Correlation density matrix: An unbiased analysis of exact diagonalizations

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Given the ground-state wave function for an interacting lattice model, we define a "correlation density matrix" (CDM) for two disjoint separated clusters A and B to be the density matrix of their union minus the direct product of their respective density matrices. The CDM can be decomposed systematically by a numerical singular-value decomposition to provide a systematic and unbiased way to identify the operator(s) dominating the correlations, even unexpected ones.

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I. INTRODUCTION

The ground state of a strongly interacting, quantum-mechanical lattice model (with spin, boson, or fermion degrees of freedom) is characterized by long-range order, power-law correlations, or the lack of these. When such a system is studied numerically, it may be unclear *a priori* what kind of correlation will be dominant especially in cases where exotic order or disorder are possible, such as the doped square-lattice Hubbard model or (better) the highly frustrated $s=1/2$ kagome antiferromagnet; in the latter system spin-spin, spin-Peierls, spin-nematic, or chiral-order parameters were all serious candidates.[1] Before computing the ground-state correlations, one must first guess which operators are important—a choice which is necessarily biased by one's prior knowledge or preconceptions and is problematic for hidden or exotic orders.

In contrast, approaches based on the density matrix (DM) of a cluster of several sites are unbiased—apart from specification of that cluster—since the DM specifies the expectation of every operator local to the cluster including the "key operator(s)" meaning those having long-range order (i.e., order parameter) or having strong correlations. For exact diagonalizations (ED) of interacting systems, the DM was used as a diagnostic to compare different system sizes[2] or truncations of the Hilbert space.[3]

Here we propose an application of the density matrix as a way to uncover correlations/orders from numerics *without* requiring any foreknowledge of what kinds to expect. Consider two small disjoint clusters A and B (identical apart from a translation), either cluster having a Fock-Hilbert space of dimension D. Let $\hat{\rho}^{AB}$ be the many-body density matrix for the disconnected "supercluster" $A\cup B$, constructed from the whole system's ground-state wave function by tracing out all other sites, with $\hat{\rho}^{A}$ and $\hat{\rho}^{B}$ similarly defined. Then we define the *correlation density matrix* (CDM) to be

$$\hat{\rho}^{C} \equiv \hat{\rho}^{AB} - \hat{\rho}^{A} \otimes \hat{\rho}^{B}. \tag{1}$$

If there were no correlations between clusters A and B, then $\hat{\rho}^{AB}=\hat{\rho}^{A}\otimes\hat{\rho}^{B}$ and $\hat{\rho}^{C}=0$.

The CDM defined in Eq. (1) contains all possible intercluster correlations.[4] Write the ("connected") correlation of the fluctuations of any two operators as $\langle\hat{P}\hat{Q}\rangle_{c}\equiv\langle\hat{P}\hat{Q}\rangle - \langle\hat{P}\rangle\langle\hat{Q}\rangle$; then if $\hat{P}(A)$ and $\hat{Q}(B)$ act on clusters A and B,

$$\langle\hat{P}(A)\hat{Q}(B)\rangle_{c} = \mathrm{Tr}[\hat{\rho}^{C}\hat{P}(A)\hat{Q}(B)]. \tag{2}$$

II. INDEX RELABELING AND THE OPERATOR SINGULAR-VALUE DECOMPOSITION

The key notion underlying our processing of the CDM is, given the $D\times D$ matrix representing an operator on a cluster's D dimensional Hilbert space, to rewrite it as an D^2-component *vector* of complex numbers using fused indices[5] $(a',a)\leftrightarrow\alpha(a',a)$, $(b',b)\leftrightarrow\beta(b',b)$. Say that $\hat{\rho}^{C}$ is known in terms of the product states $|a'\rangle|b'\rangle$ and $|a\rangle|b\rangle$ of the occupation-number basis on the clusters.[6] Then

$$\hat{\rho}^{C} = \sum_{a',b',a,b} \hat{\rho}^{C}_{a'b',ab}|a'\rangle|b'\rangle\langle a|\langle b| \equiv \sum_{\alpha\beta} C_{\alpha\beta}\hat{g}_{\alpha}\hat{h}_{\beta}, \tag{3}$$

where $\hat{\rho}^{C}_{a'b',ab}\equiv C_{\alpha(a',a),\beta(be,b)}$. Here $\hat{g}_{\alpha}\equiv|a'\rangle\langle a|$ and $\hat{h}_{\beta}\equiv|b'\rangle\langle b|$ are bases for the respective clusters A and B, manifestly orthonormal in terms of the *Frobenius norm*

$$\|\hat{P}\|_{F}^{2} \equiv \sum_{a',a} |P_{a',a}|^{2} = \mathrm{Tr}(\hat{P}^{\dagger}\hat{P}) \tag{4}$$

for any operator $\hat{P}$, and the *Frobenius inner product*

$$(\hat{P},\hat{Q})_{F} \equiv \sum_{a',a} P^{*}_{a',a}Q_{a',a} = \mathrm{Tr}(\hat{P}^{\dagger}\hat{Q}). \tag{5}$$

[In the fused-index notation, Eqs. (4) and (5) take on the usual form of a vector norm and vector inner product.]

Next numerical singular-value decomposition (SVD) can be made of $C_{\alpha\beta}$ as a matrix of complex numbers:

$$C_{\alpha\beta} = \sum_{\nu} \sigma_{\nu}U_{\nu\alpha}V_{\nu\beta}, \tag{6}$$

where U and V are unitary matrices and $\{\sigma_{\nu}:\nu=1,\ldots,D^2\}$ are the singular values. [Equation (6) can also be written in the matrix form $C=U^{T}\Sigma V$ where $\Sigma\equiv\mathrm{diag}(\{\sigma_{\nu}\})$.] Substituting Eq. (6) into Eq. (3), we obtain the operator singular-value decomposition,

$$\hat{\rho}^{C} = \sum_{\nu=1}^{D^2} \sigma_{\nu}\hat{X}_{\nu}(A)\hat{Y}_{\nu}(B). \tag{7}$$

This (simple but powerful) expression is the key formula of our Brief Report. Each term represents the correlated quan-

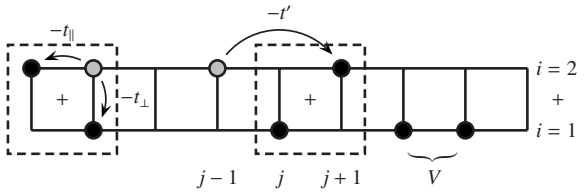

FIG. 1. Model: spinless fermions, with hardcore excluding nearest neighbors on a ladder, with longitudinal hopping $t_\parallel \equiv 1$, transverse hopping $t_\perp$, and correlated hopping t'. The correlation density matrix involves two clusters, each of 2×2 sites, with their centers (marked +) separated by r. This ladder has length $L=8$, with periodic boundary conditions as indicated by the + at right edge.

tum fluctuations of Frobenius-orthonormalized basis operators,[7] $\hat{X}_\nu \equiv \Sigma_\alpha U_{\nu\alpha}\hat{g}_\alpha$ on cluster A and $\hat{Y}_\nu \equiv \Sigma_\beta V_{\nu\beta}\hat{h}_\beta$, on cluster B.

Recalling Eq. (2), we can rewrite any correlation

$$\langle \hat{P}(A)\hat{Q}(B)\rangle_c = \sum_\nu \sigma_\nu [\hat{X}_\nu^\dagger, \hat{P}(A)]_F [\hat{Y}_\nu^\dagger, \hat{Q}(B)]_F \tag{8}$$

in terms of Frobenius inner products (5). In particular, $\langle \hat{X}_\nu(A)^\dagger \hat{Y}_\tau(B)^\dagger\rangle_c = \sigma_\nu \delta_{\nu\tau}$. Thus $\{\hat{X}_\nu(A)^\dagger\}$ and $\{\hat{Y}_\nu(B)^\dagger\}$ are the natural bases into which operators $\hat{P}(A)$ and $\hat{Q}(B)$ should be decomposed. Each $|\sigma_\nu|$ is a normalized measure of the strength of the corresponding intercluster ground-state correlation. By convention, we order the singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{D^2} \geq 0$. This ordering gives a means of approximating $\hat{\rho}^C$ by retaining just the first few terms in expansion (7).

Observe that $\|\hat{\rho}^C\|^2 = \Sigma_\nu |\sigma_\nu|^2$ is a basis-invariant measure of the total correlations between A and B. Since[8]

$$\|\hat{\rho}^C\|_F^2 = \|\hat{\rho}^{AB}\|_F^2 - \|\hat{\rho}^A\|_F^2 \|\hat{\rho}^B\|_F^2, \tag{9}$$

it follows that $\|\hat{\rho}^C\|_F^2 \leq 1 - 1/D^2 \approx 1$, which gives a standard of comparison for numerically obtained σ_ν's.

The CDM typically inherits various symmetries from the input wave function (ultimately from the Hamiltonian) such as spin rotations, lattice rotations/reflections, or fermion number conservation.[9] The matrix $C_{\alpha\beta}$ breaks up into symmetry-labeled blocks, which (as with diagonalization) can be singular-value decomposed independently. Each term in expansion (7) is thus assigned to a sector according to the quantum numbers carried by $\hat{X}_\nu$ and $\hat{Y}_\nu$, and each sector is interpreted as representing a different kind of correlation.

A convenient test bed to study CDM properties is a noninteracting system (including BCS states) for which density matrices can be calculated exactly.[10] We analytically checked the CDM and its operator SVD for a free Fermi sea in one dimension (Ref. 11, chapters 5 and 6), finding the expected Fermi-like (FL) correlations with an $r^{-1/2}$ envelope and charge-density-wave-like (CDW) correlations with an r^{-2} envelope.

III. LADDER MODEL: LIMITING REGIMES AND OPERATOR CLASSES

We now test the CDM method on a toy system (Fig. 1) in which spinless fermions hop on a two-leg ladder of length L;

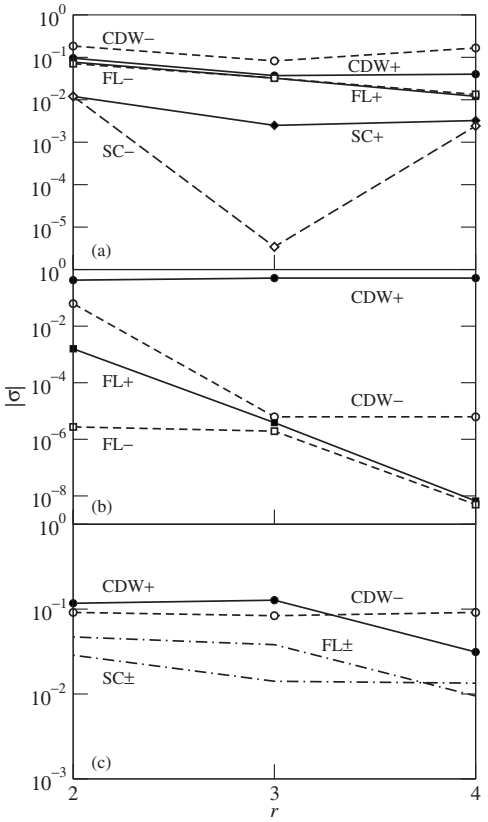

FIG. 2. Each plot shows (on a log scale) the magnitude of the largest singular value for each symmetry sector of operators. The symmetries are labeled "CDW" for number operator (or any combination $c_i^\dagger c_j$ in the same cluster); "FL" for single creation/annihilation (i.e., the correlation function is a two-point Green's function); "SC" for superconducting (combination $c_i^\dagger c_j^\dagger$ in same cluster). The symmetry label $\pm$ denotes even/oddness under exchanging the legs of the ladder. In every case, there are four particles on a ladder of length $L=8$ and twist boundary condition averaging was used. (a) No-passing ladder with $t_\perp = 0.1$, $t' = 0$; (b) rung-fermion case (each fermion delocalized on a rung) with $t_\perp = 100$, $t' = 0$; SC singular values do not appear since they are $\sim 10^{-15}$. (c) Boson pair state: $t_\perp = 0$, $t' = 100$.

they are forbidden to occupy adjacent sites (i.e., the nearest-neighbor repulsion is $V=\infty$). Three kinds of hopping amplitudes appear: $t_\parallel \equiv 1$ along legs, $t_\perp$ along rungs, and t' a "correlated hop" conditioned on a second fermion, $-t'(c_j^\dagger c_i + c_i^\dagger c_j)\hat{n}_k$; here i and j are two steps apart on the same leg, and $\hat{n}_k$ is the number operator for the site between i and j on the opposite leg (which would block the $t_\parallel$ hops).

The phase diagram (see Ref. 11, Fig. 8.1) may be understood through the three limiting cases in which one hopping dominates. (a) $t_\parallel$ dominant ("no-passing" limit): the leg index is a conserved flavor; the model reduces to a free-fermion chain (with fermions on alternate legs), (b) $t_\perp$ dominant ("rung-fermion" limit): each fermion delocalizes on a rung, so at low energy the model maps to reduces to a fermion chain with nearest neighbors excluded, and (c) t' dominant ("paired" limit): fermions bind into effective (p-wave) boson pairs (in one dimension, with nearest neighbors excluded). Regime (c) must be dominated by superconductivity at large length scales.

TABLE I. Correlation behaviors in limiting-case models. Row labels (a, b, and c) correspond to the panels in Fig. 2. Columns "Sim" summarize behaviors inferable from Fig. 2: "large," "medium," or "small" indicate singular values roughly constant with r, i.e., possible long-range order (values over 10^{-1}, 10^{-2}, or 10^{-3}, respectively). Singular values decaying with r are labeled "d(fast)" or "d(slow)." Columns are labeled by the symmetry sectors as in Fig. 2. For comparison, the columns "Th" are from semianalytic computations of Ref. 12; exp=exponential decay, LRO=long-range order. For the pairing limit (c), the FL correlation exponent varies with filling n, with $\alpha(n=1/4)\approx 1.1$.

	CDM singular values							
	CDW^+		CDW^-		$FL^{\pm}$		$SC^{\pm}$	
	Sim	Th	Sim	Th	Sim	Th	Sim	Th
a	Medium	r^{-2}	Large	$r^{-1/2}$	d(slow)	Exp	Small	$r^{-2.5}$
b	Large	LRO?	~0?		d(fast)	r^{-1}	0	$r^{-2.2}$??
c	d(slow)	r^{-2}	Medium	$r^{-\alpha}$	d(slow)	Exp	Small	$r^{-1/2}$

Each of the three limiting cases maps nontrivially to free fermions. Elsewhere[12] we derived from these maps a semianalytic method ("intervening particle expansion") to calculate various correlation functions; the results of Ref. 12 have illuminated the present calculation. The asymptotic behaviors (as expected) are that of a Luttinger liquid: power-law decays, with possibilities of commensurate locking when the filling is a rational fraction.

We performed exploratory exact diagonalizations using periodic boundary conditions, with four fermions on a ladder of length $L=8$, the smallest (nontrivial) case at 1/4 filling. [This is the most interesting filling and the hardest, since the Hilbert space is largest at filling 1/4: see Ref. 13(b), appendix.] The largest block matrix for a sector is 27×27. (As in our earlier ED studies on the square lattice,[2,13] the spinlessness and the neighbor exclusion greatly limit the Hilbert space compared to, e.g., a Hubbard system of the same dimensions.) To minimize finite-size effects on the density matrices, it was necessary to use phase-twist boundary conditions[14] (i.e., to thread flux through the "ring" of sites) and average over 21 distinct phase angles. (See Ref. 2 and Sec. 8.2.4 of Ref. 11.)

Each of our two clusters is 2×2 (two adjacent rungs) as shown in Fig. 1, the smallest cluster that can capture superconducting correlations; each cluster's Hilbert space has dimension $D=7$. The operators $\{\hat{X}_\nu, \hat{Y}_\nu\}$ emerging from the operator singular-value decomposition are classified into three main categories according to the fermion number change ΔF they carry: (i) CDW, $\Delta F=0$, e.g., the number operator $\hat{n}_i$ on site i (Ref. 15); (ii) FL, $\Delta F=\pm 1$, e.g., the operator $c_i^\dagger$ on a site. The two-point Green's function, the dominant long-range correlation in a Fermi sea, belongs with this operator sector. (iii) SC (superconducting), $\Delta F=\pm 2$; such operators are the order parameters for superconductivity. In addition, each operator can be even or odd under exchange of the ladder's legs, which we denote by appending "+" or "−."

Generically, the basis operators $\{\hat{X}_\nu, \hat{Y}_\nu\}$ do not take the minimal form one would adopt in defining a correlation function (even in the *free*-fermion case). Instead, complicated terms are admixed.[16] For example, the dominant operator in the FL sector not only has single creation operators $c_i^\dagger$, but terms $c_i^\dagger \hat{n}_j$.

IV. NUMERICAL RESULTS AND CONCLUSIONS

Figure 2 presents the numerical singular values for the CDM in the three limits; the decay behaviors of the different correlations are summarized in Table I, where they are compared with our knowledge from the intervening particle expansion.[12] Due to the limited system sizes for ED, the CDM analysis cannot determine the dominant kind of correlation at large distances. That is practically impossible for Luttinger liquids in any case: for the hardcore boson chain (related to our models) the asymptotic (superfluid) correlations may dominate only after 50–100 sites.[17] Table I shows there is a general correspondence between the decay rate of known correlations and that of the singular values; the degree of correlation in Fig. 2 tends to be overestimated due to the very small range of r.

The rung-fermion case (b) at filling 1/4 breaks translational symmetry, with period-2 long-range order. Examination of Fig. 2(b) indeed shows the corresponding contrast with the other two cases: the singular value for the order-parameter operator (CDW+) is nondecaying and saturates the bound $\sigma=1/2$, whereas other kinds of singular values are orders of magnitude smaller.

In the boson-pair case (c), as t' grows large (the boson-pair limit), a crossover is expected to asymptotic SC correlations; but Fig. 2(c) shows that CDW correlations still dominate at all accessible distances, similar to hardcore bosons.[17] A partial success of the CDM analysis is that the SC singular values are visibly larger than in the other cases, competitive with FL correlations; absent any other knowledge of this system, the SC order parameter would be flagged for further study (e.g., analytic or by quantum Monte Carlo).

In all three cases, most correlations decay generically[12] as $C(r)\sim \cos(2mk_F r+\delta)/|r|^x$, where $2mk_F$ is an even multiple of the Fermi wave vector and x is some correlation exponent. Over a small range of r, the with oscillations with r obscure the asymptotic r dependence of the singular values. We conjecture each such correlation is associated with a *pair* of singular values, oscillating 90° out of phase inside the same envelope. Ideally, then, one should plot $[\Sigma'_\nu \sigma_\nu^2]^{1/2}$, where "$\Sigma'$" runs over just one symmetry sector to obtain a monotonic decay as $1/|r|^x$. In practice, for reasons we do not understand, this gave little or no improvement.

To conclude, we have introduced a tool for analyzing exact-diagonalization ground states, using the density matrix of a pair of clusters to extract *all* their correlations in an unbiased fashion. Furthermore, via singular-value decomposition, the kind of operator dominating the correlations could be identified using Eq. (7). There are two regimes where asymptotic decays are not at issue and the correlation density matrix based on exact diagonalization should be effective. First, for systems believed to have negligible correlations beyond the nearest neighbor—e.g., quantum-spin liquids in highly frustrated antiferromagnets[1]—the CDM is the foolproof way to confirm the absence of *any* correlations. Second, in systems having long-range order [such as our case (b)], the CDM detects the symmetry breaking. On the other hand, critical states [such as the Luttinger liquids of our cases (a) and (c) above] are the *least* promising systems for study by CDM (or any other method), so long as system size is limited by dependence on ED. But when the CDM and density-matrix renormalization-group methods are married,[18] the asymptotic scaling becomes accessible for one-dimensional systems.

Another unbiased method has been proposed to discover the symmetry breaking operator from ED using the density matrix.[19] It differs from the CDM in two ways: (i) it is based on the DM of just one cluster; (ii) it requires not only the ground state's wave function, but that of several low-lying eigenstates which are conjectured to be linear combinations of symmetry broken states (and degenerate in the thermodynamic limit). That method is meant only for cases of long-range order, whereas in principle the CDM identifies the strongest correlations even in disordered phases.

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[4] We do not know any property of the CDM that distinguishes the case of purely classical correlations from that of quantum entanglement between A and B.

[5] The change of viewpoint in using the fused index in Eq. (3) is a species of "partial transpose," but not at all the one introduced by A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).

[6] As noted in Ref. 11, Sec. 6.3.2, a basis state for $A \cup B$ in the operation-number basis may differ from the direct product $|a\rangle|b\rangle$ by a fermion sign, since the creation operators defining it may come in a different order. A similar technicality appears in the extraction of any cluster density matrix from a wave function for the whole system: see Ref. 2.

[7] Observe that since $\mathrm{Tr}(\hat{\rho}^{AB})=\mathrm{Tr}(\hat{\rho}^{A})=\mathrm{Tr}(\hat{\rho}^{B})=1$ is true of any density matrix, we always have $\mathrm{Tr}(\hat{\rho}^{C})\equiv 0$. Then since $\mathrm{Tr}_A(\hat{\rho}^{C})\equiv \mathrm{Tr}_B(\hat{\rho}^{C})=0$, it follows that $\mathrm{Tr}\,\hat{X}_\nu=\mathrm{Tr}\,\hat{Y}_\nu=0$ for each of the SVD operators.

[8] Equation (9) follows because [using Eqs. (4) and (5)] $(\hat{\rho}^{AB},\hat{\rho}^{A}\otimes\hat{\rho}^{B})_F=\langle\hat{\rho}^{A}\otimes\hat{\rho}^{B}\rangle=\langle\hat{\rho}^{A}\rangle\langle\hat{\rho}^{B}\rangle=\|\hat{\rho}^{A}\|^2\|\hat{\rho}^{B}\|^2$. We achieve the bound when $\hat{\rho}^{AB}$ describes a pure state (norm 1), while every eigenvalue of $\hat{\rho}^{A}$ (and necessarily of $\hat{\rho}^{B}$) is $1/D$, i.e., when $A\cup B$ is in a maximally entangled state.

[9] Our density matrices are averaged over degenerate ground states, if any, to restore all symmetries, as explained in Ref. 2.

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[15] Strictly speaking, a CDW operator is *even* under conjugation and is distinguished from *staggered-flux* (SF) operators that are *odd*. SF correlations characterize "*d*-density wave" states with an ordered spatial pattern of (orbital) currents, which have been realized in various spin-full ladder models. [See U. Schöllwock, S. Chakravarty, J. O. Fjaerestad, J. B. Marston, and M. Troyer, Phys. Rev. Lett. **90**, 186401 (2003), and references therein.] Unfortunately, our implementation did not distinguish these cases: "CDW" in our results incorporates the "SF" operators.

[16] This is reminiscent of the admixed terms in the quasiparticle creation operator of a Landau-Fermi liquid or perhaps of the extra terms in a scaling operator of the renormalization group.

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