

# Exchange-Correlation Energies from Pairing Matrix Fluctuation and Particle-Particle-Random Phase Approximation

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We formulate an adiabatic connection for the exchange-correlation energy in terms of pairing matrix fluctuation. This connection opens new channels for density functional approximations based on pairing interactions. Even the simplest approximation to the pairing matrix fluctuation, the particle-particle Random Phase Approximation (pp-RPA), has some highly desirable properties. It has no delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than particle-hole RPA, and eliminates static correlation error for singly bound systems. Most significantly, the pp-RPA is the first known functional that has an explicit and closed-form dependence on the occupied and unoccupied orbitals and captures the energy derivative discontinuity in strongly correlated systems. These findings illustrate the potential of including pairing interactions within a density functional framework.

Ref: . [arXiv:1306.4957](https://arxiv.org/abs/1306.4957) Exchange-Correlation Energy from Pairing Matrix Fluctuation and the Particle-Particle Random Phase Approximation, [Helen van Aggelen](#), [Yang Yang](#), [Weitao Yang](#)