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 \textit{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 \(r\). 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” \(\hat{\rho}_{\text{corr}}(r) \equiv \hat{\rho}_{AB} - \hat{\rho}_A \otimes \hat{\rho}_B\). Using singular-value decomposition we can write \(\hat{\rho}_{\text{corr}} = \sum_i \lambda_i \hat{\Phi}_i(A) \hat{\Phi}^\prime_i(B)\), where \(\hat{\Phi}_i\) and \(\hat{\Phi}^\prime_i\) 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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