

TABLE I: Comparison of convergence of GW -RPA correlation energies for the He and B atoms. The RPA correlation energy is computed using the standard integral of Eq. (53) (third column) or the plasmon form of Eq. (38) (fourth column). All energies are in Hartrees. N_{max} is the number of single-particle state included in the calculations for each angular momentum and spin channel. The single particles energies and wave functions are from the LSDA.

Atom	N_{max}	integral	plasmon
He	25	-0.1038	-0.0804
He	50	-0.0916	-0.0805
He	100	-0.0849	-0.0806
He	150	-0.0830	-0.0806
He	200	-0.0819	-0.0806
B	50	-0.4126	-0.2129
B	100	-0.3600	-0.2171
B	200	-0.2844	-0.2175
B	300	-0.2584	-0.2175

the exact RPA energy of Eq. (38) in the second to last row in each table. For completeness, we also include the other energy terms to show their relative importance and their variation with single-particle theory, discussed further below. The Hartree energy reported in the table is the one based on the actual, non-spherical electron density (*i.e.* based on m -dependent occupancies $f_{nlm\sigma}$ as opposed to the spherical density in most DFT atomic calculations).

We begin by considering our main approximate form of Eq. (45). As we can see from comparing to the exact RPA energy, and especially when comparing to the static versions, the basic approximation underlying Eqs. (44) and (45) is a relatively good one: the absolute correlation energy of Eq. (45) differs by at most 0.1 Ha from the exact RPA one. This shows that the fundamental approximation of assuming high-frequency screening is reasonable even in atoms. For solids and extended systems where the Coulomb interaction shows true long-ranged behavior (as opposed to atoms), plasma modes are of higher energies than interband energies and the situation should be further improved.

As explained above, the approximate form of Eq. (45) is as computationally expensive to calculate as the exact RPA plasmon form but is additionally very difficult to converge. To obtain the values in the tables, we had to perform the following steps simultaneously: (i) increase the size of the radial axis to make for a denser continuum, (ii) increase the number of one-particle states entering the calculation to ensure a fixed level of convergence with increasing radial axis, and (iii) exclude contributions to $W_t(\Delta_t)$ from transitions t' that were within a small energy window δ of Δ_t (*i.e.*, $|\Delta_{t'} - \Delta_t| < \delta$) while sending $\delta \rightarrow 0$.

Moving on to the approximations that assume static screening, we see that they overes-