Numerical Algorithms for Accelerating GW and BSE Calculations

Team Members: Chao Yang, Andrew Canning, Jack Deslippe, Jeff Neaton, Steven Louie (LBNL), Yousef Saad (University of Minnesota), Alex Demkov , Jim Chelikowsky (University of Texas at Austin)

Develop efficient algorithms and implementations to accelerate excited and ground state electronic structure calculation within the GW and BSE formalism on DOE leadership class supercomputers. Leverage the development in SciDAC FASTmath institute on eigenvalue and linear equation solvers to improve the performance of PARSEC and BerkeleyGW software packages

Excited States and GW Formalism

Excited states of complex materials via Green's function formalism of many-body perturbation theory

- Dyson's equation for quasi-particle energies E_n^{QP} and wavefunctions ψ_n^{QP} (a nonlinear eigenvalue problem)

$$\left[-\frac{1}{2}\nabla^2 + V_{\{ion\}} + V_H + \Sigma\left(E_n^{QP}\right)\right]\psi_n^{QP} = E_n^{QP}\psi_n^{QP}$$

- Self-energy approximation:

$$\Sigma(r,r',\omega) = i\int \frac{d\omega'}{2\pi} e^{\{-i\delta\omega'\}} G(r,r';\omega-\omega')W(r,r';\omega')$$

- Dielectric matrix and screened Coulomb interaction
  - $\epsilon_{G,G'} = \delta_{G,G'} - v(q+G')P_{G,G'}(q;\omega)$
  - $P(r,r',\omega) = \Sigma_{\{n,m\}} \frac{f_n - f_m}{\epsilon_n - \epsilon_m - \omega}\psi_n(r)\psi_m^*(r)\psi_n^*(r')\psi_m(r')$
  - $W_{\{G,G'\}}(q,\omega) = \epsilon_{\{G,G'\}}^{\{-1\}}(q;\omega)v(q+G')$

Eigenvectors for Polarizability Matrix

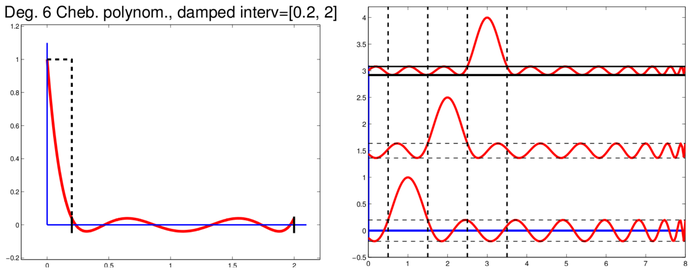
- $P(r,r',\omega) = \Sigma_{\{n,m\}} \frac{f_n - f_m}{\epsilon_n - \epsilon_m - \omega}\psi_n(r)\psi_m^*(r)\psi_n^*(r')$
- Need both occupied and unoccupied (empty) states
- The number of eigenpairs required can easily reach thousands or tens of thousands

Our approaches (spectrum slicing)

- Polynomial filtering + subspace iteration
- Multiple shift-invert Lanczos with implict restart
- Contour integral based subspace iteration
- Need initial estimate of the density of state

(See FASTmath poster on eigensolver)

Polynomial Filtering



- Extremal versus interior eigenvalues
- Exploit multiple levels of parallelism on leadership class machines
- Reduce the cost of orthogonalization and Rayleigh-Ritz calculation by limiting the size of each slice
- Need to worry about missing eigenvalues and double counting

Polarizability without Unoccupied States

- Construct a "localized" basis for the occupied states (e.g., maximum locallized Wannier functions) Φ
- Rewrite P as

$$\hat{P} = \Phi^* P \Phi = \sum_i (D_i^v \Phi)^* P^c \boxed{H_v(\omega)^{-1} P^c (D_i^v \Phi)},$$

where $P^c = I - P^v$ is the projector associated with the unoccupied states, D_i^v =diag(ψ_i^v) and $H_v(\omega) = H + (\omega - \epsilon_c)$

Steinheimer equation

$$W = V + WPV$$

where V is the Coulomb interaction, P is polarizability, and $WPVe_j = V\Delta n$, Δn is the induced electron density that satisfy the self consistent equations

$$\Delta n = 2\sum_i \psi_i^v \odot \Delta\psi_i^v$$

$$H_v \Delta\psi_i^v = -P^c(\psi_i^v \odot w_i)$$

- Must solve shifted linear systems with multiple right hand sides. Krylov subspace is shift invariant, we may recycle the subspace for multiple linear systems
- Develop preconditioners to accelerate convergence

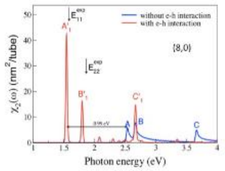
Bethe-Salpeter Eigenvalue Problem

$$\left(E_{ck}^{\{QP\}} - E_{vk}^{QP}\right)A_{vck}^S + \sum_{v'c'k'} \langle vck|K^{eh}|v'c'k'\rangle = \Omega^S A_{vck}^S$$

- Hamiltonian has structure, eigenvalues come in pairs
- Solve the eigenvalue problem by structure preserving minimization algorithm if a few eigenstates are needed
- When a large number of eigenstates are needed, use polynomial filtering or contour integral projection method to reduce the dimension of the problem first before solving a dense eigenvalue problem by ScaLAPACK

Future Plans

- Deploy the latest development in eigensolvers by SciDAC FASTmath institute in both PARSEC and BerkelyGW
- Develop customized acceleration strategies to speedup DFT unoccupied states calculation required by the existing GW/BSE algorithms
- Develop and test algorithms that do not require unoccupied states
- Performance optimization for leadership class machines
- Applications



More Information: contact Chao Yang, LBNL, CYang@llnl.gov, 510-486-6424