p. t.

model Hamiltonian:

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$$H_0 \approx H_c$$

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$$\Longrightarrow$$

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$$\Longrightarrow \mathbb{H}_c$$

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$$H_0 \Phi_\sigma = \mathcal{E}_\sigma \Phi_\sigma \quad \text{(known e.f.s)}$$

$$\Rightarrow \mathbb{H}_c = \left[\langle \Phi_\sigma | H_c | \Phi_\tau \rangle \right]$$

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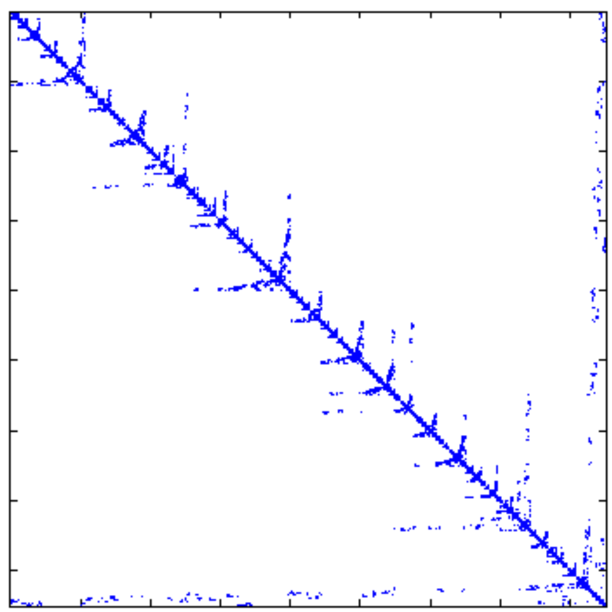

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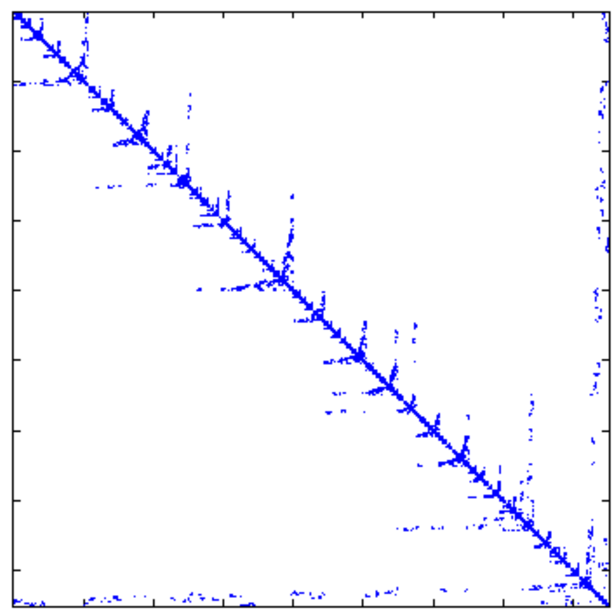
$=$  sparse

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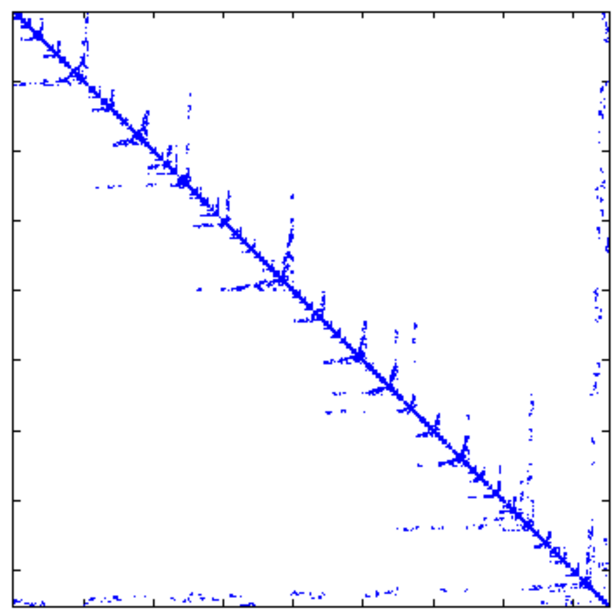

sparse,
diagonally
dominant

for weakly correlated systems

for weakly correlated systems $(\Phi \approx \Psi)$

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$$H_0 = f_p^p \tilde{a}_p^p$$

for weakly correlated systems $(\Phi \approx \Psi)$

$H_0 = f_p^p \tilde{a}_p^p$ works fine

for weakly correlated systems $(\Phi \approx \Psi)$

$$H_0 = f_p^p \tilde{a}_p^p \quad \text{works fine}$$

$$H_0 \Phi = 0 \cdot \Phi$$

for weakly correlated systems $(\Phi \approx \Psi)$

$$H_0 = f^p_p \tilde{a}^p_p \quad \text{works fine}$$

$$H_0 \Phi = 0 \cdot \Phi \qquad H_0 \Phi^{ab\cdots}_{ij\cdots} = \varepsilon^{ab\cdots}_{ij\cdots} \Phi^{ab\cdots}_{ij\cdots}$$

for weakly correlated systems $\quad (\Phi \approx \Psi)$

$$H_0 = f_p^p \tilde{a}_p^p \quad \text{works fine}$$

$$H_0 \Phi = 0 \cdot \Phi \qquad H_0 \Phi_{ij\ldots}^{ab\ldots} = \varepsilon_{ij\ldots}^{ab\ldots} \Phi_{ij\ldots}^{ab\ldots}$$

super convenient

Subspace

Projection operator

Subspace

Projection operator

"model space"

Subspace

"model space"

$\operatorname{span}\{\Phi\}$

Projection operator

Subspace

"model space" → contains qualitative approx. for Ψ

$\text{span}\{\Phi\}$

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"orthogonal space"

$\mathrm{span}\{\Phi_i^a\} \cup \{\Phi_{ij}^{ab}\} \cup \ldots$

Subspace

Projection operator

contains qualitative approx. for Ψ

"model space"

$\mathrm{span}\{\Phi\}$

contains last little bit of Ψ to eek out quant. accuracy

"orthogonal space"

$\mathrm{span}\{\Phi_i^a\} \cup \{\Phi_{ij}^{ab}\} \cup \ldots$

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contains qualitative approx. for Ψ

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Projection operator

$P = |\Phi\rangle\langle\Phi|$

Subspace

Projection operator

contains qualitative approx. for Ψ

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$\text{span}\{\Phi\}$

$$P = |\Phi\rangle\langle\Phi|$$

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"orthogonal space"

$\text{span}\{\Phi_i^a\} \cup \{\Phi_{ij}^{ab}\} \cup \ldots$

$$Q = 1 - P$$

$$P + Q = 1$$

$P + Q = 1 \qquad P^2 = P$

$$P + Q = 1 \qquad P^2 = P \qquad Q^2 = Q$$

$$P+Q=1 \qquad P^2=P \qquad Q^2=Q \qquad PQ=QP=0$$

$$P + Q = 1 \qquad P^2 = P \qquad Q^2 = Q \qquad PQ = QP = 0$$

with intermediate normalization:

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with intermediate normalization:

$$P\Psi = \Phi$$

$$P + Q = 1 \qquad P^2 = P \qquad Q^2 = Q \qquad PQ = QP = 0$$

with intermediate normalization:

$$P\Psi = \Phi \qquad Q\Psi = \Psi - \Phi$$

Q

$$Q = \sum_{k} \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1 \cdots a_k \\ i_1 \cdots i_k}} \left| \Phi^{a_1 \cdots a_k}_{i_1 \cdots i_k} \right\rangle \left\langle \Phi^{a_1 \cdots a_k}_{i_1 \cdots i_k} \right|$$

$$Q = \sum_{\substack{a\\i}} |\Phi_i^a\rangle\langle\Phi_i^a| + \left(\frac{1}{2!}\right)^2 \sum_{\substack{ab\\ij}} |\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}| + \left(\frac{1}{3!}\right)^2 \sum_{\substack{abc\\ijk}} |\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}| + \ldots$$

the resolvent:

the resolvent:

$$R_0 = -H_0^{-1}$$

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$$R_0 = -H_0^{-1}\Big|_{\text{ortho. space}}$$

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$$R_0 = -H_0^{-1}\Big|_{\text{ortho. space}}$$

why?

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why?

$$H_0\Big|_{\text{model space}} = 0$$

the resolvent:

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why?

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singular $\iff$ non-invertible

R_0

$$R_0 = -H_0^{-1} Q$$

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$$= \sum_k \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1 \cdots a_k \\ i_1 \cdots i_k}} (-H_0)^{-1} \left| \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right\rangle \left\langle \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right|$$

$$R_0 = -H_0^{-1} Q$$

$$= \sum_k \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1 \cdots a_k \\ i_1 \cdots i_k}} \left(-\mathcal{E}_{i_1 \cdots i_k}^{a_1 \cdots a_k}\right)^{-1} \left| \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right\rangle \left\langle \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right|$$

$$R_0 = -H_0^{-1} Q$$

$$= \sum_k \left(\frac{1}{k!}\right)^2 \sum_{\substack{a_1 \cdots a_k \\ i_1 \cdots i_k}} \left(+\mathcal{E}_{a_1 \cdots a_k}^{i_1 \cdots i_k}\right)^{-1} \left| \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right\rangle \left\langle \Phi_{i_1 \cdots i_k}^{a_1 \cdots a_k} \right|$$

$$R_0 = -H_0^{-1} Q$$

$$= \sum_{\substack{a \\ i}} \frac{|\Phi_i^a\rangle\langle\Phi_i^a|}{\varepsilon_a^i}$$

$$+ \left(\frac{1}{2!}\right)^2 \sum_{\substack{ab \\ ij}} \frac{|\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}|}{\varepsilon_{ab}^{ij}}$$

$$+ \left(\frac{1}{3!}\right)^2 \sum_{\substack{abc \\ ijk}} \frac{|\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}|}{\varepsilon_{abc}^{ijk}}$$

$$+ \ \ldots$$

note that

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$$R_0 \Phi^{ab\cdots}_{ij\cdots}$$

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$$R_0\, \Phi^{ab\cdots}_{ij\cdots} = \left(\mathcal{E}^{ij\cdots}_{ab\cdots}\right)^{-1} \Phi^{ab\cdots}_{ij\cdots}$$

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$$R_0 \Phi$$

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and

$$R_0 \Phi = 0 \cdot \Phi$$

consider

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$$R_0 X_1 \cdots X_n |\Phi\rangle$$

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$$= R_0 \vdots \overline{X_1 \cdots X_n} \vdots |\Phi\rangle$$

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observations:

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$$= R_0 \vdots \overline{X_1 \cdots X_n} \vdots |\Phi\rangle$$

observations:

1. complete contractions vanish

consider

$$R_0 X_1 \cdots X_n |\Phi\rangle$$

$$= R_0 : \overline{X_1 \cdots X_n} : |\Phi\rangle$$

observations:

each term must be able to fully contract one of these

$$|\Phi_{ij\cdots}^{ab\cdots}\rangle\langle\Phi|\tilde{a}^{ij\cdots}_{ab\cdots}$$

such terms will have the form

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$$\text{const} \times \tilde{a}^{b_1 \cdots b_m}_{j_1 \cdots j_m} |\Phi\rangle$$

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$\Longrightarrow$

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$$= \text{const} \times |\Phi^{b_1 \cdots b_m}_{j_1 \cdots j_m}\rangle$$

$$\Longrightarrow \quad R_0 \times \text{const} \times |\Phi^{b_1 \cdots b_m}_{j_1 \cdots j_m}\rangle$$

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$$= \text{const} \times \frac{|\Phi^{b_1 \cdots b_m}_{j_1 \cdots j_m}\rangle}{\mathcal{E}^{j_1 \cdots j_m}_{b_1 \cdots b_m}}$$

Perturbation theory:

analyze dependence of Ψ or

$O = \langle \Psi | \hat{O} | \Psi \rangle$ on $V_c \equiv H_c - H_0$

"fluctuation potential"

Perturbation theory:

Perturbation theory:

$$H(\lambda) \equiv H_0 + \lambda V_c$$

Perturbation theory:

on/off switch

$$H(\lambda) \equiv H_0 + \lambda V_c$$

Perturbation theory:

on/off switch

$$H(\lambda) \equiv H_0 + \lambda V_c \qquad \lambda = 1$$

Perturbation theory:

on/off switch

$$H(\lambda) \equiv H_0 + \lambda V_c \qquad \lambda = 1 \text{ "on"}$$

Perturbation theory:

on/off switch

$$H(\lambda) \equiv H_0 + \lambda V_c$$

$\lambda = 1$ "on"

$\lambda = 0$

Perturbation theory:

on/off switch

$$H(\lambda) \equiv H_0 + \lambda V_c$$

$\lambda = 1$ "on"

$\lambda = 0$ "off"

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$$H(\lambda)\Psi(\lambda) = E(\lambda)\Psi(\lambda)$$

Perturbation theory:

on/off switch

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$\lambda = 0$ "off"

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

$$\Psi(\lambda) = \sum_{n=0}^{\infty} \lambda^n \Psi^{(n)}$$

Perturbation theory:

on/off switch

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$$E(\lambda) = \sum_{n=0}^{\infty} \lambda^n E_c^{(n)}$$

Perturbation theory:

on/off switch

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$\lambda = 1$ "on"

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$$\Psi(\lambda) = \sum_{n=0}^{\infty} \lambda^n \Psi^{(n)} \qquad \Psi^{(n)} \to \frac{1}{n!}\left.\frac{\partial^n \Psi(\lambda)}{\partial \lambda^n}\right|_0$$

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Perturbation theory:

on/off switch

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$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

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project by Φ:

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

project by Φ:

$$\lambda \langle \Phi | V_c | \Psi(\lambda) \rangle = E(\lambda)$$

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

project by Φ:

$$\lambda \langle \Phi | V_c | \Psi(\lambda) \rangle = E(\lambda)$$

$$\Longrightarrow$$

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

project by Φ:

$$\lambda \langle \Phi | V_c | \Psi(\lambda) \rangle = E(\lambda)$$

$$\Longrightarrow \langle \Phi | V_c | \Psi^{(n)} \rangle = E^{(n+1)}$$

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

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operate R_0 on both sides:

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

operate R_0 on both sides:

$$R_0 H_0 \Psi(\lambda) + R_0 \lambda V_c \Psi(\lambda) = E(\lambda) R_0 \Psi(\lambda)$$

$$H(\lambda)\Psi(\lambda) = E(\lambda)\Psi(\lambda)$$

operate R_0 on both sides:

$$\underbrace{R_0 H_0 \Psi(\lambda)}_{-Q\Psi(\lambda)} + R_0 \lambda V_c \Psi(\lambda) = E(\lambda) R_0 \Psi(\lambda)$$

$$H(\lambda)\,\Psi(\lambda) = E(\lambda)\,\Psi(\lambda)$$

operate R_0 on both sides:

$$\underbrace{R_0 H_0 \Psi(\lambda)}_{-Q\Psi(\lambda) = -\Psi(\lambda) + \Phi} + R_0 \lambda V_c \Psi(\lambda) = E(\lambda) R_0 \Psi(\lambda)$$

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operate R_0 on both sides:

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$$\Longrightarrow \Psi(\lambda)$$

$$H(\lambda)\Psi(\lambda) = E(\lambda)\Psi(\lambda)$$

operate R_0 on both sides:

$$\underbrace{R_0 H_0 \Psi(\lambda)}_{-Q\Psi(\lambda) = -\Psi(\lambda) + \Phi} + R_0 \lambda V_c \Psi(\lambda) = E(\lambda) R_0 \Psi(\lambda)$$

$$\Longrightarrow \Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda)$$

$$\Psi(\lambda) = \Phi + R_0\left(\lambda V_c - E(\lambda)\right)\Psi(\lambda)$$

$$E^{(n+1)} = \langle \Phi | V_c | \Psi^{(n)} \rangle$$

$$\Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda)$$

$$E^{(n+1)} = \langle \Phi | V_c | \Psi^{(n)} \rangle$$

1. $E^{(1)}$

$$\Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda)$$

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1. $E^{(1)}$ 2. $\Psi^{(1)}$

$$\Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda)$$

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1. $E^{(1)}$ 2. $\Psi^{(1)}$ 3. $E^{(2)}$

$$\Psi(\lambda) = \Phi + R_0(\lambda V_c - E(\lambda))\Psi(\lambda)$$

$$E^{(n+1)} = \langle \Phi | V_c | \Psi^{(n)} \rangle$$

1. $E^{(1)}$ 2. $\Psi^{(1)}$ 3. $E^{(2)}$ 4. $\Psi^{(2)}$

end.