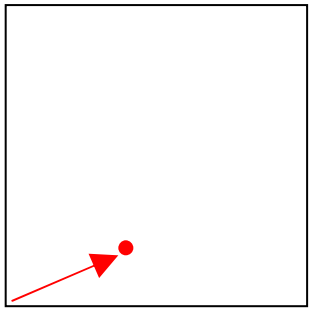
GW-HS

GW – Haydock – Sternheimer

2

GWHS basic steps

Choose k_0 for $\Sigma(k_0)$



GWHS basic steps

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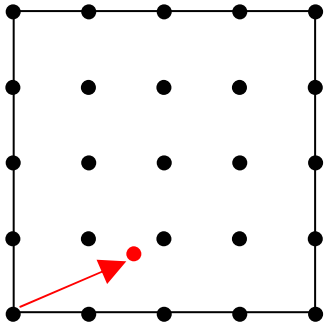
Generate uniform {q} grid for
the screened Coulomb interaction W



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Generate uniform $\{k_0-q\}$ grid for
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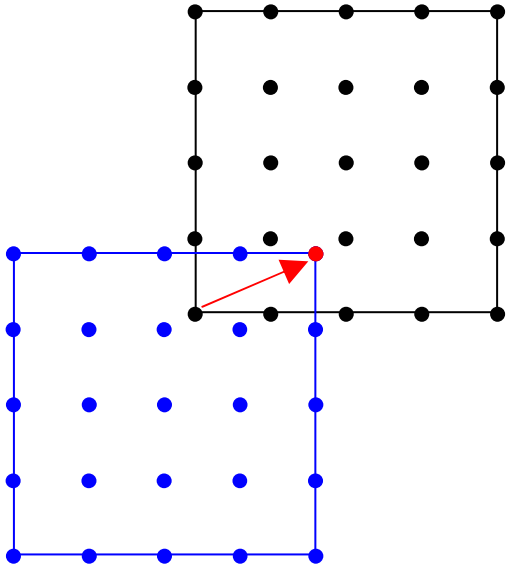

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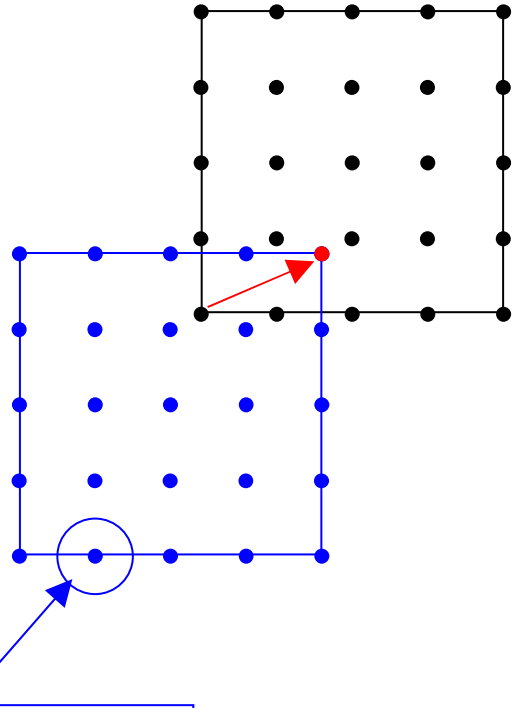
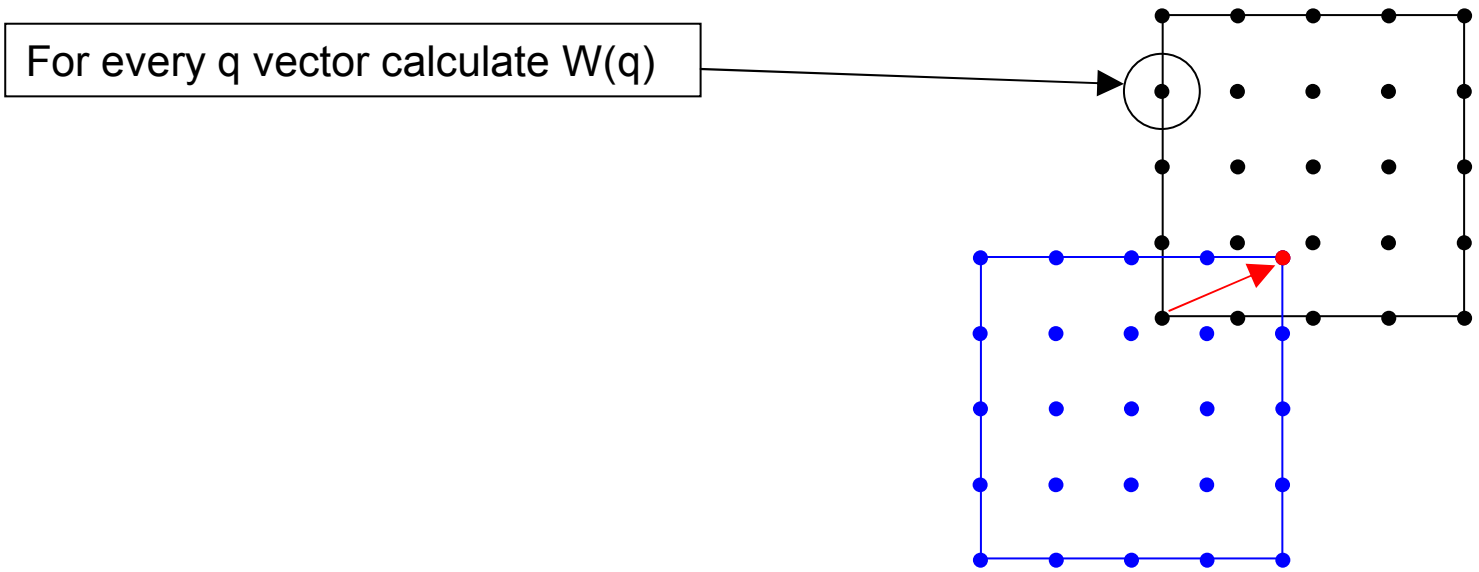


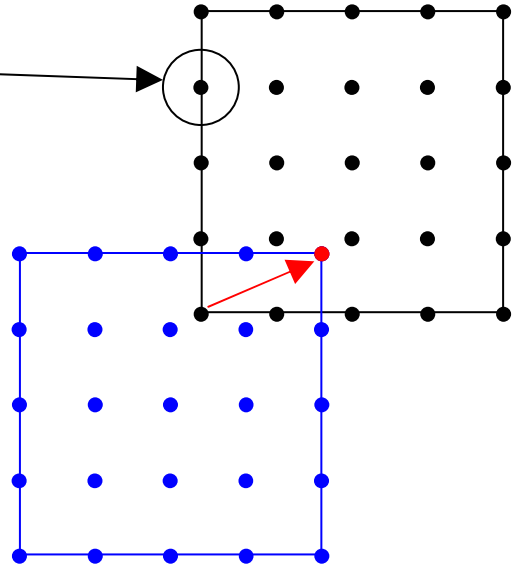
Calculate Green's function for every k_0-q point

GWHS basic steps



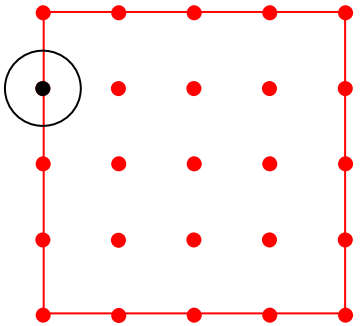
GWHS basic steps

For every q vector calculate W(q)



We need the variation of the charge density
→ BZ integral

Set {k} grid equal to {q} grid



Solve Sternheimer for every k of {k}.

This requires also the k+q eigenstates → fold k+q into {k} grid using G-vector maps

GWHS basic steps

- The occupied wavefunctions are calculated only once at the beginning on the {q} grid
- If we change k_0 for $\Sigma(k_0)$, we only need to re-compute the Green's function,
  the screened Coulomb stays unchanged

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What about the frequency ?

Same idea:

Choose w_0 for $\Sigma(w_0)$

Generate uniform {w} grid for
the screened Coulomb interaction W

Generate uniform {w_0-w} grid for
the Green's function G

- If we change w_0 there is no extra cost since Haydock is frequency-independent

GWHS basic steps

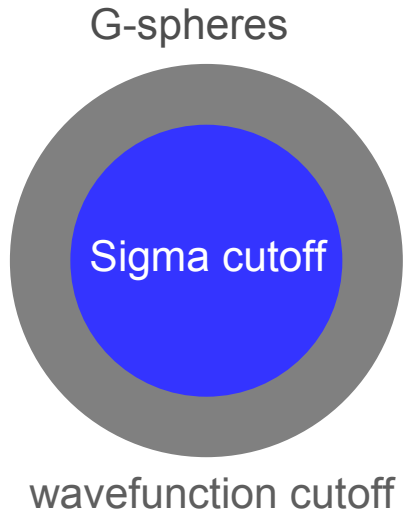
Direct product in real space: $\Sigma(r,r') = G(r,r')\, W(r,r')$

Determine Green's function for every (G,G'), small cutoff
Determine W(G,G') for every G, small cutoff

FFT of Green's function to coarse real-space grid
FFT of W to coarse real-space grid

Σ = G W product in real space

I-FFT of Σ to G-space (small cutoff)



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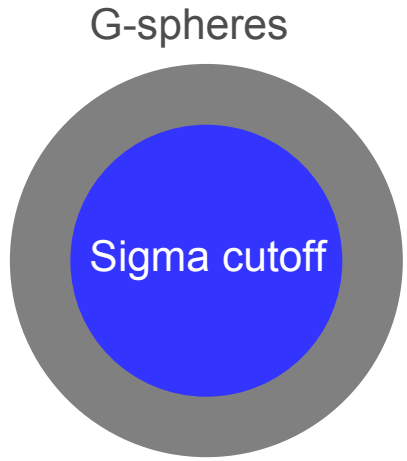

Haydock works fine in G-space

Work in progress

- Frequency integration
  (need to use disk to store W at each frequency)

- Restart of Sternheimer at various q and w with previous guess
  I do not get any improvement in convergence – need to understand

- Is G-basis optimal or we can still exploit the periodic sinc functions?

TODO

- Comparison with BerkeleyGW: plasmon-pole?
- scaling test on silicon supercell

scaling

Green's function

N_q x 4 x (N_{Gs} x (N_{Gs} -1)/2 Lanczos chains)

each chain:

$N_{it\_lanczos}$ x (2 scalar products + 1 Hamiltonian application)

Screened Coulomb

N_w x N_q x N_{Gs} x (N_{it_SCF} x (N_q x 4 x CG sequences))

each sequence:

N_{it_CG} x N_{occ} x (2 scalar products + 1 Hamiltonian application)

TOTAL

$4 \times N_q \times N_{Gs} \times (N_w \times N_{it\_SCF} \times N_q \times N_{it\_CG} \times N_{occ} + (N_{Gs} - 1)/2 \times N_{it\_lanczos})$
x (2 scalar products + 1 Hamiltonian application)

Scaling of Hybertsen/Louie

Calculation of empty states	$N_{Gs} \times N_{occ} \times N_{empty} \times N_q \times N_q$ scalar products
Optical matrix elements	$N_{empty} \times N_q$ (CG sequences) each sequence: N_{it_CG} x (2 scalar products + 1 Hamiltonian application)
Inversion of epsilon	$N_w \times N_q \times 4/3(N_{Gs})^3$ (assuming inversion by LU decomposition)

TOTAL $N_q \times N_{empty} \times (N_{Gs} \times N_{occ} \times N_q + 2 \times N_{it\_CG})$ (scalar products)

$+ N_q \times N_{empty} \times N_{it\_CG}$ (Hamiltonian application)

$+ N_q \times N_w \times (N_{Gs})^3$

Comparison

Assumption

Large systems, Gamma point sampling

Hybertsen/Louie	$N_{Gs} \times N_{occ} \times$	N_{empty} (scalar product)
Haydock/Sternheimer	$N_{Gs} \times N_{occ} \times$	$4 \times N_{it\_SCF} \times N_{it\_CG}$ (Hamiltonian application)

N_{at}^2

N_{empty} (scalar product) – This goes as $N_{Gb} \times N_{empty}$

$4 \times N_{it\_SCF} \times N_{it\_CG}$ (Hamiltonian application) – This goes as $N_{Gb} \times \log N_{Gb}$

H = T + V

T is applied in $O(N_G)$ operations

V requires 3 FFTs and 1 $O(N_G)$ operation. FFTs take $3N_G \log N_G$ operations

Comparison

Assumption

Large systems, Gamma point sampling

Hybertsen/Louie	$N_{Gs} \times N_{occ} \times N_{Gb} \times N_{empty}$
Haydock/Sternheimer	$N_{Gs} \times N_{occ} \times N_{Gb} \times \log N_{Gb} \times 12 \times N_{it\_SCF} \times N_{it\_CG}$

Hybertsen/Louie	N_{at}^4	
Haydock/Sternheimer	$N_{at}^3 \log N_{at}$	– PLANEWAVES

Comparison

Assumption

Large systems, Gamma point sampling

Hybertsen/Louie	$N_{Gs} \times N_{occ} \times N_{Gb} \times N_{empty}$
Haydock/Sternheimer	$N_{Gs} \times N_{occ} \times N_{Gb} \times \log N_{Gb} \times 12 \times N_{it\_SCF} \times N_{it\_CG}$

Hybertsen/Louie	N_{at}^4	
Haydock/Sternheimer	$N_{at}^3 \log N_{at}$	– PLANEWAVES
	N_{at}^3	– LOCAL ORBITALS

$H\psi$ in local orbitals is a O(N) operation

Comparison

CONCLUSION

- Planewaves: The use of $H\psi$ operations instead of sums over empty states has a better scaling thanks to FFTs – O (NlogN)

- Local orbitals: The use of $H\psi$ operations instead of sums over empty states has a better scaling thanks to sparseness O(N)

Hbar