Slides for Patryk's Notes

Patryk Kozlowski

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Outline

Booth GW Supermatrix

$$\boldsymbol{H}^{G_0W_0} = \begin{pmatrix} \boldsymbol{F} & \boldsymbol{W}^< & \boldsymbol{W}^> \\ \boldsymbol{W}^{\dagger<} & \boldsymbol{d}^< & \boldsymbol{0} \\ \boldsymbol{W}^{\dagger>} & \boldsymbol{0} & \boldsymbol{d}^> \end{pmatrix} \tag{1}$$

where $\boldsymbol{F}$ is the Fock matrix, $\boldsymbol{W}^<$ and $\boldsymbol{W}^>$ are the lesser and greater components of the RPA screened Coulomb interaction, defined as

$$W^<_{pk\nu} = \sum_{ia}(pk|ia)\left(X^\nu_{ia} + Y^\nu_{ia}\right) \quad \text{and} \quad W^>_{pc\nu} = \sum_{ia}(pc|ia)\left(X^\nu_{ia} + Y^\nu_{ia}\right) \tag{2}$$

and the auxiliary blocks $\boldsymbol{d}^<$ and $\boldsymbol{d}^>$ are defined as

$$d^<_{k\nu,l\nu'} = \left(\epsilon_k - \Omega_\nu\right)\delta_{k,l}\delta_{\nu,\nu'} \quad \text{and} \quad d^>_{c\nu,d\nu'} = \left(\epsilon_c + \Omega_\nu\right)\delta_{c,d}\delta_{\nu,\nu'} \tag{3}$$

Garnet GW via auxiliary bosons

They used a basis of particle-hole excitations, approximated as bosons. So $\hat{a}_a^\dagger \hat{a}_i \approx \hat{b}_\nu^\dagger$ and $\hat{a}_i^\dagger \hat{a}_a \approx \hat{b}_\nu$ Define

$$\hat{H}^{\mathrm{eB}} = \hat{H}^{\mathrm{e}} + \hat{H}^{\mathrm{B}} + \hat{V}^{\mathrm{eB}} \tag{4}$$

where $\hat{H}^{\mathrm{e}}$ is the electronic Hamiltonian, $\hat{H}^{\mathrm{B}}$ is the bosonic Hamiltonian, and $\hat{V}^{\mathrm{eB}}$ is the electron-boson coupling term, given as

$$\hat{H}^e = \sum_{pq} f_{pq} \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} \tag{5}$$

$$\hat{H}^B = \sum_{\nu\mu} A_{\nu\mu} \hat{b}_\nu^\dagger \hat{b}_\mu + \frac{1}{2} \sum_{\nu\mu} B_{\nu\mu} \left(\hat{b}_\nu^\dagger \hat{b}_\mu^\dagger + \hat{b}_\nu \hat{b}_\mu \right) \tag{6}$$

$$\hat{V}^{eB} = \sum_{pq,\nu} V_{pq\nu} \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} \left(\hat{b}_\nu^\dagger + \hat{b}_\nu \right) \tag{7}$$

Form in bosonic basis

Originally $\hat{H}^{\mathrm{B}}$ in the bosonic basis was

$$\hat{H}^{\mathrm{B}}\left(\hat{b},\hat{b}^{\dagger}\right) = -\frac{1}{2}\operatorname{tr}\mathbf{A} + \frac{1}{2}\begin{pmatrix} \mathbf{b}^{\dagger} & \mathbf{b} \end{pmatrix}\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix}\begin{pmatrix} \mathbf{b} \\ \mathbf{b}^{\dagger} \end{pmatrix} \tag{8}$$

$$= \sum_{\nu\mu} A_{\nu\mu}\hat{b}_{\nu}^{\dagger}\hat{b}_{\mu} + \frac{1}{2}\sum_{\nu\mu} B_{\nu\mu}\left(\hat{b}_{\nu}^{\dagger}\hat{b}_{\mu}^{\dagger} + \hat{b}_{\nu}\hat{b}_{\mu}\right) \tag{9}$$

But if we redefine the basis via a Bogoliubov transformation

$$\begin{pmatrix} \overline{\mathbf{b}} \\ \overline{\mathbf{b}}^{\dagger} \end{pmatrix} = \begin{pmatrix} \mathbf{X} & -\mathbf{Y} \\ -\mathbf{Y} & \mathbf{X} \end{pmatrix}^{T}\begin{pmatrix} \mathbf{b} \\ \mathbf{b}^{\dagger} \end{pmatrix} \tag{10}$$

Effect of transformation on Hamiltonians

Then

$$\hat{H}^{\mathrm{B}}\left(\overline{\mathbf{b}},\overline{\mathbf{b}}^{\dagger}\right) = -\frac{1}{2}\operatorname{tr}\mathbf{A} + \frac{1}{2}\left(\overline{\mathbf{b}}^{\dagger}\overline{\mathbf{b}}\right)\begin{pmatrix} \Omega\mathbf{1} & 0 \\ 0 & \Omega\mathbf{1} \end{pmatrix}\begin{pmatrix} \overline{\mathbf{b}} \\ \overline{\mathbf{b}}^{\dagger} \end{pmatrix} \tag{11}$$

$$= \sum_{\nu}\Omega_{\nu}\overline{b}_{\nu}^{\dagger}\overline{b}_{\nu} + E_{\mathrm{RPA}}^{c} \tag{12}$$

$$\tag{13}$$

Because $\hat{b}_{\nu} + \hat{b}_{\nu}^{\dagger} = \sum_{\mu}\left(\mathbf{X}_{\mu}^{\nu} + \mathbf{Y}_{\mu}^{\nu}\right)\left(\hat{\overline{b}}_{\nu} + \hat{\overline{b}}_{\nu}^{\dagger}\right)$, we also get

$$\hat{V}^{\mathrm{eB}}\left(\overline{\mathbf{b}},\overline{\mathbf{b}}^{\dagger}\right) = \sum_{pq,\nu} W_{pq,\nu}\left\{\hat{a}_{p}^{\dagger}\hat{a}_{q}\right\}\left(\overline{b}_{\nu} + \overline{b}_{\nu}^{\dagger}\right) \tag{14}$$

Supermatrix construction

We then build the supermatrices **H** and **S** with matrix elements,

$$H_{IJ} = \langle 0_{\mathrm{F}} 0_{\mathrm{B}} | \left[C_I, \left[\tilde{H}^{\mathrm{eB}}, C_J^\dagger \right] \right] | 0_{\mathrm{F}} 0_{\mathrm{B}} \rangle$$
$$S_{IJ} = \langle 0_{\mathrm{F}} 0_{\mathrm{B}} | \left[C_I, C_J^\dagger \right] | 0_{\mathrm{F}} 0_{\mathrm{B}} \rangle$$

where $\left\{ C_I^\dagger \right\} = \left\{ \underbrace{a_i}_{1h}, \underbrace{a_a}_{1p}, \underbrace{a_i b_\nu^\dagger}_{2h1p}, \underbrace{a_a b_\nu}_{1p2p} \right\}$ and $|0\rangle_{\mathrm{F}}$ and $|0\rangle_{\mathrm{B}}$ are the Fermi and boson vacuums. Then constructing $-\boldsymbol{S}^{-1}\boldsymbol{H}$ yields Booth's ED. Derivation is in my notes. Nothing too complicated, but long due to many Wick contractions.

Realization of the idea

Describe the bosons via an auxiliary basis, scaling linearly with system size.

$$\hat{b}_\nu^\dagger \approx \sum_Q^{N_{\mathrm{AB}}} C_\nu^Q \hat{b}_Q^\dagger, \quad \hat{b}_\nu \approx \sum_Q^{N_{\mathrm{AB}}} C_\nu^Q \hat{b}_Q \tag{15}$$

Use RI technique to get the C_ν^Q coefficients. Define

$$(ia \mid jb) \approx \sum_L R_{ia}^L R_{jb}^L \tag{16}$$

Then $C_\nu^Q = \sum_{LM} R_\nu^L \left[\mathbf{S}^{-1/2}\right]_{LM} P_M^Q$ with
$S_{LM} = \sum_\nu R_\nu^L R_\nu^M = \sum_Q P_L^Q E_Q P_M^Q$

Realization of the idea continued

- 1. Get the excitation energies $\boldsymbol{\Omega}$ and vectors $\boldsymbol{X} + \boldsymbol{Y}$ by solving the symmetrized Casida eigenproblem in $O(N_{AB}^3)$ time
- Recall last week we identified using $\mathbf{T} = \boldsymbol{\Omega}^{\frac{1}{2}} (\mathbf{A} - \mathbf{B})^{-\frac{1}{2}} (\mathbf{X} + \mathbf{Y})$ to get excitation vectors as problematic; but that was in a different context and now we have explicit access to $\boldsymbol{\Omega}$ and $\boldsymbol{A} - \boldsymbol{B}$, so we can do this
- 2. Transform the excitation vectors into a screened Coulomb interaction in $O(N_{\text{orb}}^2 N_{\text{AB}}^2)$ time, where $N_{\text{orb}} = O + V$
- 3. Diagonalize the Hamiltonian with a Davidson procedure in $\mathcal{O}\left(N_{\text{orb}}^2\, N_{\mathrm{AB}}\right) / \mathcal{O}\left(N_{\text{orb}}\, N_{\mathrm{AB}}^2\right)$ time for each root

Interestingly, their highest scaling step is 2.

Equation of motion formalism

Define an oscillator that satisfies

$$[H, O^\dagger] = \omega O^\dagger, \qquad [H, O] = -\omega O, \qquad [O, O^\dagger] = 1 \tag{17}$$

With the arbitrary operator R we have

$$\langle\phi|[R,[H,O^\dagger]]|\phi\rangle = \omega\langle\phi|[R,O^\dagger]|\phi\rangle \tag{18}$$

$$\langle\phi|[R,[H,O]]|\phi\rangle = -\omega\langle\phi|[R,O]|\phi\rangle \tag{19}$$

$$\implies \langle\phi|\left[R,H,O^\dagger\right]|\phi\rangle = \omega\langle\phi|\left[R,O^\dagger\right]|\phi\rangle \tag{20}$$

where we have defined the double commutator as

$$2\left[R,H,O^\dagger\right] = \left[R,\left[H,O^\dagger\right]\right] + \left[[R,H],O^\dagger\right] \tag{21}$$

This approach can save because we exploit Hermiticity and the commutator is of lower-rank than the product, so we don't need to know much about the wavefunction to get good matrix elements.

The particle hole approximation leads to RPA

Define the excitation operator $\hat{O}^\dagger = \sum_{ai}\left(Y_{ai}\, a_a^\dagger a_i - Z_{ia}\, a_i^\dagger a_a\right)$. Then,

$$A_{ai,bj} = \langle\phi|\left[a_i^\dagger a_a,\ H,\ a_b^\dagger a_j\right]|\phi\rangle \tag{22}$$

$$B_{ai,bj} = -\langle\phi|\left[a_i^\dagger a_a,\ H,\ a_j^\dagger a_b\right]|\phi\rangle \tag{23}$$

$$U_{ai,bj} = \langle\phi|\left[a_i^\dagger a_a,\ a_b^\dagger a_j\right]|\phi\rangle \tag{24}$$

or in matrix form

$$\begin{pmatrix} A & B \\ B^\dagger & A^* \end{pmatrix}\begin{pmatrix} Y \\ Z \end{pmatrix} = \omega \begin{pmatrix} U & 0 \\ 0 & -U^* \end{pmatrix}\begin{pmatrix} Y \\ Z \end{pmatrix}. \tag{25}$$

Then if we choose the basis that diagonalizes the single-particle Hamiltonian, we get the RPA equations

$$A_{aibj} = \langle 0_\mathrm{F}|a_a^\dagger \left[H, a_b^\dagger a_i\right]|0_\mathrm{F}\rangle = \delta_{ab}\delta_{ij}\left(\varepsilon_i - \varepsilon_a\right) + V_{ajib} \tag{26}$$

$$B_{aibj} = \langle 0_\mathrm{F}|a_a^\dagger \left[H, a_b a_i^\dagger\right]|0_\mathrm{F}\rangle = V_{abij} \tag{27}$$

$$U_{aibj} = \langle 0_\mathrm{F}|a_a^\dagger \left[H, a_b a_i\right]|0_\mathrm{F}\rangle = \delta_{ab}\delta_{ij}. \tag{28}$$

The BSE problem

We want to solve the problem

$$\boldsymbol{L}^{-1} = \boldsymbol{L}_0^{-1} - \boldsymbol{\Xi}^{\text{eh}} \tag{29}$$

$$\implies \begin{pmatrix} \mathcal{A}(\omega) & \mathcal{B}(\omega) \\ \mathcal{B}(\omega) & \mathcal{A}(\omega) \end{pmatrix} \begin{pmatrix} \boldsymbol{X}^m \\ \boldsymbol{Y}^m \end{pmatrix} = \Omega^m \begin{pmatrix} \boldsymbol{X}^m \\ \boldsymbol{Y}^m \end{pmatrix} \tag{30}$$

with

$$\mathcal{A}_{\mu\nu} \equiv \mathcal{A}_{ai,bj} = \underbrace{\left(\epsilon_a^{QP} - \epsilon_i^{QP}\right) \delta_{ab}\delta_{ij} + (ai|jb)}_{\tilde{A}_{ai,bj}} - \Xi_{ab,ji}(\omega) \tag{31}$$

$$\mathcal{B}_{\mu\nu} \equiv \mathcal{B}_{ai,bj} = (ai|bj) - \Xi_{bi|aj}(\omega) \tag{32}$$

BSE@GW approximates the kernel as the screened Coulomb interaction

$$\boldsymbol{\Xi}(\omega) \approx \boldsymbol{\Xi}_{GW}(\omega) = W(\omega) \tag{33}$$

Common to do $\boldsymbol{\Xi}_{GW}(\omega) \approx W(\omega = 0)$, which introduces errors

Tim's full frequency and frequency free BSE@TDA

In TDA, the upfolded 2p Hamiltonian is given by

$$\mathcal{H} = \begin{pmatrix} \tilde{\mathbf{A}} & -\mathbf{V}^{\mathrm{h}} & -\mathbf{V}^{\mathrm{h}} \\ \left(\mathbf{V}^{\mathrm{h}}\right)^{\dagger} & \mathbf{D} & \mathbf{0} \\ (\mathbf{V}^{\mathrm{e}})^{\dagger} & \mathbf{0} & \mathbf{D} \end{pmatrix} \tag{34}$$

The single excitation block $\tilde{A}$ was defined last slide; the rest is:

$$\mathbf{D}_{iajb,iajb} = [-\boldsymbol{E}_{\mathrm{occ}}] \oplus_{\mathsf{kron}} \boldsymbol{E}_{\mathrm{vir}} \oplus_{\mathsf{kron}} \mathbf{S} \tag{35}$$

$$V^{\mathrm{h}}_{ia,ldkc} = \sqrt{2}\,(il|kc)\,\delta_{ad} \tag{36}$$

$$V^{\mathrm{e}}_{ia,ldkc} = \sqrt{2}\,(kc|ad)\,\delta_{il} \tag{37}$$

Here, **S** is the direct RPA matrix in the TDA. Claim: this downfolds to 31, thus preserving full frequency dependence; I have not been able to prove this yet.

Where I am stuck in the derivation

$$\mathcal{A}(\omega) = \tilde{\mathbf{A}} - \mathbf{V}^{\mathrm{e}}(\omega\mathbf{I} - \mathbf{D})^{-1}(\mathbf{V}^{\mathrm{h}})^{\dagger} - \mathbf{V}^{\mathrm{h}}(\omega\mathbf{I} - \mathbf{D})^{-1}(\mathbf{V}^{\mathrm{e}})^{\dagger} \tag{38}$$

$$\tag{39}$$

This implies the kernel shoulld be

$$K^{(\mathrm{p})}_{abij}(\omega) = \mathbf{V}^{\mathrm{e}}(\omega\mathbf{I} - \mathbf{D})^{-1}(\mathbf{V}^{\mathrm{h}})^{\dagger} + \mathbf{V}^{\mathrm{h}}(\omega\mathbf{I} - \mathbf{D})^{-1}(\mathbf{V}^{\mathrm{e}})^{\dagger} \tag{40}$$

$$= \frac{\mathbf{V}^{\mathrm{e}}\tilde{\boldsymbol{X}}(\boldsymbol{V}^{\mathrm{h}}\tilde{\boldsymbol{X}})^{\dagger}}{\omega\mathbf{I} - (-\boldsymbol{E}_O \oplus \boldsymbol{E}_V \oplus \boldsymbol{\Omega}_{OV})} + \frac{\boldsymbol{V}^{\mathrm{h}}\tilde{\boldsymbol{X}}(\boldsymbol{V}^{\mathrm{e}}\tilde{\boldsymbol{X}})^{\dagger}}{\omega\mathbf{I} - (-\boldsymbol{E}_O \oplus \boldsymbol{E}_V \oplus \boldsymbol{\Omega}_{OV})} \tag{41}$$

$$\tag{42}$$

I should be getting

$$K^{(\mathrm{p})}_{abij}(\omega) = 2\sum_{m}^{\Omega_m > 0} (ij|\rho_m)\,(ab|\rho_m)\left[\frac{1}{\omega - (E_b - E_i) - \Omega_m} + \frac{1}{\omega - (E_a - E_j) - \Omega\right. \tag{43}$$

where $(pq|\rho_m) = \sum_{ia} X^m_{ia}(pq|ia)$.

Starting from QRPA

If ground state $|\phi\rangle$ is the quasiparticle vacuum

$$|\tilde{\phi}\rangle = \prod_{\nu>0}\left(U_\nu + V_\nu a^\dagger_\nu a^\dagger_{\bar{\nu}}\right)|-\rangle \tag{44}$$

with quasiparticles (satisfying $U_\nu^2 + V_\nu^2 = 1$) defined by:

$$\alpha^\dagger_\nu = U_\nu a^\dagger_\nu - V_\nu a_{\bar{\nu}} \tag{45}$$

$$\alpha^\dagger_{\bar{\nu}} = U_\nu a^\dagger_{\bar{\nu}} + V_\nu a_\nu \tag{46}$$

Then $\alpha_\nu|\tilde{\phi}\rangle = 0$

Starting from QRPA continued

Define excitation vector as

$$O^\dagger = \sum_{\mu\nu} \left(Y_{\mu\nu} \alpha^\dagger_\mu \alpha^\dagger_\nu + Z_{\mu\nu} \alpha_\mu \alpha_\nu \right) \tag{47}$$

Then

$$A_{\mu\nu\mu'\nu'} = \langle\phi| \left[\alpha_\nu \alpha_\mu, H, \alpha^\dagger_{\mu'} \alpha^\dagger_{\nu'} \right] |\phi\rangle, \tag{48}$$

$$B_{\mu\nu\mu'\nu'} = \langle\phi| \left[\alpha_\nu \alpha_\mu, H, \alpha_{\mu'} \alpha_{\nu'} \right] |\phi\rangle, \tag{49}$$

$$U_{\mu\nu\mu'\nu'} = \langle\phi| \left[\alpha_\nu \alpha_\mu, \alpha^\dagger_{\mu'} \alpha^\dagger_{\nu'} \right] |\phi\rangle. \tag{50}$$

Form of H^{eB}

Define

$$\hat{H}^{\mathrm{eB}} = \hat{H}^{\mathrm{e}} + \hat{H}^{\mathrm{B}} + \hat{V}^{\mathrm{eB}} \tag{51}$$

where $\hat{H}^{\mathrm{e}}$ is the electronic Hamiltonian, $\hat{H}^{\mathrm{B}}$ is the bosonic Hamiltonian, and $\hat{V}^{\mathrm{eB}}$ is the electron-boson coupling term, given as

$$\hat{H}^{e} = \sum_{pq} f_{pq} \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} \tag{52}$$

$$\hat{H}^{B} = \sum_{\nu\mu} A_{\nu\mu} \hat{b}_\nu^\dagger \hat{b}_\mu + \frac{1}{2} \sum_{\nu\mu} B_{\nu\mu} \left(\hat{b}_\nu^\dagger \hat{b}_\mu^\dagger + \hat{b}_\nu \hat{b}_\mu \right) \tag{53}$$

$$\hat{V}^{eB} = \sum_{pq,\nu} V_{pq\nu} \left\{ \hat{a}_p^\dagger \hat{a}_q \right\} \left(\hat{b}_\nu^\dagger + \hat{b}_\nu \right) \tag{54}$$