Calculating the energies of quasiparticles in very large systems using GPU-implemented stochastic GW

Tim Duong,1 Phillip Thomas,2 Minh Nguyen,1 Barry (Yangtao) Li,1 and Daniel Neuhauser1
1Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, California, 90095, USA
2Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

**Linear Scaling Stochastic Functional Theory**

Density functional theory (DFT) is a method that determines the electronic density of many-body systems and calculates various electronic properties of those systems through functionals of that density. The recently developed stochastic density functional theory (sDFT) uses the stochastic sampling of random combinations of occupied and unoccupied states to approximate the electronic density. This density is formally made from the occupied states by applying a low-pass energy filter that uses a Chebyshev polynomial expansion onto the stochastic orbitals to obtain filtered stochastic orbitals that approximate the electronic density. This process can run these calculations separately and in parallel. With the superior parallelization of GPUs due to their greater number of parallel threads, sGW can now be run much more efficiently. Our GPU-implemented sGW specifically uses Nvidia CUDA technology for these calculations and will be tested on systems such as chronophores and silicon clusters of varying sizes.

**Linear Scaling Stochastic GW**

The GW approximation is an efficient method for describing quasiparticles and quasiparticle behavior. It makes use of the self-energy term and approximates it as the product of the Green’s function, G, and the polarization potential, W. This project specifically deals with one-shot GW in which only the first iteration of GW is used rather than the summation, ignoring the self-consistency in G and W when performing the approximation.

\[
\Sigma^P (r_1, r_2, t; \epsilon) = i \hbar G_0 (r_1, r_2, t) W^P (r_1, r_2; t; \epsilon)
\]

\[
i \hbar G_0 (r_1, r_2, t) \equiv \langle r_1 | e^{-i \hbar \tau_{st}/\hbar} P_\tau (t) | r_2 \rangle
\]

\[
W^P (r_1, r_2; t; \epsilon) \equiv \langle r_1 | u_C \otimes \chi (t; \epsilon) \otimes u_C | r_2 \rangle
\]

**Stochastic GW (sGW)** employs methods similar to sDFT in which stochastic sampling is used to calculate the Green’s function and screened coulomb interaction. As with sDFT, this enables linear scaling with the system size and greatly improves on the fourth-order scaling of the traditional GW approximation.

In this project, sGW is used to obtain the energies of quasiparticles. These energies are then used to correct the HOMO/LUMO energy gap from sDFT, resulting in a method that can more accurately design theoretical materials in computer-simulated experiments.

\[
\epsilon_{QP} (\epsilon) = \epsilon + \Sigma^P (\omega_{QP}; \epsilon) + \Sigma^X (\epsilon) - \Sigma^C (\epsilon)
\]

**Major References**


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