BSE in

http://www.exciting-code.org

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Outline

- Review BSE
- Implementation within LAPW and exciting
  - Elements of the BSE
    - Direct interaction term
    - Exchange interaction term
  - Screened Coulomb interaction
    - q-dependent screening
    - Singularities
- TDDFT kernel from BSE
- Parallelization

BSE

- e-h eigenvalue problem (effective electron-hole Hamiltonian)

$$\sum_{v'c'\mathbf{k}'} H_{vc\mathbf{k},v'c'\mathbf{k}'} A^{\lambda}_{v'c'\mathbf{k}'} = \mathcal{E}^{\lambda} A^{\lambda}_{vc\mathbf{k}}$$

- macroscopic dielectric function including excitonic effects

$$\epsilon^{\alpha\alpha}_{\mathrm{M}}(\omega) = 1 - \frac{8\pi}{V} \sum_{\lambda} |t^{\alpha}_{\lambda}|^2 \left[\frac{1}{\omega - \mathcal{E}_{\lambda} + i\delta} + \frac{1}{-\omega - \mathcal{E}_{\lambda} - i\delta} \right]$$

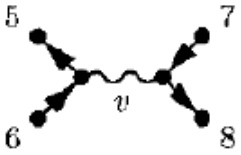
$$t^{\alpha}_{\lambda} = \sum_{vc\mathbf{k}} A^{\lambda}_{vc\mathbf{k}} \frac{\langle v\mathbf{k}|\hat{p}_{\alpha}|c\mathbf{k}\rangle}{\varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}}}$$

The BSE Hamiltonian

- Three parts

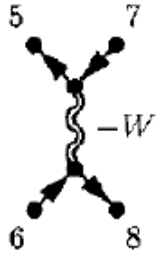
$$H^{\mathrm{eff}} = H^{\mathrm{diag}} + H^{\mathrm{x}} + H^{\mathrm{dir}}$$

- Repulsive exchange interaction



$$H^{\mathrm{x}}_{vc\mathbf{k},v'c'\mathbf{k}'} = \int \mathrm{d}^3r\mathrm{d}^3r'\psi_{v\mathbf{k}}(\mathbf{r})\psi^*_{c\mathbf{k}}(\mathbf{r})\bar{v}(\mathbf{r},\mathbf{r}')\psi^*_{v'\mathbf{k}'}(\mathbf{r}')\psi_{c'\mathbf{k}'}(\mathbf{r}')$$

- Attractive direct interaction



$$H^{\mathrm{dir}}_{vc\mathbf{k},v'c'\mathbf{k}'} = -\int \mathrm{d}^3r\mathrm{d}^3r'\psi_{v\mathbf{k}}(\mathbf{r})\psi^*_{c\mathbf{k}}(\mathbf{r}')W(\mathbf{r},\mathbf{r}')\psi^*_{v'\mathbf{k}'}(\mathbf{r})\psi_{c'\mathbf{k}'}(\mathbf{r}')$$

- Diagonal part

$$H^{\mathrm{diag}}_{vc\mathbf{k},v'c'\mathbf{k}'} = (E_{c\mathbf{k}} - E_{v\mathbf{k}})\delta_{vv'}\delta_{cc'}\delta_{\mathbf{k}\mathbf{k}'}$$

The BSE Hamiltonian

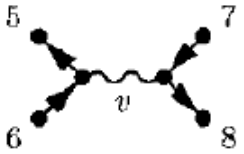
- H(+) resonant part
- H(–) anti-resonant part
- H(#), H(#') coupling parts (beyond Tamm-Dancoff approximation, not yet implemented)

$$H^{\text{eff}} = \begin{pmatrix} H^{(+)}_{v_1 c_2, v_3 c_4} & H^{(\#)}_{v_1 c_2, c_3 v_4} \\ H^{(\#')}_{c_1 v_2, v_3 c_4} & H^{(-)}_{c_1 v_2, c_3 v_4} \end{pmatrix}$$

The BSE Hamiltonian

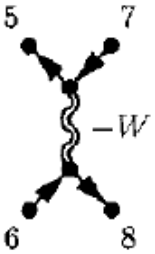
Effective e-h Hamiltonian

$$H^{\text{eff}} = H^{\text{diag}} + H^{\text{x}} + H^{\text{dir}}$$

- exchange part <vc| 

|v'c'>

$$H^{\text{x}}_{vc\mathbf{k},v'c'\mathbf{k}'} = \frac{1}{V}\sum_{\mathbf{G}} M^{*}_{vc\mathbf{k}}(\mathbf{G})\bar{v}_{\mathbf{G}}(0)M_{v'c'\mathbf{k}'}(\mathbf{G})$$

- direct part <vc| 

|v'c'>

$$H^{\text{dir}}_{vc\mathbf{k},v'c'\mathbf{k}'} = -\frac{1}{V}\sum_{\mathbf{G}\mathbf{G}'} M^{*}_{vv'\mathbf{k}}(\mathbf{q}+\mathbf{G})W'_{\mathbf{G}\mathbf{G}'}(\mathbf{q})M_{cc'\mathbf{k}}(\mathbf{q}+\mathbf{G}')$$

Common ingredients

- Exchange and direct part of BSE Hamiltonian can be written in terms of:

$$M_{nn'\mathbf{k}}(\mathbf{q}+\mathbf{G}) = \langle n\mathbf{k}|e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}}|n'\mathbf{k}+\mathbf{q}\rangle$$

$$P^{j}_{nn'\mathbf{k}} = \langle n\mathbf{k}|-i\nabla_j|n'\mathbf{k}\rangle$$

wave function within APW-like basis sets

Atomic like basis functions in muffin-tin: **spherical harmonics** expansion

$$\phi^{\mathrm{MT}}_{n\mathbf{k}}(\mathbf{r}) = \sum_{\alpha lmp} A^{\alpha}_{lmp}(n\mathbf{k}) u^{\alpha}_{lp}(r_\alpha) Y_{lm}(\hat{\mathbf{r}}_\alpha)$$

$$A^{\alpha}_{lmp}(n\mathbf{k}) = \sum_{\mathbf{G}} c_{n\mathbf{k}+\mathbf{G}} A^{\alpha}_{lmp}(\mathbf{k}+\mathbf{G})$$

α … atom

n … band index

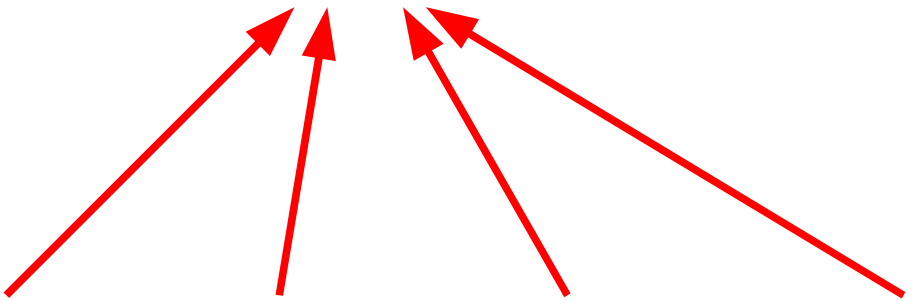
$$\phi^{\mathrm{I}}_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{n\mathbf{k}+\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}$$

Plane waves for interstitial region, slow changes in wave function

Controlling the Hamiltonian

$$H_{vc\mathbf{k},v'c'\mathbf{k}'}$$

Space of transitions: $vc\mathbf{k}$



```
@nstlbse="start_v,stop_v,start_c,stop_c"
```

(**c** counts from Fermi level)

Screening

- Make use of TDDFT response at ω=0

$$\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G}\mathbf{G}'} - \chi^0_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) v_{\mathbf{G}'}(\mathbf{q})$$

$$\chi^{\mathrm{KS}}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \frac{1}{V} \sum_{nm\mathbf{k}} \frac{f_{n\mathbf{k}} - f_{m\mathbf{k}+\mathbf{q}}}{\varepsilon_{n\mathbf{k}} - \varepsilon_{m\mathbf{k}+\mathbf{q}} + \omega + i\delta} M_{nm\mathbf{k}}(\mathbf{q},\mathbf{G}) M^*_{nm\mathbf{k}}(\mathbf{q},\mathbf{G}')$$

- Statically screened Coulomb interaction

$$W_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) = \epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) v_{\mathbf{G}'}(\mathbf{q})$$

Screened interaction at Gamma-point

- Subcell average on spherical Lebedev-Laikov grids (Freysoldt, CPC 2007)

$$W'_{\mathbf{GG'}}(\mathbf{q}) = \frac{1}{V_q}\int_{V_\mathbf{q}} \mathrm{d}^3 p W_{\mathbf{GG'}}(\mathbf{p})$$

$$\int_{V_\mathbf{q}} \mathrm{d}^3 p\, f(\mathbf{p}) = \int \mathrm{d}\hat{\Omega}_\mathbf{p} \int \mathrm{d}p \lambda_\mathbf{q}(p, \hat{\Omega}_\mathbf{p})\, f(\mathbf{q}+\mathbf{p})$$

- Head of W: $W'_{00}(0) = \frac{1}{V_q}\int \mathrm{d}\hat{\Omega}_\mathbf{p} \epsilon^{-1}_{00}(\hat{\Omega}_\mathbf{p}) \int \mathrm{d}p \lambda_\Gamma(p, \hat{\Omega}_\mathbf{p}) \frac{4\pi^2}{p^2}$

- Approximation for head $\frac{1}{V_q}\int \mathrm{d}^3 p \frac{4\pi^2}{q^2} = \frac{2}{\pi} V q_s$

Effective subcell radius: q_s

Controlling the screening

$$\tilde{\epsilon}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) = \sum_{v'c'\mathbf{k}'}$$

Space of transitions

@gqmax

@nemtpy="N_c"

BSE for core-levels

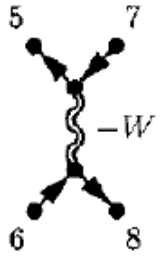
Trick: Treat core states as local orbitals valence states. More information:

- Claudia's talk (tomorrow)
- Weine's tutorial (tomorrow)

TDDFT with a xc-kernel derived from BSE

MBPT xc kernel

- TDDFT kernel derived from BSE (Nanoquanta groups), excitonic part, approximation to 1st order in W:



$$H^{\mathrm{dir}}_{vc\mathbf{k},v'c'\mathbf{k}'} = -\int \mathrm{d}^3r\mathrm{d}^3r'\psi_{v\mathbf{k}}(\mathbf{r})\psi^*_{c\mathbf{k}}(\mathbf{r}')W(\mathbf{r},\mathbf{r}')\psi^*_{v'\mathbf{k}'}(\mathbf{r})\psi_{c'\mathbf{k}'}(\mathbf{r}')$$

- Yields to 1st order in W:

$$f_{\mathrm{xc}}^{\text{e-h}} \approx \chi_{\mathrm{QP}}^{-1} GGWGG \chi_{\mathrm{QP}}^{-1}$$

MBPT xc kernel

- Reformulation of TDDFT Dyson equation (Sottile, PRL 2003)

$$\chi_{\mathbf{G}\mathbf{G}'}(\omega) = \sum_{\mathbf{G}_1\mathbf{G}_2} \chi^0_{\mathbf{G}\mathbf{G}_1}(\omega)\Big[\chi^0_{\mathbf{G}_1\mathbf{G}_2}(\omega) - \sum_{\mathbf{G}_3} \chi^0_{\mathbf{G}_1\mathbf{G}_3} v_{\mathbf{G}_3} \chi^0_{\mathbf{G}_3\mathbf{G}_2} - T^{\mathrm{xc}}_{\mathbf{G}_1\mathbf{G}_2}\Big]^{-1} \times \chi^0_{\mathbf{G}_2\mathbf{G}'}.$$

- Reformulation of xc kernel part

$$T^{\mathrm{xc}}_{\mathbf{G}\mathbf{G}'}(\omega) = \sum_{vc\mathbf{k}} \sum_{v'c'\mathbf{k}'} \frac{M_{vc\mathbf{k}}(\mathbf{G}) W_{vc\mathbf{k},v'c'\mathbf{k}'} M^*_{v'c'\mathbf{k}'}(\mathbf{G}')}{(\varepsilon_{v\mathbf{k}} - \varepsilon_{c\mathbf{k}} + \omega + i\delta)(\varepsilon_{v'\mathbf{k}'} - \varepsilon_{c'\mathbf{k}'} + \omega + i\delta)}$$

$$T_{\mathrm{xc}} = \chi^0 f_{\mathrm{xc}} \chi^0$$

Important parameters

(input/xs/)

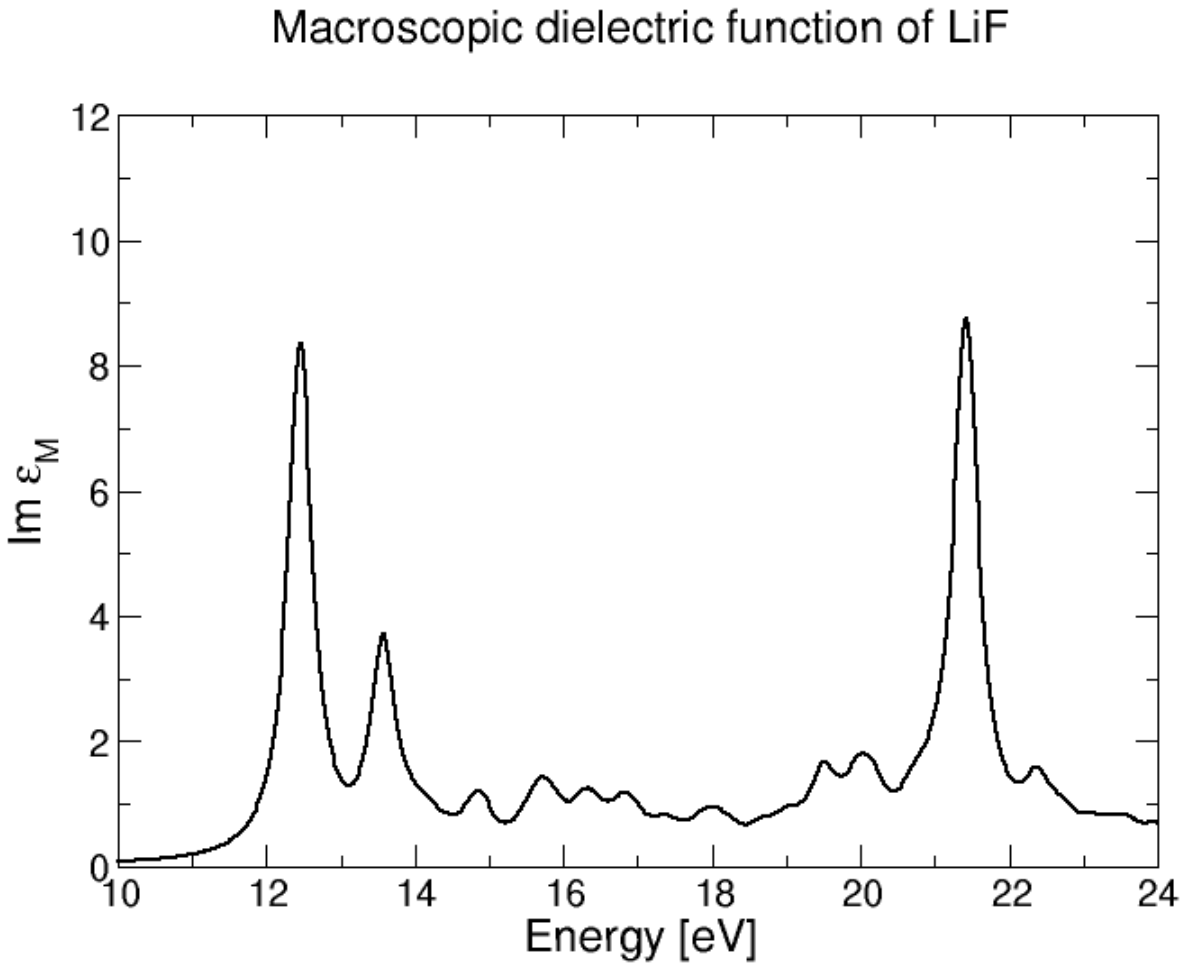
- **@ngridk, @ngridq** k/q-point grid sizes
- **@rgkmax** $|G+k|_{max}R_{min}$ basis set size for wavefunction
- **screening/@nempty** #unocc. states for screening
- **@gqmax** $|G+q|_{max}$ local field effects size
- **energywindow** range of energies for spectrum
- **bse/@nstlbse** ranges for occupied and unocc. states in BSE Hamiltonian
- **bse/@bsetype** type of BSE Hamiltonian (RPA, singlet, triplet)

In practice:

```
<xs xstype="BSE"
 ngridq="4 4 4"
 ngridk="4 4 4" vkloff="0.05 0.15 0.25
 gqmax="3">

   <energywindow intv="0.0 1.0"
    points="1200" />

   <screening screentype="full"
    nempty="115" />

   <BSE bsetype="singlet"
    nstlbsemat="1 5 1 4"
    nstlbse="1 5 1 4"/>

   <qpointset>
      <qpoint>0.0 0.0 0.0</qpoint>
   </qpointset>

</xs>
```

data

templates



Parallelization

MPI parallelization

- Wavefunctions: – #k-points
- Matrix elements – #k-points
- screening – #q-points
- Exchange interaction – #k-points
- Direct interaction – #(kk')-pairs
- Diagonalization – *not yet*

Data parallelism throughout – no side effects

Now grab your coffee and we meet at the excercises...