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A Non-Local, Energy-Optimized Kernel: Recovering Second-Order Exchange and Beyond in Extended Systems JEFFERSON BATES, SAVIO LARICCHIA[1], ADRIENN RUZSINSZKY, Temple University — The Random Phase Approximation (RPA) is quickly becoming a standard method beyond semi-local Density Functional Theory that naturally incorporates weak interactions and eliminates self-interaction error. RPA is not perfect, however, and suffers from self-correlation error as well as an incorrect description of short-ranged correlation typically leading to underbinding. To improve upon RPA we introduce a short-ranged, exchange-like kernel that is one-electron self-correlation free for one and two electron systems in the high-density limit. By tuning the one free parameter in our model to recover an exact limit of the homogeneous electron gas correlation energy we obtain a non-local, energy-optimized kernel that reduces the errors of RPA for both homogeneous and inhomogeneous solids. To reduce the computational cost of the standard kernel-corrected RPA, we also implement RPA renormalized perturbation theory for extended systems, and demonstrate its capability to describe the dominant correlation effects with a low-order expansion in both metallic and non-metallic systems. Furthermore we stress that for norm-conserving implementations the accuracy of RPA and beyond RPA structural properties compared to experiment is inherently limited by the choice of pseudopotential.

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