only when the matrix elements $\langle t|V|\tilde{p}\rangle$ become small. On the other hand, the dynamic case has a denominator that changes sign from positive to negative as Δ_t sweeps through the plasma energies, and the denominator itself gets large when Δ_t gets large. The dynamic screening behavior of the plasmons is missing in the static formula which assumes that no matter what the transition energy, the plasmons can screen it adiabatically. This is obviously erroneous for transitions where $\Delta_t \gtrsim \tilde{\omega}_p$. Therefore, the static formula can be improved by adding some dynamic behavior in the screening even if done approximately. This is an example of what was meant in Section 10 regarding the use of plasmon-pole models or model dielectric functions to improve the static COHSEX.

We end this section with some observations on the results in Tables II and III and their dependence on the single-particle theory. The parts of the total energy that depend only on the single-particle orbitals, *i.e.* the kinetic, electron-ion, Hartree, and Fock exchange energies, depend weakly on the choice of LSDA versus HF single-particle orbitals, changing at most $\sim$1%. This is not surprising *a posteriori* as visual comparison of the radial functions show small differences. However, the correlation energies depend more strongly on the choice of single-particle theory, and this is due to the relatively large differences between the single-particle energies. The HF-based correlation energies are smaller than the LSDA simply because HF transition energies are larger than LSDA: *e.g.*, for atomic boron the important $2s$-$2p$ transition is at 0.210 Ha in LSDA but at 0.232 Ha in HF; larger transition energies mean weaker screening and thus weaker correlation. As per Section 8, it matters greatly whether the Green's function G_0 is generated by a local or non-local potential.

The true many-body Green's function G obeys Dyson's Eq. (4) and is thus generated by a non-local (and dynamic) self-energy $\Sigma_{xc}(x, x', \omega)$. *A priori*, we would expect that a static but non-local potential $U_0(x, x')$ should generate a decent non-interacting G_0 which should be close to the true G, certainly closer than one generated by a static local potential. However, as discussed in Section 8, choosing the "best" U_0 via an optimization of the total energy functional is problematic unless constraints are imposed on U_0. The outstanding theoretical problem is what constraints to impose and which ones are the "best" ones. This obviously involves creating and justifying metrics that tells us how good each choice of constraints will be in practice.

12. SUMMARY AND OUTLOOK

Our work has focused on the correlation energy functional with Luttinger-Ward theory (specifically the Klein functional) within the GW-RPA approximation. The Green's functions used in the energy functional are of non-interacting form. The main findings in this work are threefold. First, we present the exact rewriting of the GW-RPA correlation energy functional in Eq. (38) in terms of differences between plasma and interband energies. This form is directly amenable to computation, shows good convergence properties in the atomic tests, and has prospects for having its computational scaling improved by use of matrix square root algorithms. Second, we describe the approximate rewriting of the GW-RPA correlation energy functional in Eqs. (44) and (45) where the correlation energy is written as a sum of screened interband transition contributions; the main approximation is to assume that the dominant screening dynamics are much faster than the key interband dynamics;