HEDIN EQUATIONS AND KOHN–SHAM POTENTIAL IN THE PATH–INTEGRAL FORMALISM

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- Hamiltonian: N interacting electrons in an external potential $u(\mathbf{x})$ (atoms, molecules, solids, ...):

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{\hat{\boldsymbol{p}}_i^2}{2m} + u(\hat{\boldsymbol{x}}_i) \right) + \frac{1}{2} \sum_{\substack{i,j=1 \\ (i \neq j)}}^{N} \frac{e^2}{|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|}$$

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Many Body System:		*Kohn–Sham System*:
N interacting electrons in an external potential $u(\mathbf{x})$	$\Longleftrightarrow$	N *free* electrons in an effective potential $u_{KS}(\mathbf{x})$

$$\mathcal{G}(1,1^+) = n(\mathbf{x}) = \mathcal{G}_{KS}(1,1^+)$$

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$$-\frac{\hbar^2}{2m}\nabla^2\phi_j(\mathbf{x}) + u_{KS}(\mathbf{x})\phi_j(\mathbf{x}) = \epsilon_j\phi_j(\mathbf{x})$$

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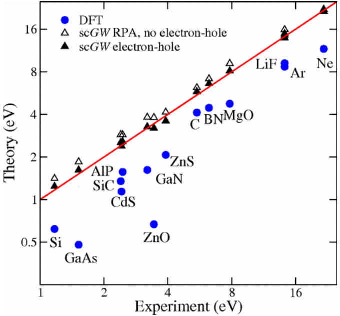
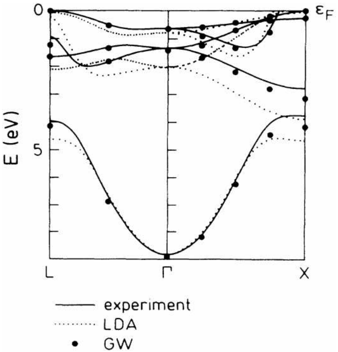
Hedin equations and DFT





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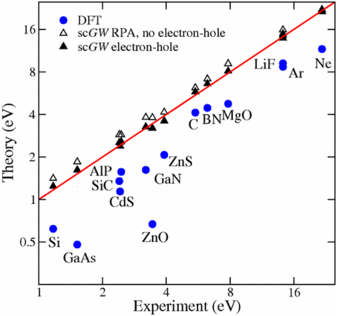

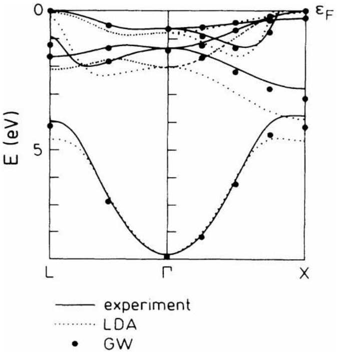

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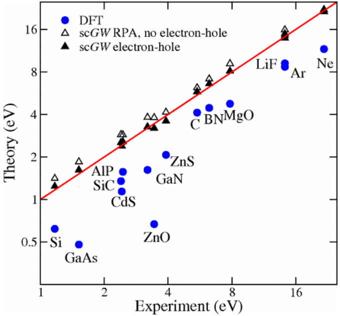

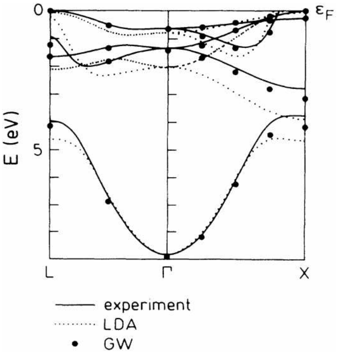

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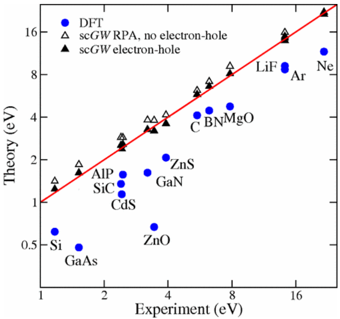

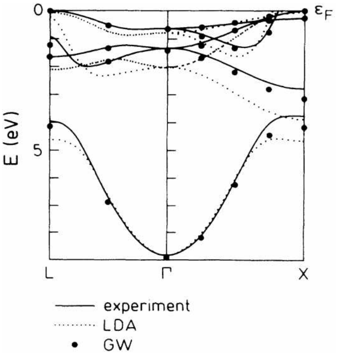

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Both theories find a natural and elegant riformulation in the functional integral formalism, for $T = 0$ and for $T \neq 0$ as well.

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$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \underset{\mathrm{Tr}[\hat{A}] = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d\mathbf{x}\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}|\hat{A}|\boldsymbol{\psi}\rangle}{\overset{\uparrow}{=}}$$

$$= \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d^3x\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}(\hbar\beta)\hat{K}} |\boldsymbol{\psi}\rangle$$

$$= \lim_{N\to\infty} \int \ldots \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\hat{\mathbb{1}}_{\mathcal{F}-}}{\uparrow\uparrow}\ldots e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\hat{\mathbb{1}}_{\mathcal{F}-}}{\uparrow\uparrow}\ldots e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} |\boldsymbol{\psi}\rangle$$

$$\left(\hat{\mathbb{1}} = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d\mathbf{x}\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|\right)$$

$$= \left\{\prod_{k=1}^{N} \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma^{(k)}(\mathbf{x}) d\psi_\sigma^{(k)}(\mathbf{x})\right\} e^{-\sum_k \int d^3x\, \bar{\psi}_\sigma^{(k)}(\boldsymbol{x})\psi_\sigma^{(k)}(\boldsymbol{x})} \cdot \prod_{j=0}^{N-1} \langle \boldsymbol{\psi}^{(j+1)}| e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} |\boldsymbol{\psi}^{(j)}\rangle \Bigg|_{\substack{\boldsymbol{\psi}^{(0)} = -\boldsymbol{\psi}^{(N)} \\ \bar{\boldsymbol{\psi}}^{(0)} = -\bar{\boldsymbol{\psi}}^{(N)}}}$$

Construction of the path–integral

Using coherent states to get a functional expression for $\mathcal{Z}$:

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \underset{\mathrm{Tr}[\hat{A}] = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d\mathbf{x}\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}|\hat{A}|\boldsymbol{\psi}\rangle}{\overset{\uparrow}{=}}$$

$$= \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d^3x\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}(\hbar\beta)\hat{K}} |\boldsymbol{\psi}\rangle$$

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$$\left(\hat{\mathbb{1}} = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\, e^{-\int d\mathbf{x}\, \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|\right)$$

$$= \left\{ \prod_{k=1}^{N} \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma^{(k)}(\mathbf{x}) d\psi_\sigma^{(k)}(\mathbf{x}) \right\} e^{-\sum_k \int d^3x\, \bar{\psi}_\sigma^{(k)}(\boldsymbol{x})\psi_\sigma^{(k)}(\boldsymbol{x})} .$$

$$\cdot \prod_{j=0}^{N-1} \langle \boldsymbol{\psi}^{(j+1)} | e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} | \boldsymbol{\psi}^{(j)} \rangle \Bigg|_{\substack{\boldsymbol{\psi}^{(0)} = -\boldsymbol{\psi}^{(N)} \\ \bar{\boldsymbol{\psi}}^{(0)} = -\bar{\boldsymbol{\psi}}^{(N)}}}$$

$$\hat{\psi}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle = \psi_\sigma^{(j)}(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle$$

Construction of the path–integral

Using coherent states to get a functional expression for $\mathcal{Z}$:

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\right] \overset{\uparrow}{=}$$

$$\mathrm{Tr}[\hat{A}] = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\; e^{-\int d\mathbf{x}\;\bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}|\hat{A}|\boldsymbol{\psi}\rangle$$

$$= \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\; e^{-\int d^3x\;\bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}|e^{-\frac{1}{\hbar}(\hbar\beta)\hat{K}}|\boldsymbol{\psi}\rangle$$

$$= \lim_{N\to\infty}\int \dots\; \langle -\boldsymbol{\psi}|e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \dots e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \dots e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}}|\boldsymbol{\psi}\rangle$$

$$\uparrow\uparrow \quad \hat{\mathbb{1}}_{\mathcal{F}-} \qquad \uparrow\uparrow \quad \hat{\mathbb{1}}_{\mathcal{F}-}$$

$$\left(\hat{\mathbb{1}} = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\; e^{-\int d\mathbf{x}\;\bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|\right)$$

$$= \left\{\prod_{k=1}^{N}\int\prod_{\sigma,\mathbf{x}} d\bar{\psi}^{(k)}_\sigma(\mathbf{x}) d\psi^{(k)}_\sigma(\mathbf{x})\right\} e^{-\sum_k\int d^3x\;\bar{\psi}^{(k)}_\sigma(\boldsymbol{x})\psi^{(k)}_\sigma(\boldsymbol{x})}\cdot$$

$$\cdot \prod_{j=0}^{N-1} \langle \boldsymbol{\psi}^{(j+1)}|e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}}|\boldsymbol{\psi}^{(j)}\rangle \Bigg|_{\substack{\boldsymbol{\psi}^{(0)}=-\boldsymbol{\psi}^{(N)} \\ \bar{\boldsymbol{\psi}}^{(0)}=-\bar{\boldsymbol{\psi}}^{(N)}}}$$

$$\uparrow \quad \hat{\psi}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle = \psi^{(j)}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle$$

$$= \left\{\prod_{k=1}^{N}\int\prod_{\sigma,\mathbf{x}} d\bar{\psi}^{(k)}_\sigma(\mathbf{x}) d\psi^{(k)}_\sigma(\mathbf{x})\right\} e^{-\sum_k\int d^3x\left\{\bar{\psi}^{(k+1)}_\sigma(\boldsymbol{x})\cdot\right.}$$

$$\left.\cdot\left[\psi^{(k+1)}_\sigma(\boldsymbol{x}) - \psi^{(k)}_\sigma(\boldsymbol{x})\right] + \frac{1}{\hbar}\frac{\hbar\beta}{N}\left(H-\mu N\right)[\bar{\psi}^{(k+1)}_\sigma(\boldsymbol{x}), \psi^{(k)}_\sigma(\boldsymbol{x})]\right\}$$

Construction of the path–integral

Using coherent states to get a functional expression for $\mathcal{Z}$:

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \underset{\uparrow}{=}$$

$$\mathrm{Tr}[\hat{A}] = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\ e^{-\int d\mathbf{x}\ \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}|\hat{A}|\boldsymbol{\psi}\rangle$$

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$$= \lim_{N\to\infty} \int \dots \ \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\uparrow\uparrow \atop \hat{\mathbb{1}}_{\mathcal{F}-}}{\dots} e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\uparrow\uparrow \atop \hat{\mathbb{1}}_{\mathcal{F}-}}{\dots} e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} |\boldsymbol{\psi}\rangle$$

$$\left(\hat{\mathbb{1}} = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\ e^{-\int d\mathbf{x}\ \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|\right)$$

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$$\hat{\psi}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle = \psi_\sigma^{(j)}(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle$$

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Last step: letting N approach ∞:

Construction of the path–integral

Using coherent states to get a functional expression for $\mathcal{Z}$:

$$\mathcal{Z} = \text{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] \underset{\uparrow}{=}$$

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$$= \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\; e^{-\int d^3x\; \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}(\hbar\beta)\hat{K}} |\boldsymbol{\psi}\rangle$$

$$= \lim_{N\to\infty} \int \ldots \langle -\boldsymbol{\psi}| e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\uparrow\uparrow \atop \hat{\mathbb{1}}_{\mathcal{F}-}}{\ldots} e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} \underset{\uparrow\uparrow \atop \hat{\mathbb{1}}_{\mathcal{F}-}}{\ldots} e^{-\frac{1}{\hbar}\frac{\hbar\beta}{N}\hat{K}} |\boldsymbol{\psi}\rangle$$

$$\left(\hat{\mathbb{1}} = \int \prod_{\sigma,\mathbf{x}} d\bar{\psi}_\sigma(\mathbf{x}) d\psi_\sigma(\mathbf{x})\; e^{-\int d\mathbf{x}\; \bar{\psi}_\sigma(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})} |\boldsymbol{\psi}\rangle\langle\boldsymbol{\psi}|\right)$$

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$$\hat{\psi}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle = \psi^{(j)}_\sigma(\boldsymbol{x})|\boldsymbol{\psi}^{(j)}\rangle$$

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Last step: letting N approach ∞: continuum limit: $\psi^{(k)}_\sigma(\boldsymbol{x}) \to \psi_\sigma(\boldsymbol{x},\tau)$...

Path–integral form of $\mathcal{Z}$

Path–integral form of $\mathcal{Z}$

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

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$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

$$\mathcal{S}[\boldsymbol{\psi},\bar{\boldsymbol{\psi}},\boldsymbol{\varphi}] = \int dx\ \bar{\psi}_\sigma(x)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu\right)\psi_\sigma(x) + $$

$$+\ \frac{1}{2}\int dx dy\ \bar{\psi}_\sigma(x)\bar{\psi}_\rho(y)\frac{e^2}{|\mathbf{x}-\mathbf{y}|}\psi_\rho(y)\psi_\sigma(x)$$

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$$+\frac{1}{2}\int dx dy\ \bar{\psi}_\sigma(x)\bar{\psi}_\rho(y)\frac{e^2}{|\mathbf{x}-\mathbf{y}|}\psi_\rho(y)\psi_\sigma(x)$$

↑

The very last step:
Hubbard–Stratonovich transformation:
from a four–fermion–fields interaction
to a two–fermion–fields plus
an auxiliary–boson–field one ($\sim$ QED):

Path–integral form of $\mathcal{Z}$

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

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↑

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$$e^{-\frac{1}{2\hbar}\mathbf{n}\cdot\mathcal{U}_0\mathbf{n}} = \int \mathcal{D}[\varphi] e^{-\frac{e^2}{2\hbar}\boldsymbol{\varphi}\cdot\mathcal{U}_0^{-1}\boldsymbol{\varphi} - \frac{ie}{\hbar}\boldsymbol{\varphi}\cdot\mathbf{n}}$$

Path–integral form of $\mathcal{Z}$

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

$$\mathcal{S}[\boldsymbol{\psi},\bar{\boldsymbol{\psi}},\boldsymbol{\varphi}] = \int dx\ \bar{\psi}_\sigma(x)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu\right)\psi_\sigma(x) +$$

$$+\ \frac{1}{2}\int dx dy\ \bar{\psi}_\sigma(x)\bar{\psi}_\rho(y)\,\frac{e^2}{|\mathbf{x}-\mathbf{y}|}\,\psi_\rho(y)\psi_\sigma(x)$$

↑

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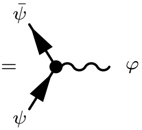

Path–integral form of $\mathcal{Z}$

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

$$\mathcal{S}[\boldsymbol{\psi},\bar{\boldsymbol{\psi}},\boldsymbol{\varphi}] = \int dx\ \bar{\psi}_\sigma(x)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu\right)\psi_\sigma(x) +$$

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↑

The very last step:
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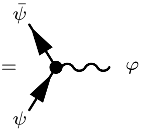

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}\right]\mathcal{D}\left[\boldsymbol{\psi}\right]\mathcal{D}\left[\boldsymbol{\varphi}\right]\exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi},\boldsymbol{\varphi}\right]$$

Path–integral form of $\mathcal{Z}$

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}_\sigma(\mathbf{x},\tau)\right] \mathcal{D}\left[\boldsymbol{\psi}_\sigma(\mathbf{x},\tau)\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi}\right]$$

$$\mathcal{S}[\boldsymbol{\psi},\bar{\boldsymbol{\psi}},\boldsymbol{\varphi}] = \int dx\ \bar{\psi}_\sigma(x)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu\right)\psi_\sigma(x) +$$

$$+\frac{1}{2}\int dxdy\ \bar{\psi}_\sigma(x)\bar{\psi}_\rho(y)\frac{e^2}{|\mathbf{x}-\mathbf{y}|}\psi_\rho(y)\psi_\sigma(x)$$

$\uparrow$

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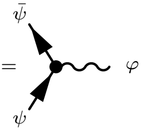

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}\right] \mathcal{D}\left[\boldsymbol{\psi}\right] \mathcal{D}\left[\boldsymbol{\varphi}\right] \exp -\frac{1}{\hbar}\mathcal{S}\left[\bar{\boldsymbol{\psi}},\boldsymbol{\psi},\boldsymbol{\varphi}\right]$$

$$\mathcal{S}[\boldsymbol{\psi},\bar{\boldsymbol{\psi}},\boldsymbol{\varphi}] = \int dx\ \bar{\psi}_\sigma(x)\left(\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu\right)\psi_\sigma(x) +$$

$$+\int dx\ \varphi(x)\left(-\frac{1}{8\pi}\nabla^2\right)\varphi(x) + ie\int dx\ \bar{\psi}_\sigma(x)\varphi(x)\psi_\sigma(x)$$

Two–points functions and generating functionals

Two–points functions and generating functionals

- Electronic Propagator:

$$-\mathcal{G}_{\sigma\sigma'}(x;x') = \langle \psi_\sigma(x)\bar{\psi}_{\sigma'}(x')\rangle_{\mathcal{Z}}$$

Two–points functions and generating functionals

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$$-\mathcal{G}_{\sigma\sigma'}(x;x') = \langle \psi_\sigma(x)\bar{\psi}_{\sigma'}(x')\rangle_{\mathcal{Z}} = \; x'$$  x

Two–points functions and generating functionals

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x

- Dressed Interaction ($\sim$ boson propagator):

$$\mathcal{U}(x;x') = \frac{e^2}{\hbar}\langle \varphi(x)\varphi(x')\rangle_{\mathcal{Z}}$$

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Linear coupling with external sources $\eta_\sigma(x)$, $\bar{\eta}_\sigma(x)$, $\rho(x)$ (Schwinger, '50): fields become derivatives...

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Linear coupling with external sources $\eta_\sigma(x)$, $\bar{\eta}_\sigma(x)$, $\rho(x)$ (Schwinger, '50): fields become derivatives...

$$\mathcal{Z}\left[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}\right] = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}\right]\mathcal{D}\left[\boldsymbol{\psi}\right]\mathcal{D}\left[\boldsymbol{\varphi}\right] e^{-\frac{1}{\hbar}\left\{\mathcal{S}+\mathcal{S}_{sorg}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}]\right\}}$$

$$\downarrow$$

$$\mathcal{S}_{sorg} = \int dx\left[\bar{\eta}_\sigma(x)\psi_\sigma(x) + \bar{\psi}_\sigma(x)\eta_\sigma(x) + ie\rho(x)\varphi(x)\right]$$

Two–points functions and generating functionals

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Linear coupling with external sources $\eta_\sigma(x)$, $\bar{\eta}_\sigma(x)$, $\rho(x)$ (Schwinger, '50): fields become derivatives...

$$\mathcal{Z}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}] = \int \mathcal{D}[\bar{\boldsymbol{\psi}}]\,\mathcal{D}[\boldsymbol{\psi}]\,\mathcal{D}[\boldsymbol{\varphi}]\,e^{-\frac{1}{\hbar}\{\mathcal{S}+\mathcal{S}_{sorg}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}]\}}$$

$$\downarrow$$

$$\mathcal{S}_{sorg} = \int dx\left[\bar{\eta}_\sigma(x)\psi_\sigma(x) + \bar{\psi}_\sigma(x)\eta_\sigma(x) + ie\rho(x)\varphi(x)\right]$$

$$\mathcal{G}_{\sigma\sigma'}(x;x') = -\frac{\hbar^2}{\mathcal{Z}}\frac{\delta^{(2)}\mathcal{Z}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}]}{\delta\bar{\eta}_{\sigma_1}(1)\delta\eta_{\sigma_{1'}}(1')} \qquad \mathcal{U}(x;x') = -\frac{\hbar}{\mathcal{Z}}\frac{\delta^{(2)}\mathcal{Z}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}]}{\delta\rho(1)\delta\rho(1')}$$

Two–points functions and generating functionals

- Electronic Propagator:

$$-\mathcal{G}_{\sigma\sigma'}(x;x') = \langle \psi_\sigma(x)\bar{\psi}_{\sigma'}(x')\rangle_{\mathcal{Z}} = \; x'$$  $$x$$

- Dressed Interaction (∼ boson propagator):

$$\mathcal{U}(x;x') = \frac{e^2}{\hbar}\langle \varphi(x)\varphi(x')\rangle_{\mathcal{Z}} = \; x'$$  $$x$$

Linear coupling with external sources $\eta_\sigma(x)$, $\bar{\eta}_\sigma(x)$, $\rho(x)$ (Schwinger, '50): fields become derivatives...

$$\mathcal{Z}\left[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}\right] = \int \mathcal{D}\left[\bar{\boldsymbol{\psi}}\right]\mathcal{D}\left[\boldsymbol{\psi}\right]\mathcal{D}\left[\boldsymbol{\varphi}\right] e^{-\frac{1}{\hbar}\left\{\mathcal{S}+\mathcal{S}_{sorg}[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}]\right\}}$$

$$\downarrow$$

$$\mathcal{S}_{sorg} = \int dx\left[\bar{\eta}_\sigma(x)\psi_\sigma(x) + \bar{\psi}_\sigma(x)\eta_\sigma(x) + ie\rho(x)\varphi(x)\right]$$

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Self–Energy and Proper Polarization

Self–Energy and Proper Polarization

Properties of the Legendre Transform:

$$\frac{\delta^{(2)}\Gamma[\boldsymbol{\psi}^{cl},\bar{\boldsymbol{\psi}}^{cl},\boldsymbol{\varphi}^{cl}]}{\delta\bar{\psi}^{cl}_{\mu}(1)\delta\psi^{cl}_{\nu}(2)} = \hbar\mathcal{G}^{-1}_{\mu\nu}(1,2)$$

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$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma^{*}\mathcal{G} \qquad \mathcal{U} = \mathcal{U}_0 + \mathcal{U}_0\Pi^{*}\mathcal{U}$$

Dyson equations

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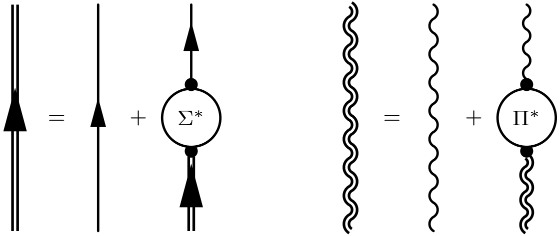

Schwinger–Dyson equations $\rightarrow$ Hedin equations

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Infinitesimal shift of the fields $\longrightarrow$ $\mathcal{Z}\left[\bar{\boldsymbol{\eta}},\boldsymbol{\eta},\boldsymbol{\rho}\right]$ doesn't change!
$\longrightarrow$ Schwinger–Dyson equations ('50):
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$$\uparrow$$

$$k(\mathbf{x},\tau) = \hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + u(\boldsymbol{x}) - \mu$$

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$$-\frac{1}{4\pi ie}\nabla^2\frac{\delta\mathcal{W}}{\delta\rho(x)} - ie\hbar\frac{\delta^{(2)}\mathcal{W}}{\delta\bar{\eta}_\sigma(x)\delta\eta_\sigma(x^+)} + ie\rho(x) = 0$$

Ward Identities $\rightarrow$ Hedin equations

Ward Identities $\to$ Hedin equations

- Begin with Schwinger–Dyson equation:

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- Derivative w.r.t. external source ($\mathcal{G}_{11'}=-\hbar\mathcal{W}^{(2)}_{\bar{\eta}_1\eta_{1'}}$ with sources to 0):

$$\left[k(1)+ie\varphi^{cl}(1)\right]\mathcal{G}_{\sigma\sigma'}(1,1')-\hbar\frac{\delta}{\delta\rho(1)}\mathcal{G}_{\sigma\sigma'}(1,1')=-\hbar\delta_{\sigma\sigma'}\delta(1-1')$$

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- Using $k(1)\delta(1-1') = -\dfrac{\delta^{(2)}\Gamma^{(0)}}{\delta \bar{\psi}^{cl}(1) \delta \psi^{cl}(1')}$ and $\Gamma_{\bar{\psi}\psi} - \Gamma^{(0)}_{\bar{\psi}\psi} = -\hbar \Sigma^*$:

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$$\Sigma^*_{\sigma\rho}(1,2) \mathcal{G}_{\rho\sigma'}(2,1') + \frac{\delta}{\delta \rho(1)} \mathcal{G}_{\sigma\sigma'}(1,1') - i\frac{e}{\hbar} \varphi^{cl}(1) \mathcal{G}_{\sigma\sigma'}(1,1') = 0$$

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- Apply functional inverse (again $\mathcal{W}^{(2)}_{\bar{\eta}_1 \eta_2} \Gamma^{(2)}_{\bar{\psi}_2 \psi_3} = -\delta_{13}$):

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$$\left[k(1)+\frac{\delta\mathcal{W}}{\delta\rho(1)}\right]\frac{\delta\mathcal{W}}{\delta\bar{\eta}_\sigma(1)}-\hbar\frac{\delta^{(2)}\mathcal{W}}{\delta\rho(1)\delta\bar{\eta}_\sigma(1)}+\eta_\sigma(1)=0$$

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$$\left[k(1)+ie\varphi^{cl}(1)\right]\mathcal{G}_{\sigma\sigma'}(1,1')-\hbar\frac{\delta}{\delta\rho(1)}\mathcal{G}_{\sigma\sigma'}(1,1')=-\hbar\delta_{\sigma\sigma'}\delta(1-1')$$

- Using $k(1)\delta(1-1')=-\frac{\delta^{(2)}\Gamma^{(0)}}{\delta\bar{\psi}^{cl}(1)\delta\psi^{cl}(1')}$ and $\Gamma_{\bar{\psi}\psi}-\Gamma^{(0)}_{\bar{\psi}\psi}=-\hbar\Sigma^*$:

$$\Sigma^*_{\sigma\rho}(1,2)\mathcal{G}_{\rho\sigma'}(2,1')+\frac{\delta}{\delta\rho(1)}\mathcal{G}_{\sigma\sigma'}(1,1')-i\frac{e}{\hbar}\varphi^{cl}(1)\mathcal{G}_{\sigma\sigma'}(1,1')=0$$

- Apply functional inverse (again $\mathcal{W}^{(2)}_{\bar{\eta}_1\eta_2}\Gamma^{(2)}_{\bar{\psi}_2\psi_3}=-\delta_{13}$):

$$\Sigma^*_{\sigma\sigma'}(1,1')=i\frac{e}{\hbar}\varphi^{cl}(1)\delta_{\sigma\sigma'}\delta(1-1')+$$
$$-\frac{1}{\hbar}\mathcal{G}_{\sigma\rho}(1,2)\frac{\delta\varphi^{cl}(3)}{\delta\rho(1)}\frac{\delta^{(3)}\Gamma}{\delta\varphi^{cl}(3)\delta\bar{\psi}^{cl}_\rho(2)\delta\psi^{cl}_{\sigma'}(1')}$$

Ward Identities $\to$ Hedin equations

- Begin with Schwinger–Dyson equation:

$$\left[k(1) + \frac{\delta \mathcal{W}}{\delta \rho(1)}\right] \frac{\delta \mathcal{W}}{\delta \bar{\eta}_\sigma(1)} - \hbar \frac{\delta^{(2)} \mathcal{W}}{\delta \rho(1) \delta \bar{\eta}_\sigma(1)} + \eta_\sigma(1) = 0$$

- Derivative w.r.t. external source ($\mathcal{G}_{11'} = -\hbar \mathcal{W}^{(2)}_{\bar{\eta}_1 \eta_{1'}}$ with sources to 0):

$$\left[k(1) + ie\varphi^{cl}(1)\right] \mathcal{G}_{\sigma\sigma'}(1,1') - \hbar \frac{\delta}{\delta \rho(1)} \mathcal{G}_{\sigma\sigma'}(1,1') = -\hbar \delta_{\sigma\sigma'} \delta(1-1')$$

- Using $k(1)\delta(1-1') = -\frac{\delta^{(2)}\Gamma^{(0)}}{\delta \bar{\psi}^{cl}(1) \delta \psi^{cl}(1')}$ and $\Gamma_{\bar{\psi}\psi} - \Gamma^{(0)}_{\bar{\psi}\psi} = -\hbar \Sigma^*$:

$$\Sigma^*_{\sigma\rho}(1,2) \mathcal{G}_{\rho\sigma'}(2,1') + \frac{\delta}{\delta \rho(1)} \mathcal{G}_{\sigma\sigma'}(1,1') - i\frac{e}{\hbar}\varphi^{cl}(1) \mathcal{G}_{\sigma\sigma'}(1,1') = 0$$

- Apply functional inverse (again $\mathcal{W}^{(2)}_{\bar{\eta}_1 \eta_2} \Gamma^{(2)}_{\bar{\psi}_2 \psi_3} = -\delta_{13}$):

$$\Sigma^*_{\sigma\sigma'}(1,1') = i\frac{e}{\hbar}\varphi^{cl}(1)\delta_{\sigma\sigma'}\delta(1-1') + \\ - \frac{1}{\hbar} \mathcal{G}_{\sigma\rho}(1,2) \frac{\delta \varphi^{cl}(3)}{\delta \rho(1)} \frac{\delta^{(3)}\Gamma}{\delta \varphi^{cl}(3) \delta \bar{\psi}^{cl}_\rho(2) \delta \psi^{cl}_{\sigma'}(1')}$$

Hedin equation for Σ^*!

Hedin equations

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- Hedin equation for the proper self–energy $\Sigma^*_{\sigma\sigma'}(1,1')$:

$$\Sigma^*_{\sigma\sigma'}(1,1') = \frac{1}{\hbar}\delta_{\sigma\sigma'}\delta(1-1')\mathcal{U}_H(1) + \Sigma^*_{xc_{\sigma\sigma'}}(1,1')$$

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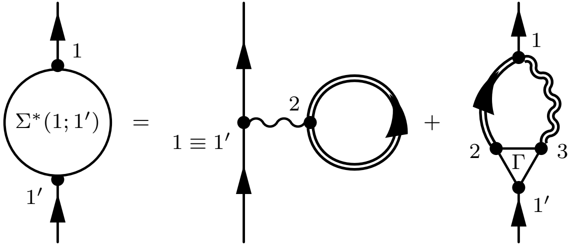

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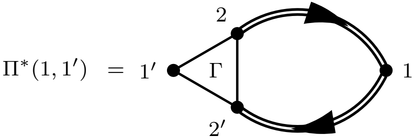

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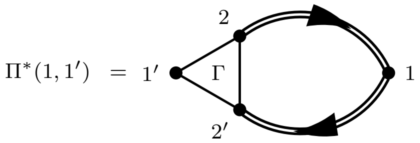

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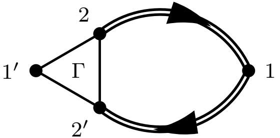

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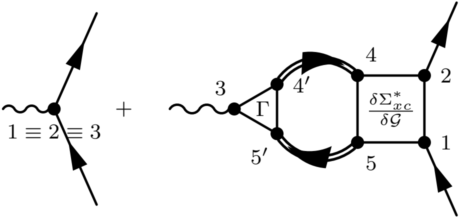

Hedin equations: approximations

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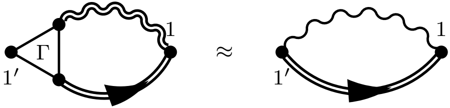

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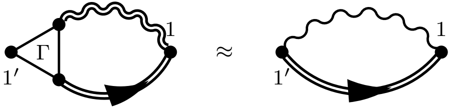

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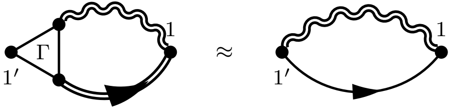

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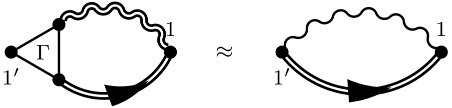

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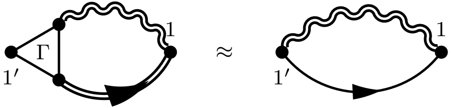

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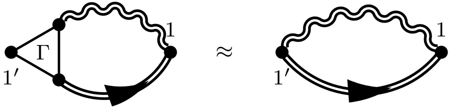

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$$\Omega = \sum_i n_i\epsilon_i - TS_s - \mu N - E_H[n(\mathbf{x})] - \int d^3x\; n(\mathbf{x})u_{xc}(\mathbf{x}) + F_{xc}[n(\mathbf{x})]$$

$$(n(\mathbf{x}) = n^*(\mathbf{x}))$$

Density Functional Theory: functional approach

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External source linearly coupled to the density (vs. coupling source/field):

$$e^{-\frac{1}{\hbar}\mathcal{W}[\boldsymbol{\theta}]} = \int \mathcal{D}\left[\boldsymbol{\varphi}\right] \mathcal{D}\left[\bar{\boldsymbol{\psi}}\right] \mathcal{D}\left[\boldsymbol{\psi}\right] e^{-\frac{1}{\hbar}\left[\mathcal{S} + \int dx\ \theta(x)\bar{\psi}_\sigma(x)\psi_\sigma(x)\right]}$$

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But our actual system corresponds to $\theta(x) = 0$ (remember $\mathcal{Z} = e^{-\beta\Omega}$):

$$\left.\frac{\delta\Gamma[\boldsymbol{n}]}{\delta n(x)}\right|_{\boldsymbol{\theta}=0} = 0$$

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$$n(x) = \langle\bar{\psi}(x)\psi(x)\rangle_{\boldsymbol{\theta}} = \frac{\delta\mathcal{W}\left[\boldsymbol{\theta}\right]}{\delta\theta(x)}$$

- Legendre Transformation: from an external–source–based description to a density–based description:

$$\Gamma\left[\boldsymbol{n}\right] = \mathcal{W}\left[\boldsymbol{\theta}\right] - \int dx\ \theta(x)\bar{\psi}_\sigma(x)\psi_\sigma(x)$$

- Equation of motion for Γ:

$$\theta(x) = -\frac{\delta\Gamma\left[\boldsymbol{n}\right]}{\delta n(x)}$$

But our actual system corresponds to $\theta(x) = 0$ (remember $\mathcal{Z} = e^{-\beta\Omega}$):

$$\left.\frac{\delta\Gamma\left[\boldsymbol{n}\right]}{\delta n(x)}\right|_{\boldsymbol{\theta}=0} = 0 \implies \left.\frac{\delta\Omega\left[\boldsymbol{n}\right]}{\delta n(x)}\right|_{\boldsymbol{n}=\boldsymbol{n}^*} = 0$$ DFT!

Density Functional Theory: functional approach

External source linearly coupled to the density (vs. coupling source/field):

$$e^{-\frac{1}{\hbar}\mathcal{W}[\boldsymbol{\theta}]} = \int \mathcal{D}\left[\boldsymbol{\varphi}\right]\mathcal{D}\left[\bar{\boldsymbol{\psi}}\right]\mathcal{D}\left[\boldsymbol{\psi}\right] e^{-\frac{1}{\hbar}\left[\mathcal{S}+\int dx\ \theta(x)\bar{\psi}_\sigma(x)\psi_\sigma(x)\right]}$$

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Moreover it is possible to prove that:

- If the source is real, $\boldsymbol{n}^*$ is a minimum ($\mathcal{W}$ is concave, Γ is convex).
- The Mermin decomposition holds: $\Omega[n(\mathbf{x})] = F[n(\mathbf{x})] + \int d^3x\ n(\mathbf{x})u(\mathbf{x})$.

Kohn–Sham Decomposition & path–integral

Go back to the path integral form of the grand–canonical partition function:

$$\mathcal{Z} = \int \mathcal{D}[\boldsymbol{\varphi}]\, \mathcal{D}[\bar{\boldsymbol{\psi}}]\, \mathcal{D}[\boldsymbol{\psi}]\, e^{-\frac{1}{\hbar}\int dx \left[\varphi(x)\left(-\frac{1}{8\pi}\nabla^2\right)\varphi(x) + \bar{\psi}(x)\left(k(x) + ie\varphi(x)\right)\psi(x)\right]}$$

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Integrate over fermion fields:
obtain an effective bosonic theory!

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Hartree field

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With this shift, a first separation occurs ($\mathcal{Z} = e^{-\beta\Omega}$):

(remember Kohn–Sham formula: $\Omega = \sum n_i\epsilon_i - TS_s - \mu N - E_H - \int n\cdot u_{xc} + F_{xc}$)

Kohn–Sham Decomposition & path–integral

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quadratic form ↓ Integrate over fermion fields: obtain an effective bosonic theory!

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Kohn–Sham Decomposition & path–integral

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Price for E_H: more difficult interaction term!

Kohn–Sham Decomposition & path–integral

$$\Omega\left[n(\mathbf{x})\right] = -E_H\left[n(\mathbf{x})\right] - \frac{1}{\beta}\ln\int\mathcal{D}\left[\boldsymbol{\varphi}\right] e^{-\frac{1}{\hbar}\left[\int dx\varphi(x)\left(-\frac{1}{8\pi}\nabla^2\right)\varphi(x) + -ie\int dx\varphi(x)n(x) - \hbar\,\mathrm{Tr}\ln\left[\frac{1}{\hbar}\left(k(x)+ie\varphi_H(x)\right)\delta(x,y)+ie\varphi(x)\delta(x,y)\right]\right]}$$

Kohn–Sham Decomposition & path–integral

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$$\left.\left.-ie\int dx\varphi(x)n(x)-\hbar\,\mathrm{Tr}\ln\left[\underbrace{\frac{1}{\hbar}\left(k(x)+ie\varphi_H(x)\right)\delta(x,y)}_{-\mathcal{G}_H^{-1}(x,y)}+ie\varphi(x)\delta(x,y)\right]\right]$$

Kohn–Sham Decomposition & path–integral

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$\downarrow$

Solution: add and remove a new field $\varphi_{xc}(x)$ with the following property:

$$\mathcal{G}_{KS}(x,x^+) = \mathcal{G}(x,x^+)$$

Kohn–Sham Decomposition & path–integral

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Kohn–Sham Decomposition & path–integral

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Kohn–Sham Decomposition & path–integral

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$$-\frac{1}{\beta}\ln\int\mathcal{D}\left[\boldsymbol{\varphi}\right]e^{-\frac{1}{\hbar}\left[\int dx\varphi(x)\left(-\frac{1}{8\pi}\nabla^2\right)\varphi(x) + \hbar\sum_{n=2}^{\infty}\frac{1}{n}\left(\frac{ie}{\hbar}\right)^n\mathrm{Tr}\left[\mathcal{G}_{KS}\delta\varphi\right]^n\right]}$$

Kohn–Sham Decomposition & path–integral

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$$-\mathcal{G}_H^{-1}(x,y) \rightarrow n_H(\mathbf{x}) \neq n(\mathbf{x})$$

$$\downarrow$$

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- The very last step:

Kohn–Sham Decomposition & path–integral

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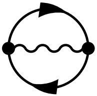

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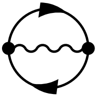

- Besides: besides RPA as far as the interaction is concerned, besides One–Loop–Expansion as far as the integral is concerned...

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Thank you for your attention

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For example:

$$\prod_{i=1}^{N} \int d\bar{\theta}_i d\theta_i e^{-\bar{\theta}_i A_{ij}\theta_j} = \det A$$

(while in the bosonic case one has $\prod_{i=1}^{N} \int_{\mathbb{R}} \frac{dz_i^* dz_i}{2\pi i} e^{-z_i^* A_{ij} z_j} = \frac{1}{\det A}$)

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