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Energy density matrix decomposition of interacting quantum systems[1] JARON KROGEL, JEONGNIM KIM, FERNANDO REBOREDO, Materials Theory Group, Oak Ridge National Laboratory — We develop energy density matrices that parallel the one-body reduced density matrix for many-body quantum systems. Just as the density matrix gives access to the number density and orbital occupations, the energy density matrix yields the energy density and orbital energy levels. The eigenvectors of the matrix provide a natural orbital partitioning of the energy density while the eigenvalues comprise a single particle like energy spectrum obeying a total energy sum rule. In systems where a single particle picture is valid (e.g. for mean-field or weak interactions), the spectrum gives the expected results. We demonstrate that the QMCPACK implementation of the energy density matrix approach is correct for the cases of the non-interacting electron gas and the spherical harmonic oscillator. We further explore the meaning of the computed spectrum in the case of the fully interacting electron gas.

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