Complex Energy Integration in Core-Electron Model

Motivation

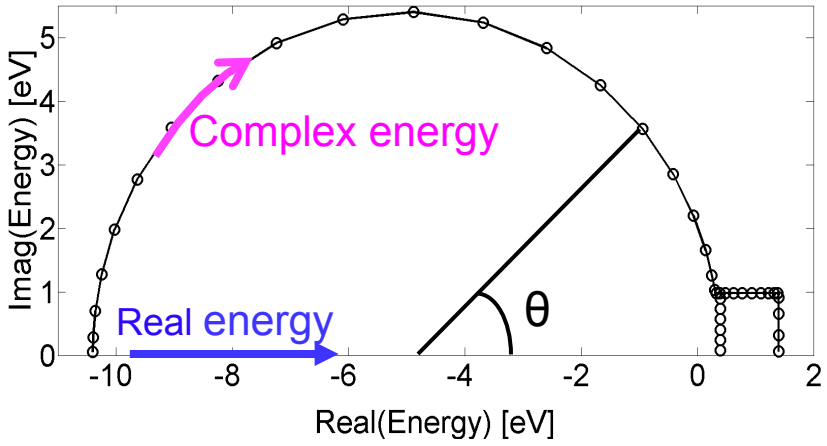
- Traditional method in charge calculation fails for TFET and broken bandgap materials
- Approximations made in distinguishing electrons and holes are unphysical in transport calculation

Approach

- Self-consistent calculation is performed using core-electron model
- All states are treated equally as electronic states
- $G^{<}$ integration is partially calculated in complex energy plane

Results

$$\rho = -\frac{1}{\pi}\int_{-\infty}^{\infty} dE\,\mathrm{Im}[G^r(E)]\,f(E-\mu_R) - \frac{1}{\pi}\int_{-\infty}^{\infty} dE\,G^r(E)\cdot\mathrm{Im}[\Sigma_L(E)]\cdot G^a(E)[f(E-\mu_L)-f(E-\mu_R)]$$



- Only around 30 energy points to cover a 10 eV energy range
- Accuracy of core-electron model + efficiency of electron-hole model