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The correlation density matrix: new tool for analyzing exact diagonalizations[1] CHRISTOPHER L. HENLEY, SIEW-ANN CHEONG, Cornell University — When a lattice model of strongly interacting spins or fermions is studied numerically, it may be unclear *a priori* what kind of correlation will be dominant – especially in cases where exotic order or disorder has been suggested (e.g. Kagomé spin-1/2 antiferromagnet, or doped square-lattice Hubbard model). To resolve this, consider two small clusters of a few sites A and B, offset by a vector $\mathbf{r}$. Let $\hat{\rho}_{AB}$ be the many-body density matrix for the disconnected cluster $A \cup B$, constructed from the whole system's ground state wavefunction by tracing out all sites except those in A or B, with $\hat{\rho}_A$ and $\hat{\rho}_B$ similarly defined. Then all possible correlations between A and B are contained in the "correlation density matrix" $\hat{\rho}_{\rm corr}(\mathbf{r}) \equiv \hat{\rho}_{\mathbf{AB}} - \hat{\rho}_{\mathbf{A}} \otimes \hat{\rho}_{\mathbf{B}}$. Using singular-value decomposition we can write $\hat{\rho}_{\rm corr} = \sum_i \lambda_i \hat{\Phi}_i(A) \hat{\Phi}'_i(B)$, where $\hat{\Phi}_i$ and $\hat{\Phi}'_i$ are normalized operators on the respective clusters; the terms represent different correlation functions, which are naturally ordered by the magnitudes $|\lambda_i|$. This permits a systematic, unbiased numerical method to identify the important correlations, given the ground state wavefunction. The procedure will be tested on ladders of spinless fermions with infinite nearest-neighbor repulsion, which are expected to have Luttinger liquid behavior.

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