarithmic corrections [32,33], for the ground states of d dimensional systems that can be simulated without a sign problem. This is because the contribution of the first term in the expansion, $\langle h_s \rangle$, to the entanglement entropy is likely to be an area law, again up to multiplicative logarithmic corrections, because the individual terms h_s themselves correspond to free fermion problems, and the averaging converges due to the lack of a sign problem. This would imply that h behaves essentially as a $d-1$-dimensional system, and thus the contribution to the entanglement entropy from higher-order terms in the expansion can be expected to scale in a similar fashion. This argument is by no means rigorous, and we leave such explorations for the future.

Before closing, we note that even though the method presented can access the Renyi entropies S_n for integer n, we presently do not know how to calculate the von Neumann entropy S_{vN}, a challenge open to other Monte Carlo schemes as well [9,10].

To summarize, we showed that the reduced density matrix for interacting fermions can be expressed rather simply in terms of free fermions, and we used this fact to develop an algorithm to calculate the Renyi entanglement entropies, and the entanglement Hamiltonian, for interacting fermionic systems in general dimensions. Our method provides an information-theoretic reformulation of the DQMC method, while opening a pathway to explore many-body entanglement in strongly correlated fermionic systems.

I thank Matthew Fisher and Max Metlitski for useful discussions and Brian Swingle, Bryan Clark, and Madhav Mani for helpful comments on the draft. This research was supported in part by the National Science Foundation under Grant No. NSF PHY11-25915.

[1] A. Kitaev and J. Preskill, Phys. Rev. Lett. **96**, 110404 (2006).
[2] M. Levin and X.-G. Wen, Phys. Rev. Lett. **96**, 110405 (2006).
[3] H. Li and F. D. M. Haldane, Phys. Rev. Lett. **101**, 010504 (2008).
[4] L. Fidkowski, Phys. Rev. Lett. **104**, 130502 (2010).
[5] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. **B424**, 443 (1994).
[6] P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.
[7] S. Ryu and T. Takayanagi, Phys. Rev. Lett. **96**, 181602 (2006).
[8] H. Casini and M. Huerta, J. Phys. A **42**, 504007 (2009).
[9] M. B. Hastings, I. Gonzalez, A. B. Kallin, and R. G. Melko, Phys. Rev. Lett. **104**, 157201 (2010).
[10] Y. Zhang, T. Grover, and A. Vishwanath, Phys. Rev. Lett. **107**, 067202 (2011).
[11] J. McMinis and N. M. Tubman, Phys. Rev. B **87**, 081108 (R) (2013).
[12] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[13] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).
[14] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).
[15] F. F. Assaad and H. G. Evertz, in *Computational Many-Particle Physics*, edited by Fehske *et al.* (Springer, Berlin, 2008).
[16] M.-C. Chung and I. Peschel, Phys. Rev. B **64**, 064412 (2001).
[17] S.-A. Cheong and C. L. Henley, Phys. Rev. B **69**, 075111 (2004).
[18] I. Peschel, J. Phys. A **36**, L205 (2003).
[19] S. Hands, I. Montvay, S. E. Morrison, M. Oevers, L. Scorzato, and J. Skellurd, Eur. Phys. J. C **17**, 285 (2000).
[20] C. Wu and S.-C. Zhang, Phys. Rev. B **71**, 155115 (2005).

[21] J. E. Hirsch, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).

[22] Y. Motome and M. Imada, J. Phys. Soc. Jpn. **66**, 1872 (1997).

[23] C. Vafa and E. Witten, Phys. Rev. Lett. **53**, 535 (1984).

[24] E. Dagotto, F. Karsch, and A. Moreo, Phys. Lett. B **169**, 421 (1986); E. Dagotto, A. Moreo, and U. Wolff, Phys. Rev. Lett. **57**, 1292 (1986).

[25] S. Hands, J. B. Kogut, M.-P. Lombardo, and S. E. Morrison, Nucl. Phys. **B558**, 327 (1999).

[26] T. Schäfer, Phys. Rev. D **57**, 3950 (1998).

[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.111.130402 for details.

[28] The only technical difference in our case is that the matrices G_s are not necessarily Hermitian, i.e., $G_s^{ij} \neq (G_s^{ji})^*$. This is because G_s can be thought of as an equal-time Green's function for a free fermion problem in the presence of a time-dependent Zeeman field $H(t) = U\sum_i (c_i^\dagger \sigma_z c_i) s(i,t)$, where $s(i,t)$ is the value of the classical Ising variable "s" at site i and time slice t. Wick's theorem, of course, continues to hold for $\rho_{A,s}$, which is all we require (see the Supplemental Material [27] for details).

[29] Note that the reduced density matrix is uniquely determined by the condition that $\langle O \rangle = \mathrm{tr}(\rho_A O)$ for all operators O. Indeed, if $\mathrm{tr}(\rho_A O) = \mathrm{tr}(\tilde{\rho}_A O)$ for all O, then one can prove $\rho_A^{\alpha\beta} = \tilde{\rho}_A^{\alpha\beta}$ element-wise by choosing appropriate O that pick out a particular element (α, β) of ρ_A, $\tilde{\rho}_A$.

[30] Explicitly, Renyi entropy S_n in the Monte Carlo is given by $S_n = -[1/(n-1)] \log \mathrm{tr}(\rho_A^n)$, where

$$\mathrm{tr}(\rho_A^n) = \sum_{\{s_\alpha\}} \prod_{\beta=1}^{n} P_{s_\beta} F_A(s_1, s_2, \ldots, s_n)$$

and

$$F_A(s_1, s_2, \ldots, s_n) = \left(\prod_{\beta=1}^{n} C_{s_\beta, A} \right) \mathrm{Det}\left(\mathbb{I} + \prod_{\gamma=1}^{n} (G_{s_\gamma, A}^{-1} - \mathbb{I})^{-1} \right).$$

Thus, one samples $F_A(s_1, s_2, \ldots, s_n)$ with the probability distribution $\prod_{\beta=1}^{n} P_{s_\beta}$, over n copies of the system.

[31] V. Alba, M. Haque, and A. M. Läuchli, Phys. Rev. Lett. **110**, 260403 (2013).

[32] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).

[33] D. Gioev and I. Klich, Phys. Rev. Lett. **96**, 100503 (2006).

[34] L. Bombelli, R. K. Koul, J. Lee, and R. D. Sorkin, Phys. Rev. D **34**, 373 (1986).

[35] M. Srednicki, Phys. Rev. Lett. **71**, 666 (1993).

[36] B. Swingle and T. Senthil, Phys. Rev. B **87**, 045123 (2013).

[37] E. Berg, M. A. Metlitski, and S. Sachdev, Science **338**, 1606 (2012).

[38] H. Widom, Operator Theory **4**, 477 (1982).

[39] B. Swingle, Phys. Rev. B **86**, 045109 (2012); Phys. Rev. Lett. **111**, 100405 (2013).

[40] M. Hohenadler, T. C. Lang, and F. F. Assaad, Phys. Rev. Lett. **106**, 100403 (2011).

[41] D. Zheng, G.-M. Zhang, and C. Wu, Phys. Rev. B **84**, 205121 (2011).

[42] N. F. Mott and R. Peierls, Proc. Phys. Soc. London **49**, 72 (1937).

[43] Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato, and G. Saito, Phys. Rev. Lett. **91**, 107001 (2003).

[44] Y. Okamoto, M. Nohara, H. Aruga-Katori, and H. Takagi, Phys. Rev. Lett. **99**, 137207 (2007).

[45] Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad, and A. Muramatsu, Nature (London) **464**, 847 (2010).

[46] S. Sorella, Y. Otsuka, and S. Yunoki, Sci. Rep. **2**, 992 (2012).

[47] F. F. Assaad and I. F. Herbut, Phys. Rev. X **3**, 031010 (2013).

[48] F. F. Assaad, Phys. Rev. B **71**, 075103 (2005).

[49] X.-G. Wen, Phys. Rev. B **65**, 165113 (2002).

[50] M. Hermele, T. Senthil, M. P. A. Fisher, P. A. Lee, N. Nagaosa, and X.-G. Wen, Phys. Rev. B **70**, 214437 (2004).

[51] F. F. Assaad, Phys. Rev. Lett. **83**, 796 (1999).

[52] S. Capponi and F. F. Assaad, Phys. Rev. B **63**, 155114 (2001)

[53] Y. Nishida, Phys. Rev. D **81**, 074004 (2010).