# Many-Body Perturbation theory: Basic concepts and approximations


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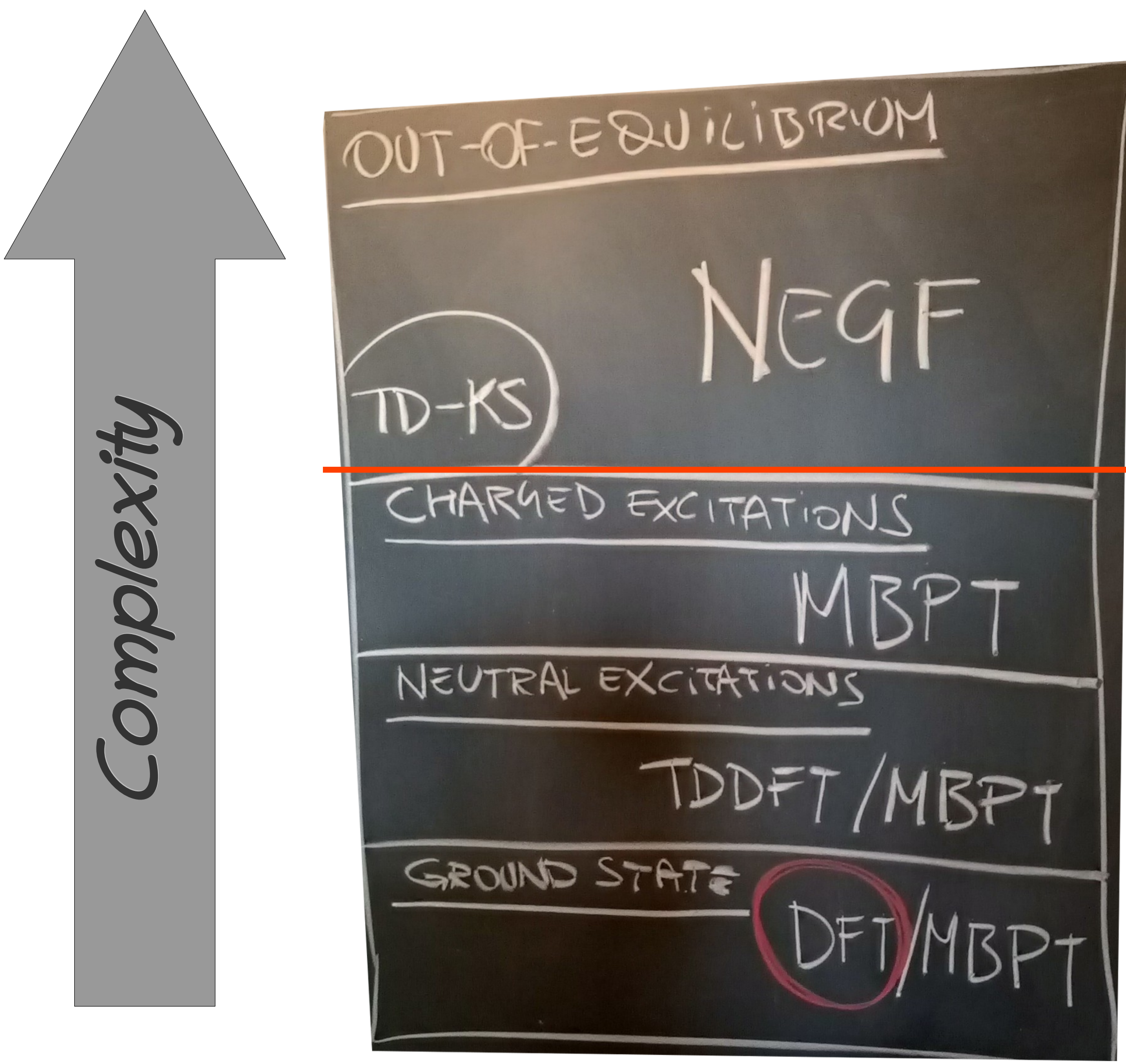
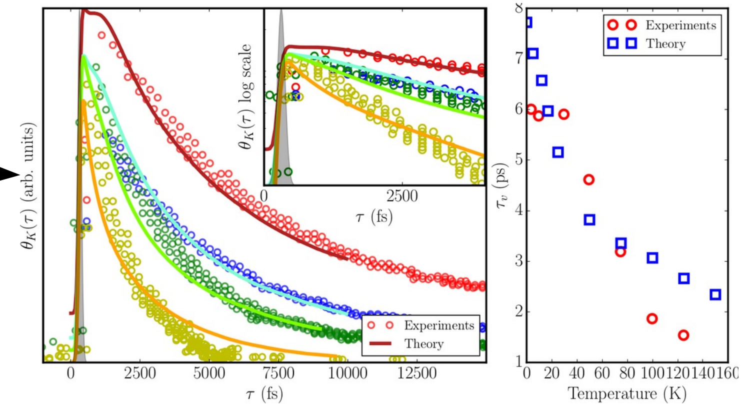
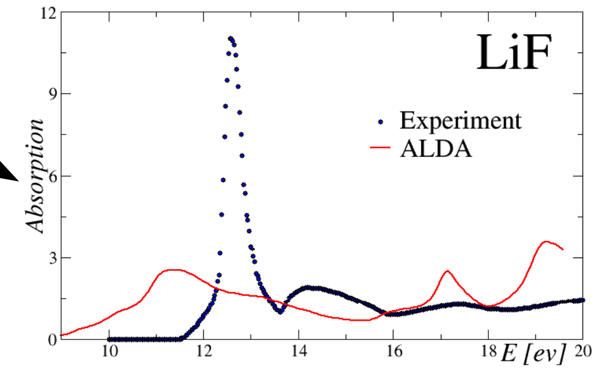
# Different physics, different approaches

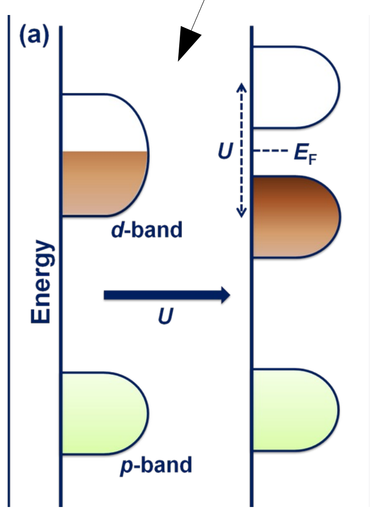


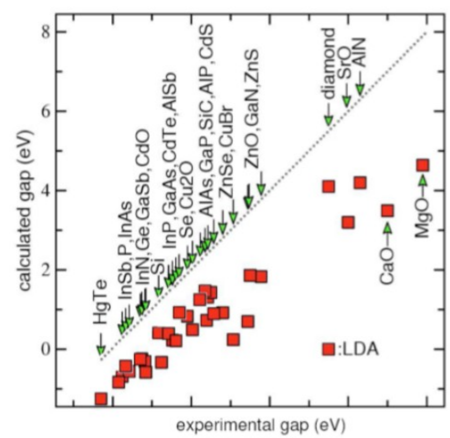


# Different physics, different approaches


Adapted from M. van Schilfgaarde *et al.* PRL **96** (2006)

Si:
0.47 eV (LDA) vs 1.1 eV (expt)

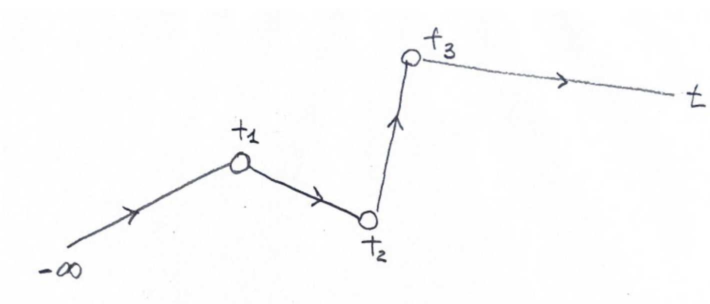
GaAs:
0.30 eV (LDA) vs 1.4 eV (expt)

# Outline

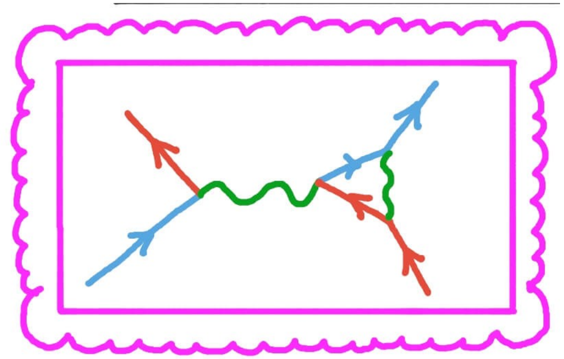
$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

The Hamiltonian

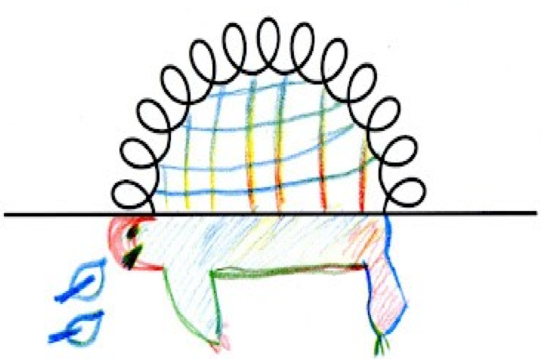
Many-Body Perturbation Theory for dummies


Lippmann-Schwinger propagators



Feynman diagrams for dummies

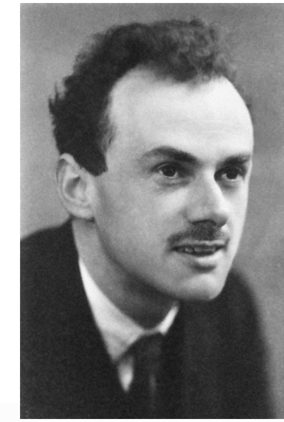


The "zoo" of MBPT approximations

# From QED to MBPT and the role of Classical Mechanics

# The "Fermi" Hamiltonian

$$\hat{H}_{int} = -\sum_{\mu=0,3} \int d\mathbf{r} \hat{\vec{j}}_{\mu}(\mathbf{r}) \hat{\vec{A}}_{\mu}(\mathbf{r})$$



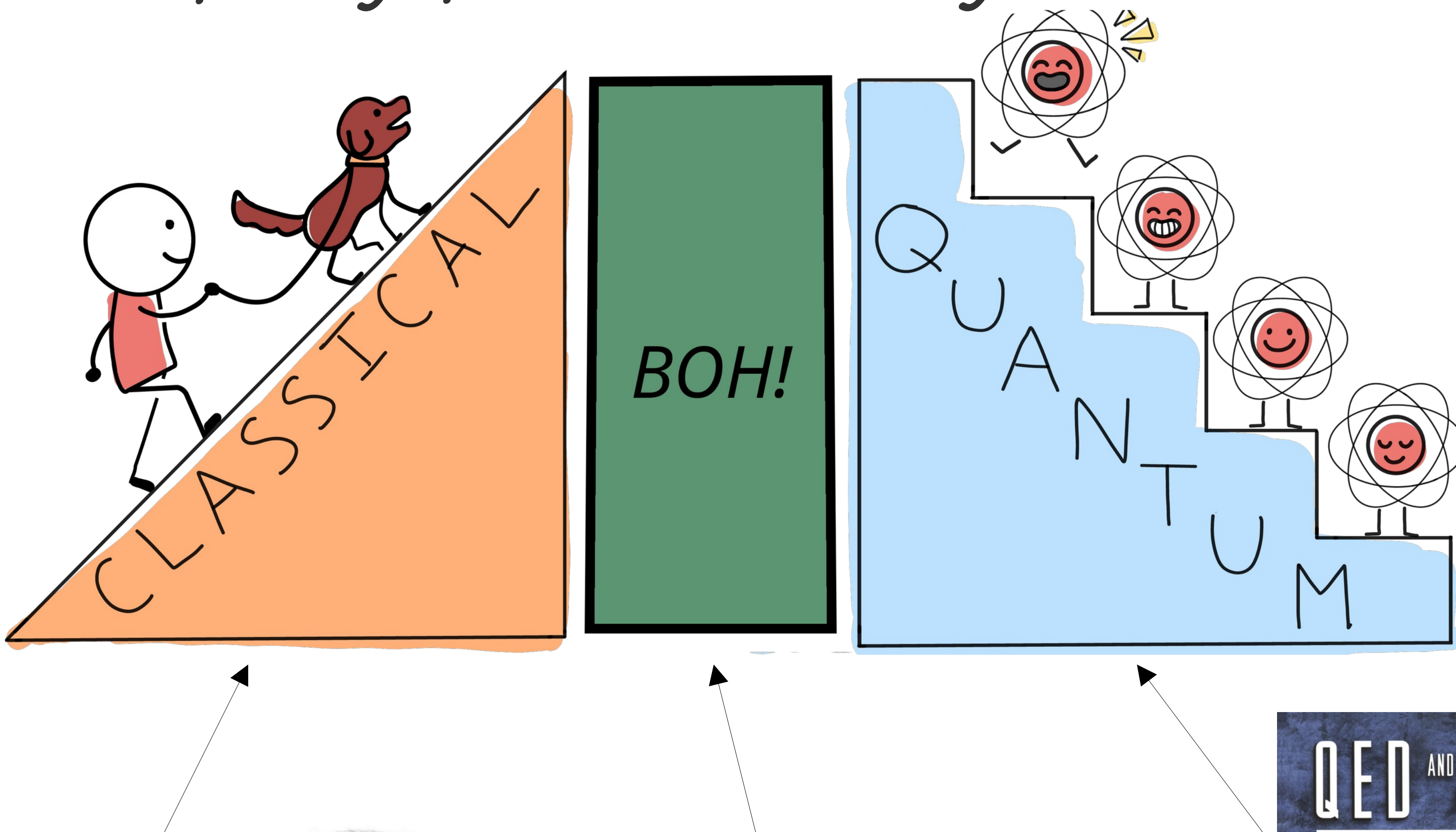
The radiation Gauge
(E. Fermi, 1932)

$$\nabla \cdot \hat{\mathbf{A}}(\mathbf{r}, \mathbf{t}) = \mathbf{0}$$

$$\nabla \cdot \mathbf{D} = \rho$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

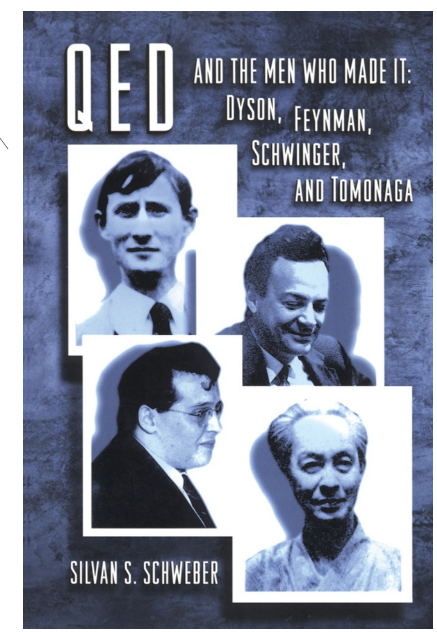
$$\hat{H}_{int} = \int d\mathbf{r}\mathbf{r}' \frac{\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \int d\mathbf{r} \hat{\vec{j}}(\mathbf{r}) \cdot \vec{A}^{\perp}(\mathbf{r})$$

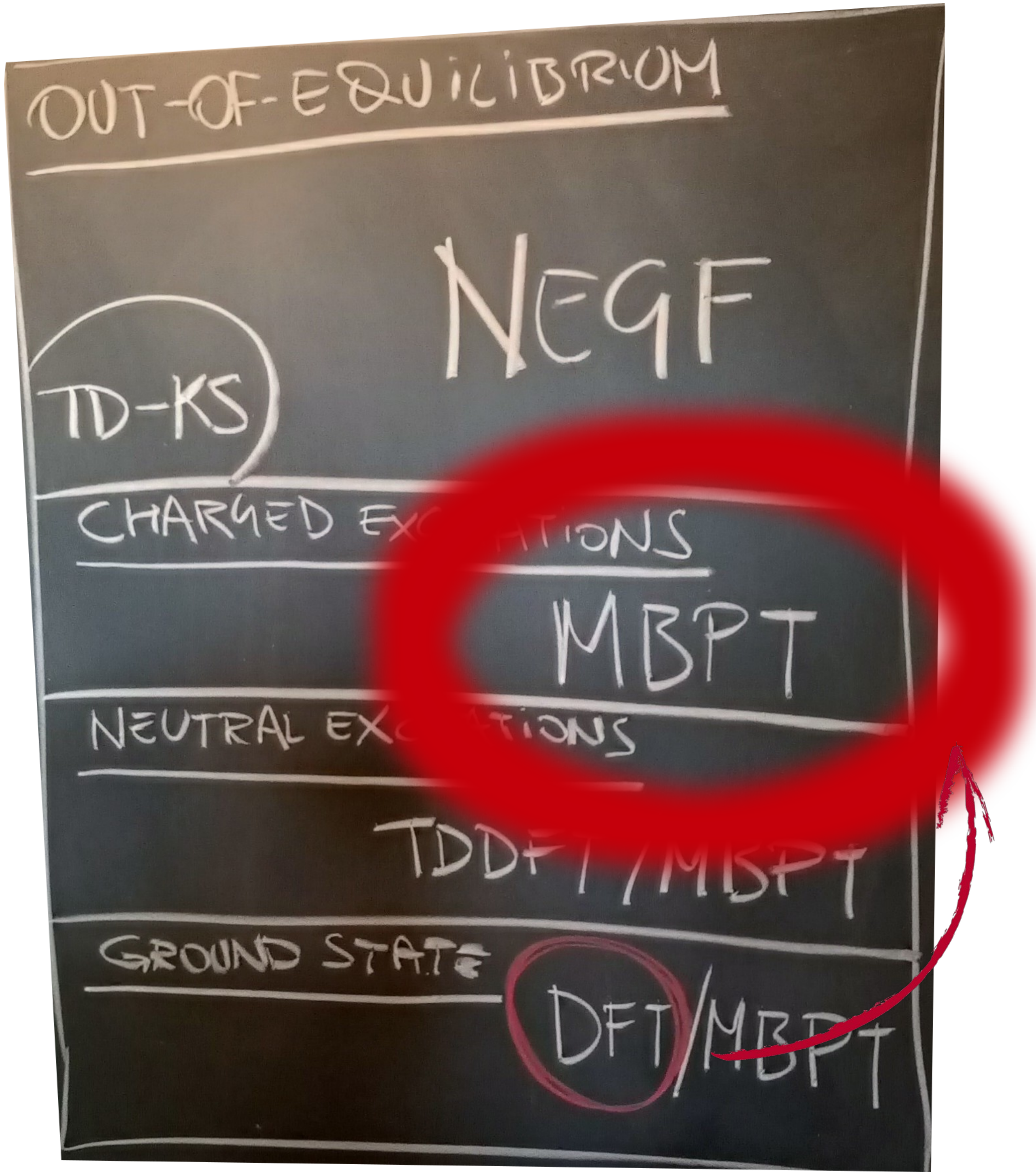
# Is MBPT a purely quantistic theory?



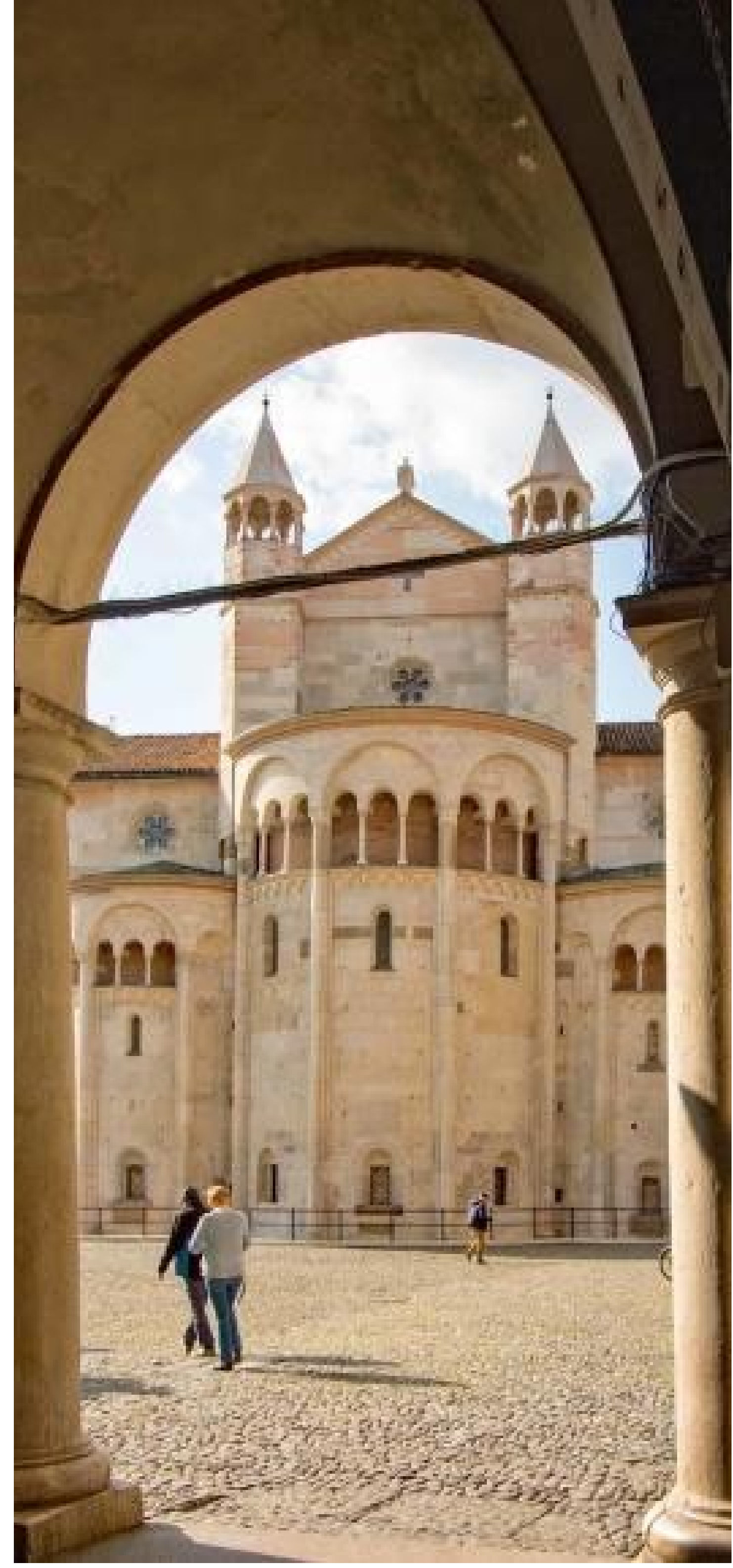

$$
\begin{aligned}
\nabla \cdot \mathbf{D} &= \rho \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{H} &= \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}
\end{aligned}
$$

MBPT



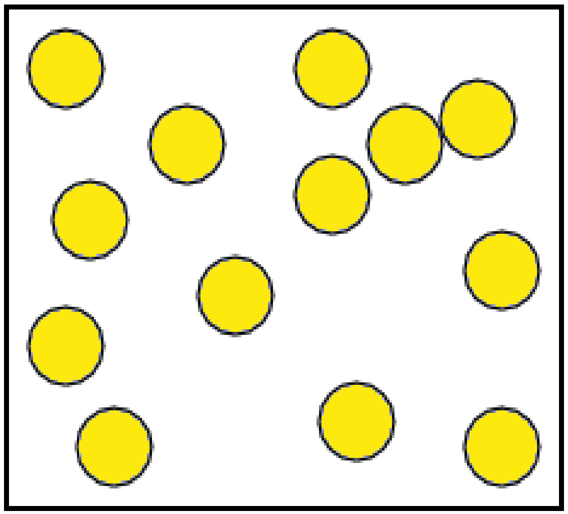


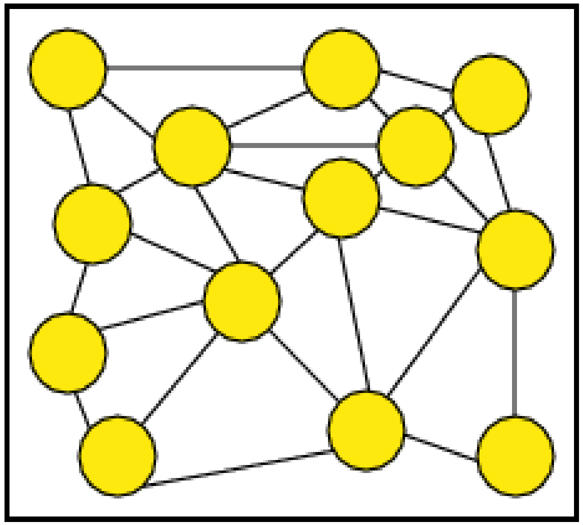

# Many-Body Perturbation Theory for dummies



# The Many-Body problem

$$H = \sum_i h(x_i, p_i) + \frac{1}{2}\sum_{i \neq j} |x_i - x_j|^{-1}$$

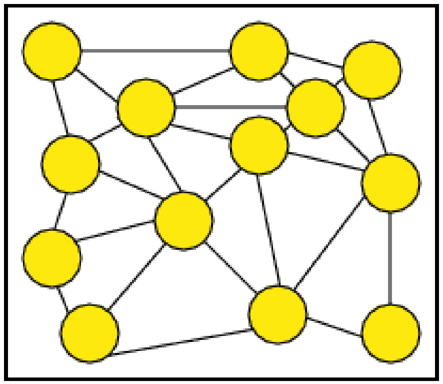




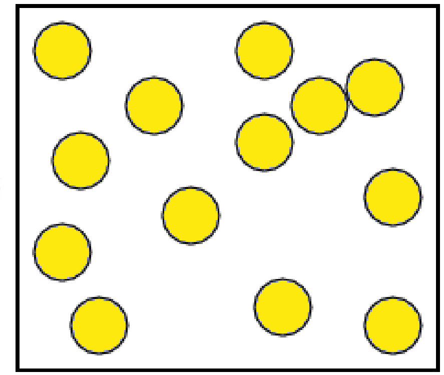
# The Many-Body problem: 1 particle approx

$H=\sum_i h(x_i)+\frac{1}{2}\sum_{i\neq j}|x_i-x_j|^{-1}$

$H=\sum_i h(x_i)$



$\hat{h}|n\rangle=\epsilon_n|n\rangle$



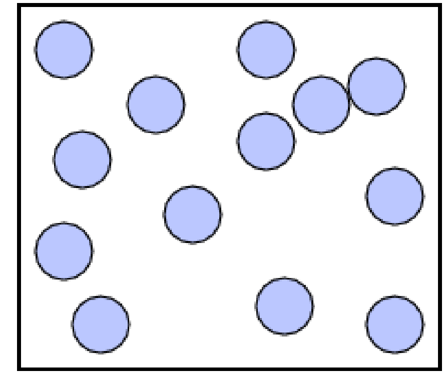
$$|N_0\rangle=\prod_{n\in filled}|n\rangle$$

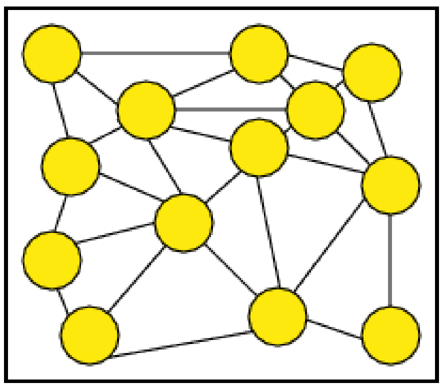
$$\langle N|\hat{A}|N\rangle\approx F_N[\{A_n\}]$$

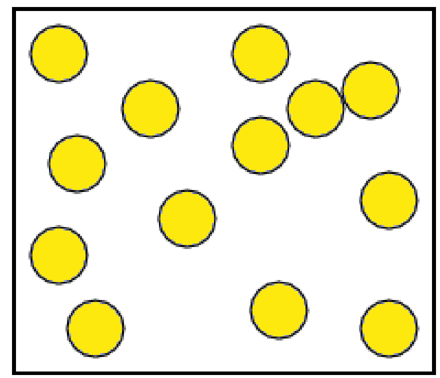
$$\langle N_0|\hat{H}\,|N_0\rangle=\sum_{n\in filled}\epsilon_n$$

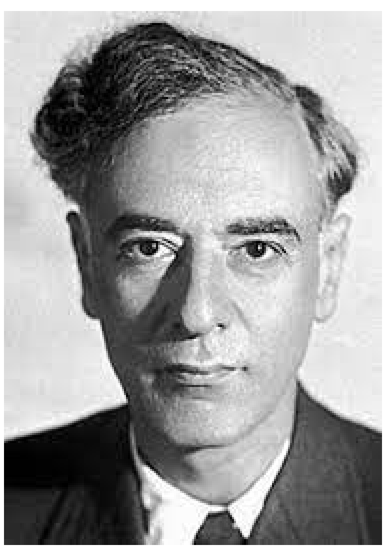
# Quasiparticles...

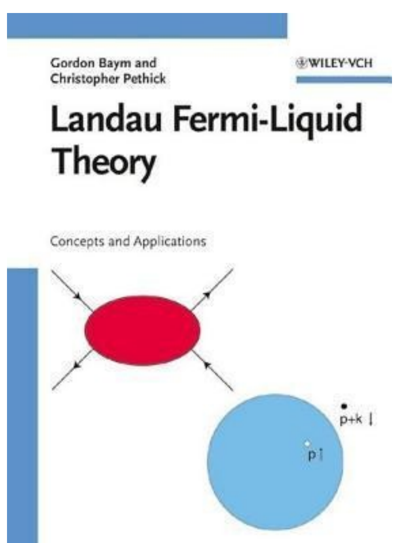
$$H = \overbrace{\sum_i h(x_i)}^{\hat{H}_0} + \frac{1}{2}\sum_{i\neq j}\left|x_i - x_j\right|^{-1} = h + H'$$







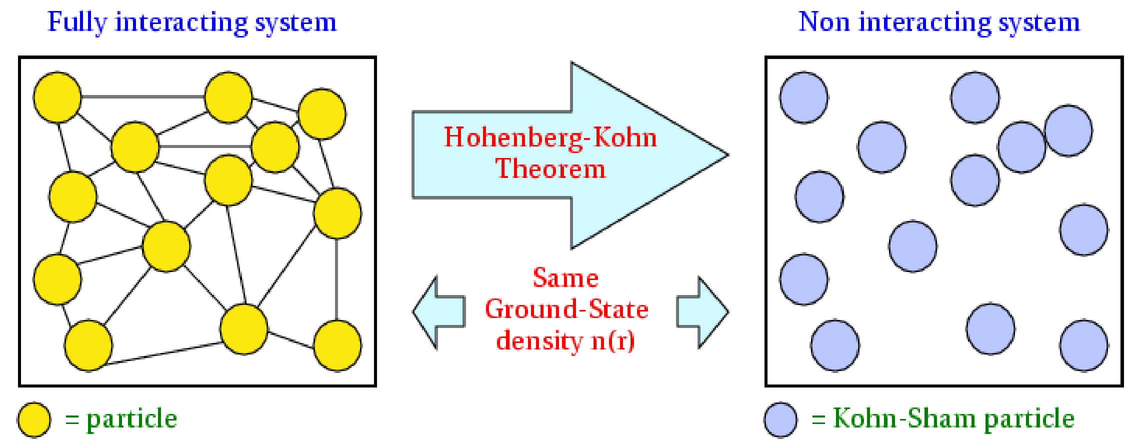



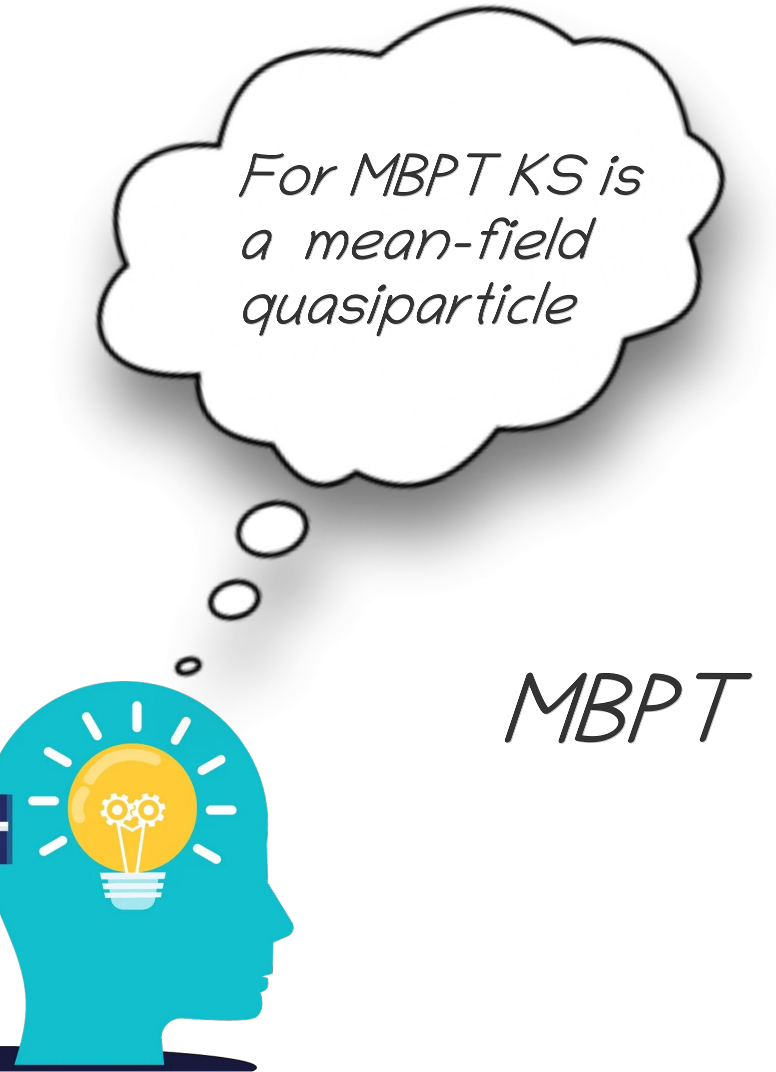



*The goal of the Many Body methods is to rewrite the fully interacting problem as an as much independent as possible counter-part*

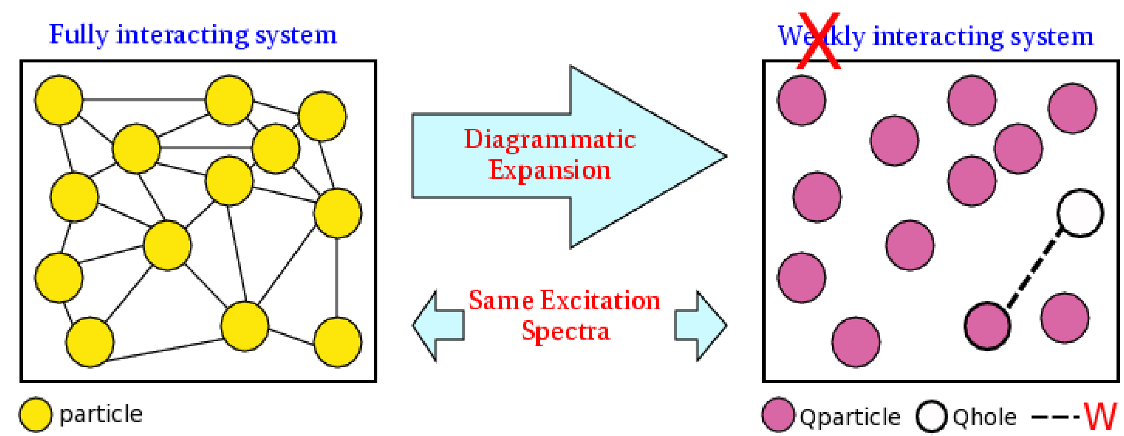
# Mean-Field and beyond

DFT




MBPT



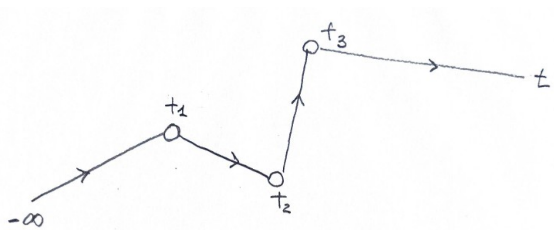
*Schrödinger equation*

$$\left(i\hbar\partial_t - \hat{H}_0\right)|\psi(t)\rangle = \hat{V}|\psi(t)$$

*Feynman path integral approach (CM trajectories)*


*Raileigh-Schrödinger Perturbation Theory (states, Dirac Notation)*

# Lippmann-Schwinger (quantum) propagation



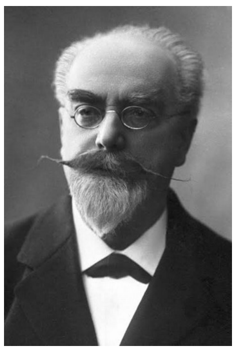

# Lippmann-Schwinger propagators

$$\left(i\hbar\partial_t - \hat{H}_0\right)|\psi(t)\rangle = e^{\eta t}\hat{V}|\psi(t)\rangle$$

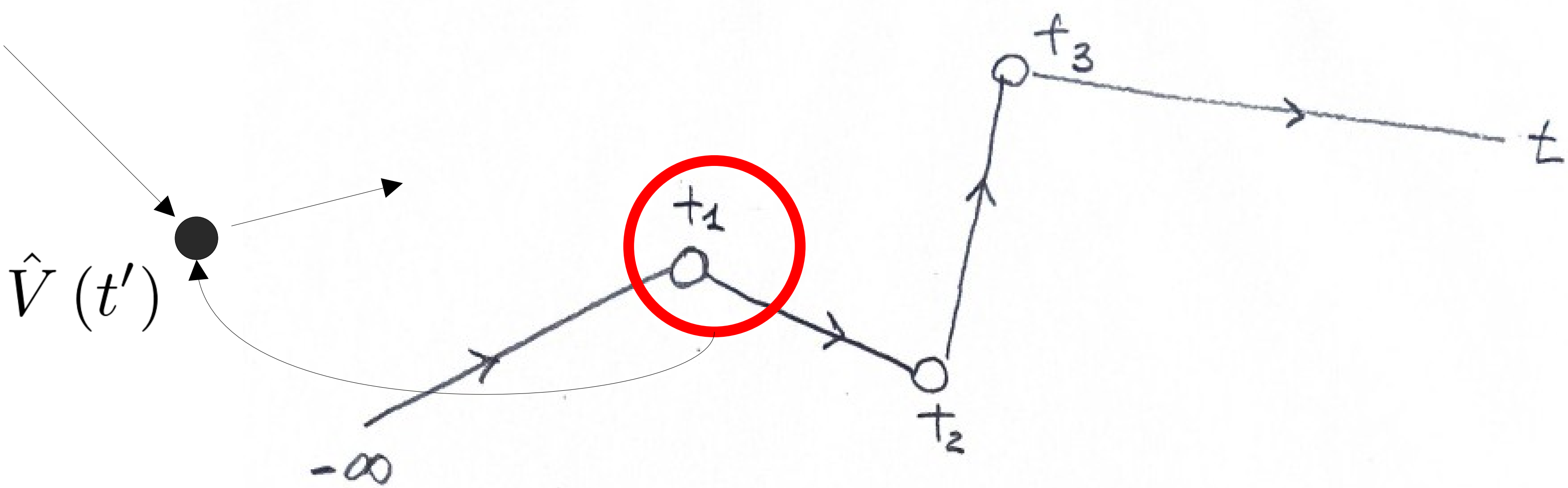
*Schrödinger equation*

$$\left(i\hbar\partial_t - \hat{H}_0\right)\hat{G}_0(t,t') = \delta(t-t')$$

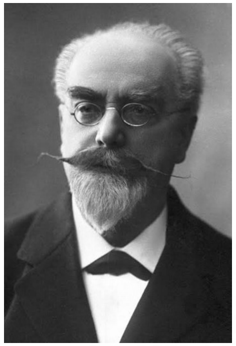
$$\hat{G}_0(t,t') = -\frac{i}{\hbar}\theta(t-t')e^{-\frac{i}{\hbar}\hat{H}_0(t-t')}$$



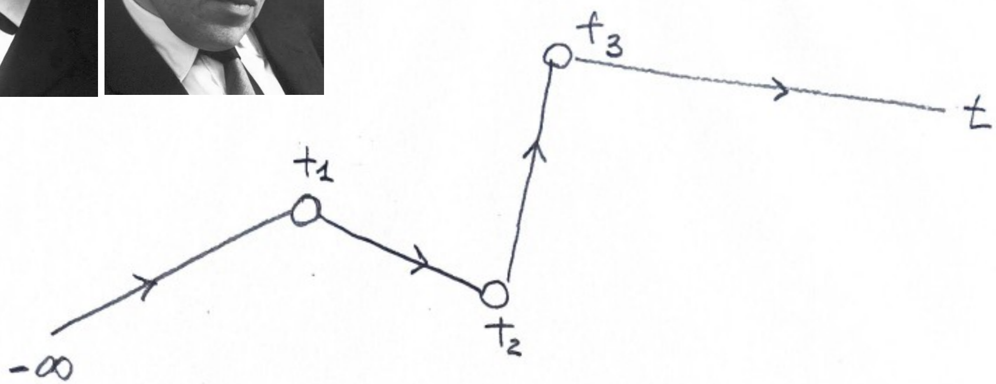
$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty}\hat{G}_0(t,t')\hat{V}(t')|\psi(t')\rangle dt'$$



# Lippmann-Schwinger propagators

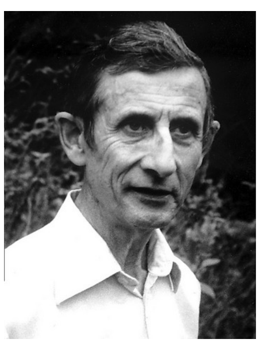


$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty} \hat{G}_0(t,t')\,\hat{V}(t')\,|\psi(t')\rangle\, dt'$$




$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty} \hat{G}_0(t,t')\,\hat{V}(t')\,|\psi(-\infty)\rangle\, dt' +$$

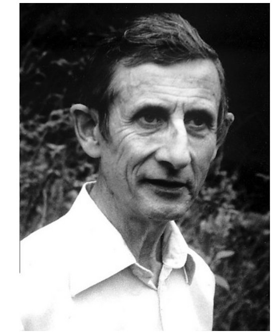
$$+ \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \hat{G}_0(t,t_1)\,\hat{V}(t_1)\,\hat{G}_0(t_1,t_2)\,\hat{V}(t_2)\,|\psi(-\infty)\rangle + \dots$$

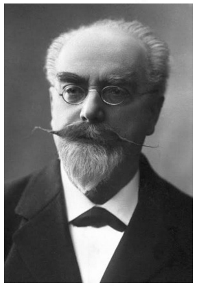


$$G_0\hat{V} + G_0\hat{V}G_0\hat{V} + \cdots = G\hat{V}$$

# *Lippmann-Schwinger propagators*

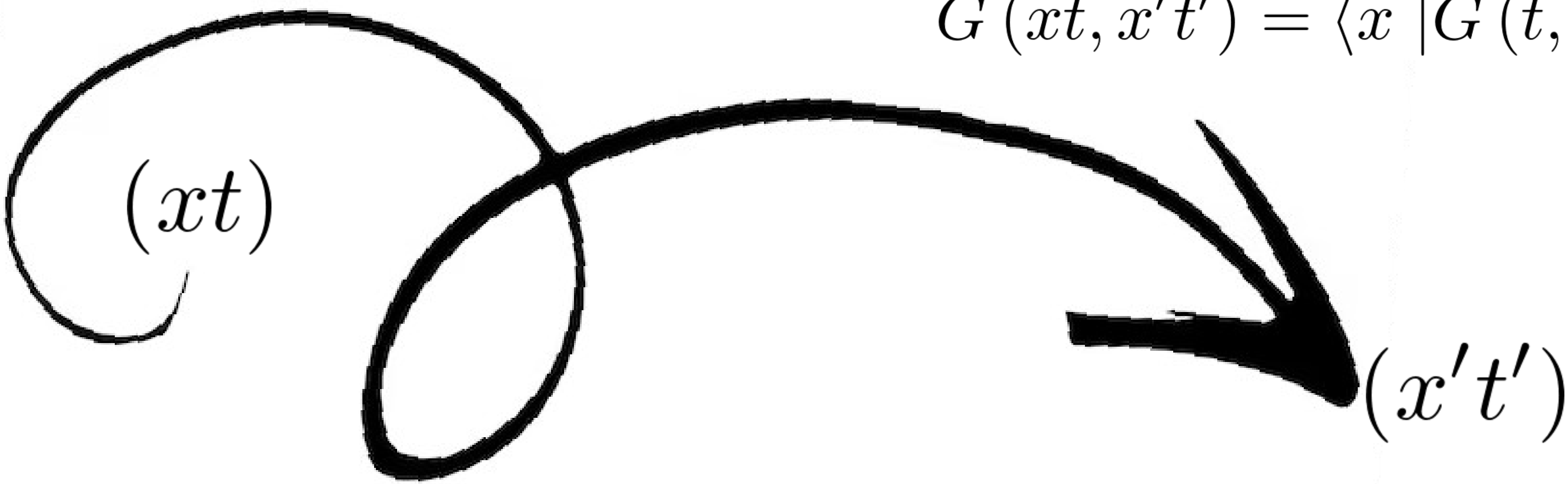
$$\hat{G}(t,t') = \hat{G}_0(t,t') + \int_{-\infty}^{\infty} \hat{G}_0\left(t,t_1\right)\hat{V}\left(t_1\right)\hat{G}(t_1,t')$$





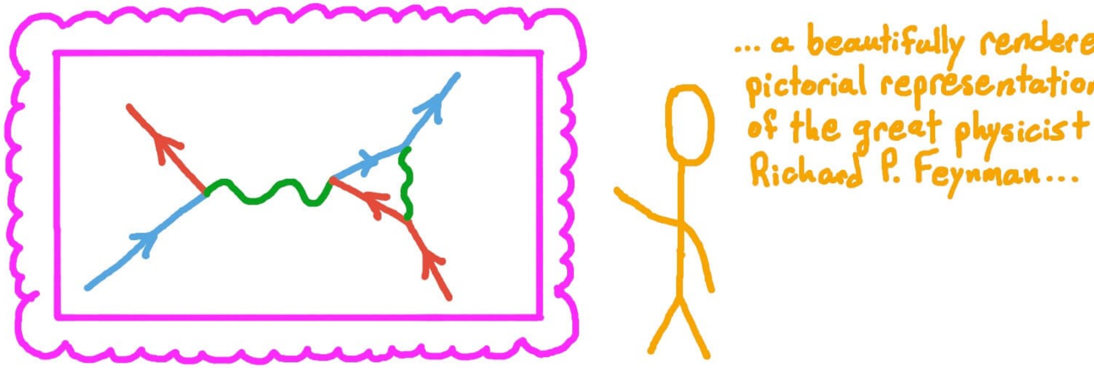
$$|\psi\left(t\right)\rangle = |\psi\left(-\infty\right)\rangle + \int_{-\infty}^{\infty} \hat{G}\left(t,t'\right)\hat{V}\left(t'\right)|\psi\left(-\infty\right)\rangle\, dt'$$

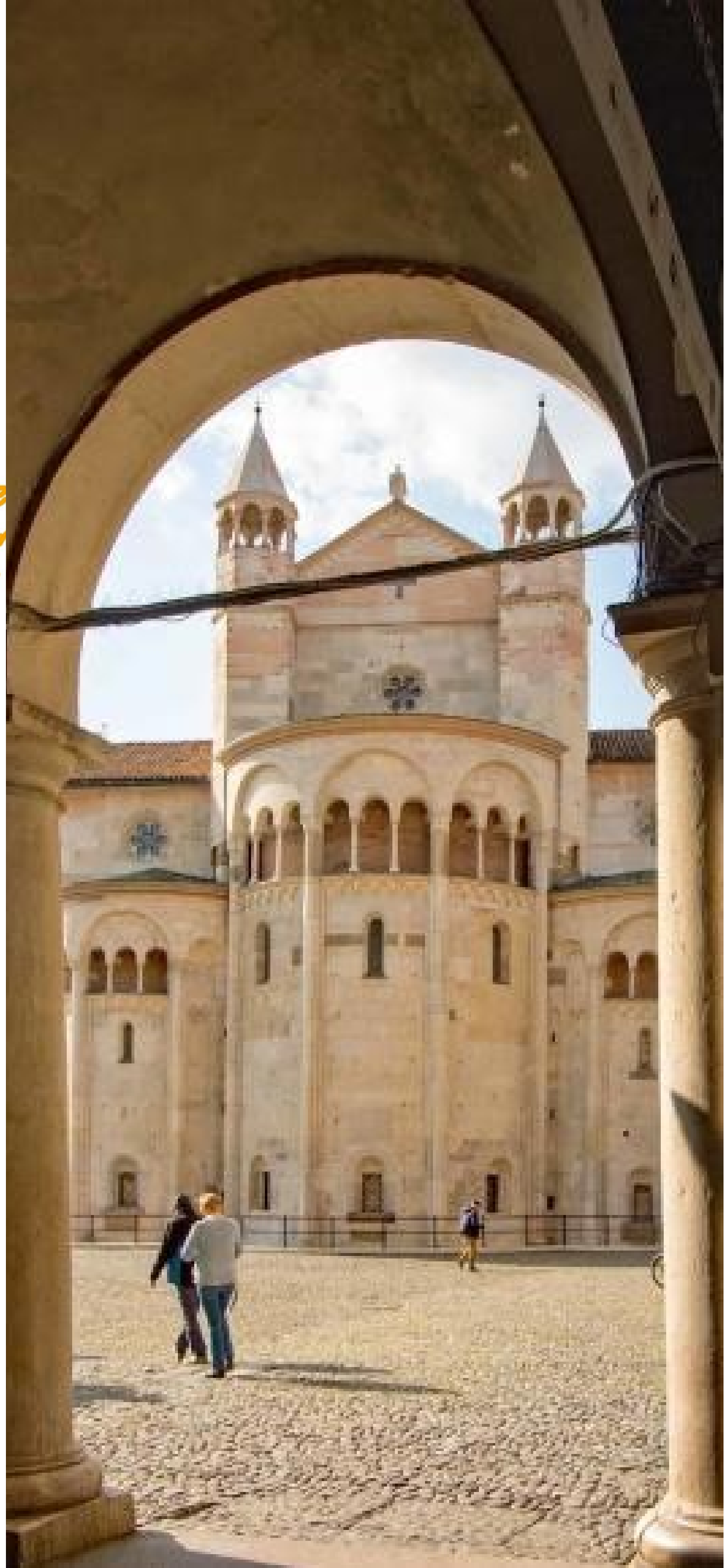
$$G\left(xt, x't'\right) = \langle x\,|\hat{G}\left(t,t'\right)|x'\rangle$$




$$|x\rangle = \hat{\psi}^{\dagger}\left(x\right)|vacuum\rangle \quad \Rightarrow \quad G\left(xt, x't'\right) = \left\langle \hat{\psi}^{\dagger}\left(xt\right)\hat{\psi}\left(x't'\right)\right\rangle$$

# FEYNMAN DIAGRAMS



Feynmann diagrams for dummies

# The time-dependent, interacting density (Kubo)

$$n(\mathbf{r},t) = \left\langle \Psi(t) \left| \hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r}) \right| \Psi(t) \right\rangle$$

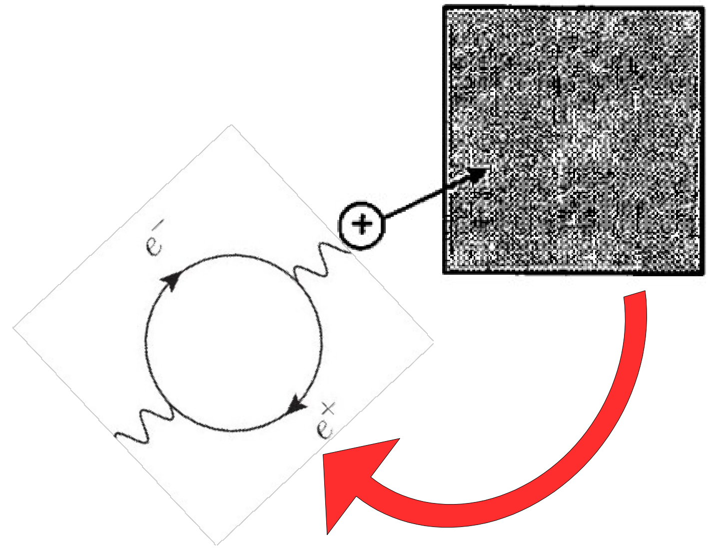
Ground State $\Psi(t) = \Psi_0$

Density Functional Theory

Semi-classical **WEAK** excitation

$$\hat{H}(t) = \hat{H}_0 + \int \hat{n}(\mathbf{r}) V(\mathbf{r},t)$$

Kubo

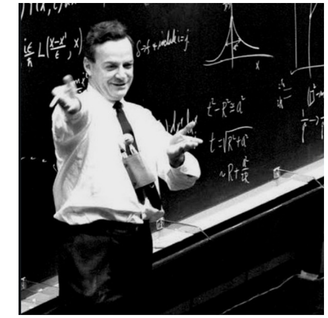



$$\mathrm{n}(\mathbf{r},\mathrm{t}) = \mathrm{n}_0(\mathbf{r}) + \int d\mathbf{r}' \int_0^t dt' \chi^R(\mathbf{r}t,\mathbf{r}'t') V(\mathbf{r}',t')$$

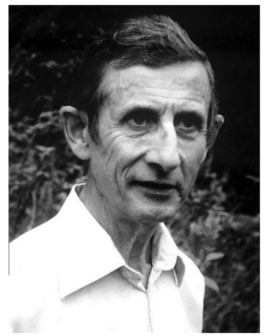
$$\chi(\mathbf{r}t,\mathbf{r}'t') = -i \left\langle \Psi \left| [\hat{n}(\mathbf{r},t), \hat{n}(\mathbf{r}',t')] \right| \Psi \right\rangle \theta(t-t')$$

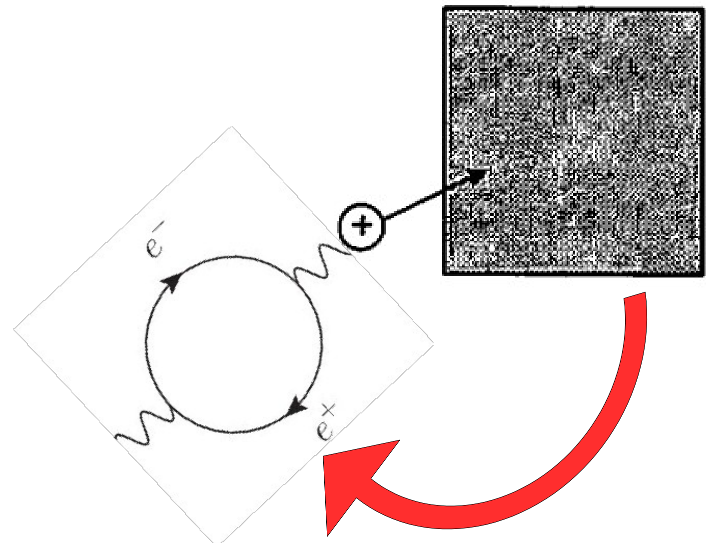
# The response (Green's) function

$$\mathrm{n}(\mathbf{r},\mathrm{t})=\mathrm{n}_0(\mathbf{r}) + \int d\mathbf{r}' \int_0^t dt' \underbrace{\chi^R(\mathbf{r}t,\mathbf{r}'t')} V(\mathbf{r}',t')$$



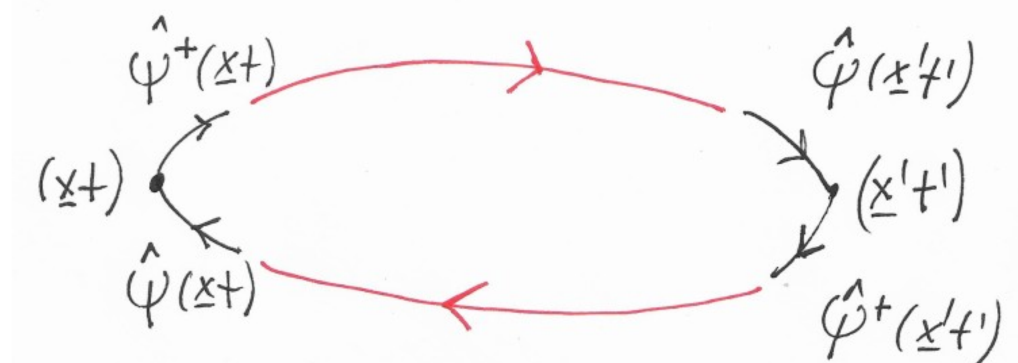
$$\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r})\hat{d}_{\mathbf{k}}$$






$\hat{\psi}^\dagger(\mathbf{r}t)$ ——▶—— $\hat{\psi}(\mathbf{r}'t')$

$$\langle \Psi \,|[\hat{n}(\mathbf{r},t),\hat{n}(\mathbf{r}',t')]|\, \Psi\rangle \approx$$



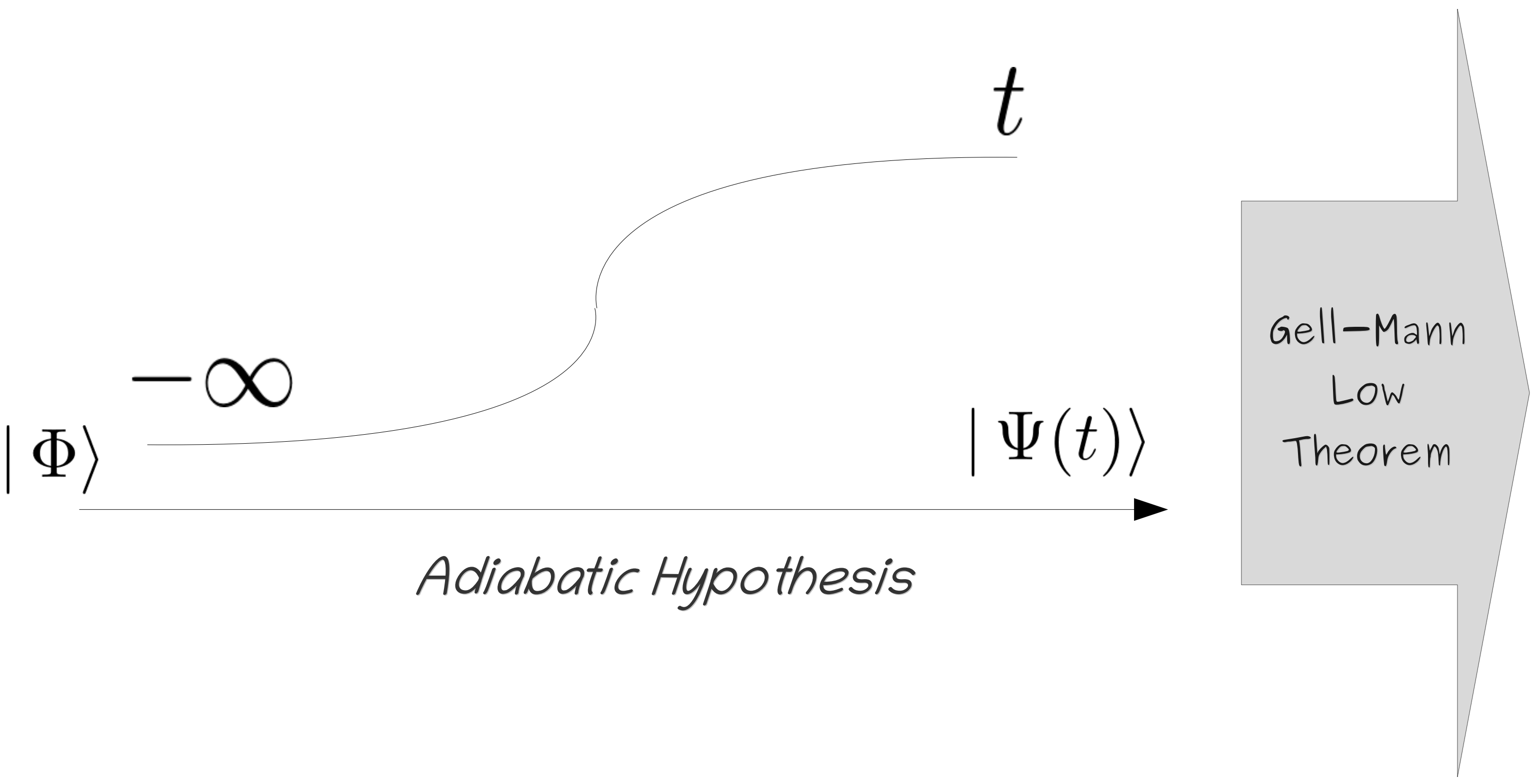

$$G(xt,x't') = \left\langle \hat{\psi}^\dagger(xt)\,\hat{\psi}(x't')\right\rangle$$

$$G(xt,x't')\,G(x't',xt)$$

# The adiabatic ansatz

$$n(\mathbf{r},t) = \left\langle \Psi(t) \middle| \hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r}) \middle| \Psi(t) \right\rangle$$

$$|\,\Psi(t)\rangle = \hat{U}(t,t_0)\ |\,\Psi(t_0)\rangle \longrightarrow \hat{U}(t,-\infty)\ |\,\Phi\rangle$$




*In equilibrium MBPT time is just the adjoint to energy. It has no link with real time.*

# The evolution operator (scattering potential)

$$\hat{H}(t) = \hat{H}_0 + \underbrace{\hat{V}(t)}$$

$$\int \hat{n}(\mathbf{r}) V(\mathbf{r}, t)$$

$$i \frac{d}{dt} \hat{U}_0(t) = \hat{H}_0 \hat{U}_0(t)$$

$$\hat{U}(t) = \hat{U}_0(t) \hat{F}(t)$$

$$\hat{F}(t) = 1 - i \int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + \underbrace{(-i)^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1}} dt_2 \hat{V}_I(t_1) \hat{V}_I(t_2) + \dots$$

*Constrained time integrals*

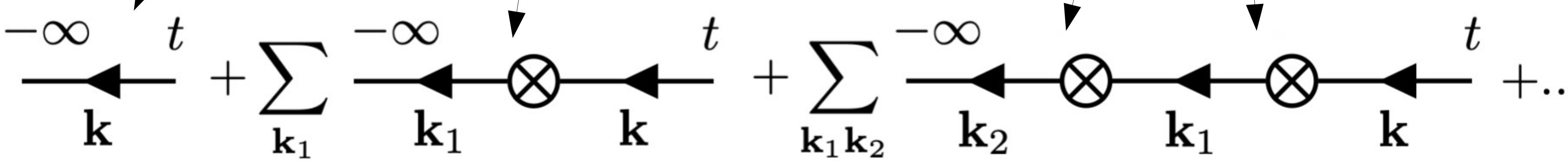
$$t > t_1 > t_2 > \cdots$$

# Half the dynamics...

$$\left\langle \Psi(t) \middle| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}_{\mathbf{k}'} \middle| \Psi(t) \right\rangle = \delta_{\mathbf{k}\mathbf{k}'} - \left\langle \Psi(t) \middle| \hat{d}_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}^\dagger_{\mathbf{k}'} \middle| \Psi(t) \right\rangle$$

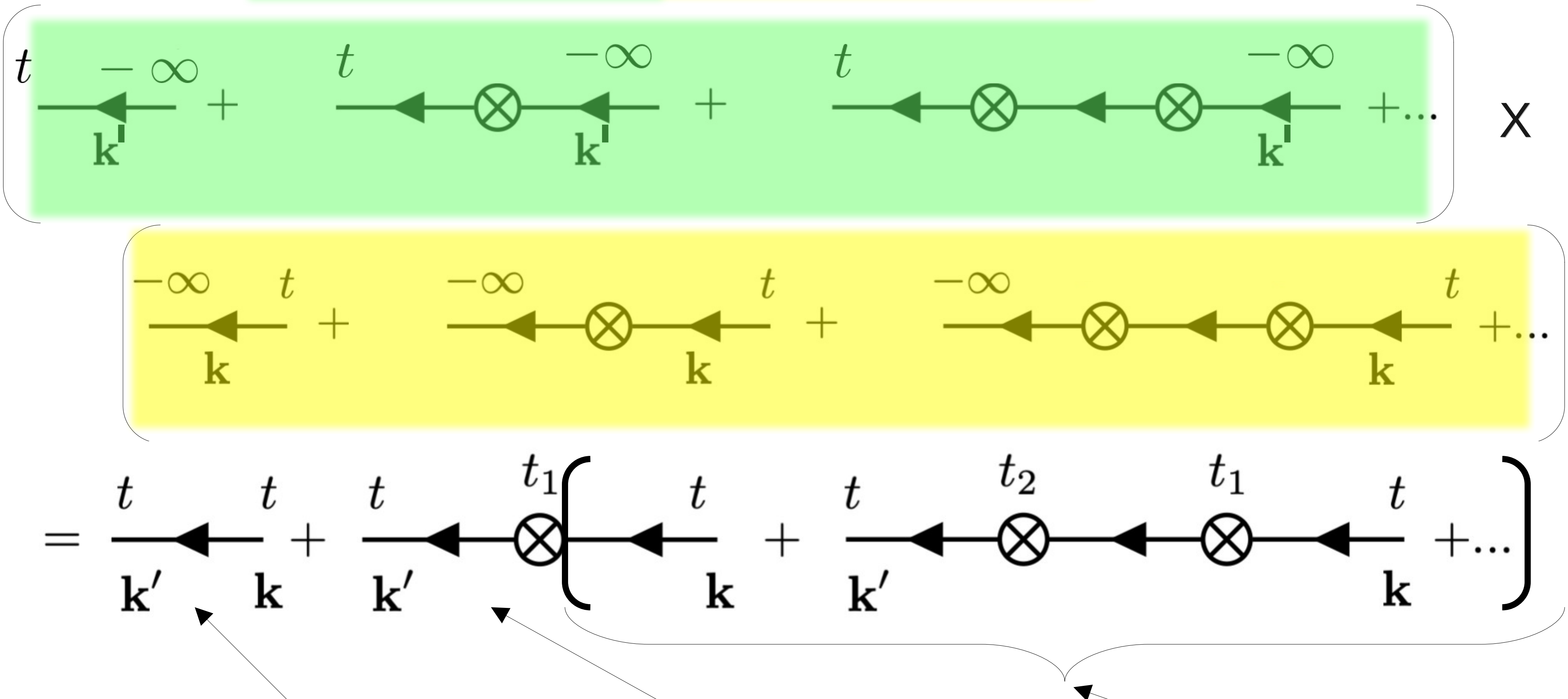
$$\hat{U}^\dagger(t) \hat{d}^\dagger_{\mathbf{k}} \middle| \Psi(t) \right\rangle = F^\dagger(t) \hat{U}_0^\dagger(t) \hat{d}^\dagger_{\mathbf{k}} \middle| \Psi(t) \right\rangle$$

$$\hat{F}(t) = 1 + i \int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + i^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_2) \hat{V}_I(t_1) + \dots$$



# The Dyson equation

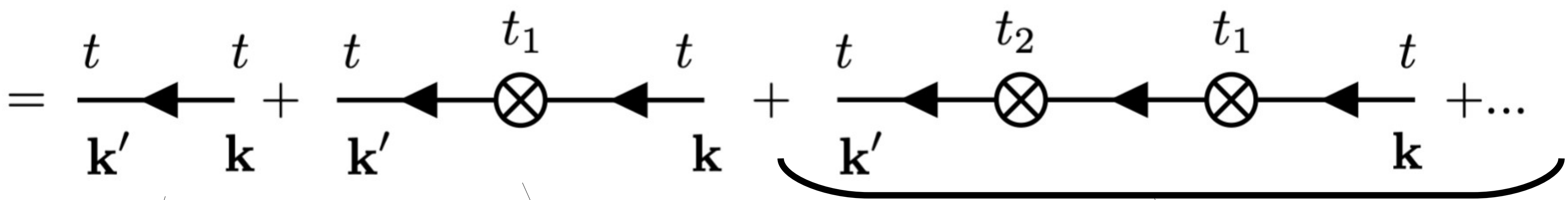
$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$




$$G_{kk'}(t,t) = G^0_{kk'}(t,t) + \sum_{qp} \int_{-\infty}^{\infty} G^0_{kq}(t,t_1)\, V_{qp}(t_1)\, G_{qk'}(t_1,t')$$

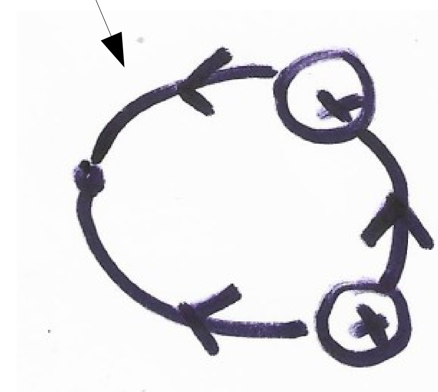
# Green's Functions: Kubo revisited

$$\left\langle \Psi(t) \left| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}^\dagger_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$




$\mathrm{n}_0(\mathbf{r})$

$\int d\mathbf{r}' \int_0^t dt' \chi^R(\mathbf{r}t, \mathbf{r}'t') V(\mathbf{r}', t')$

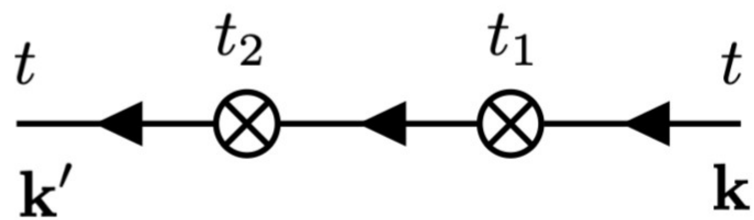


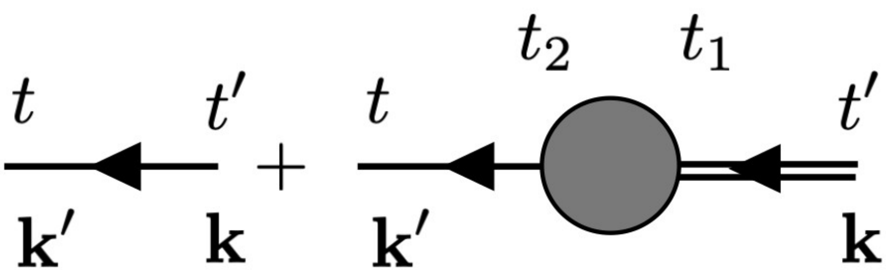
*Non-linear terms*

# Key messages

MBPT is based on a **semi-classical definition** of the elemental interactions

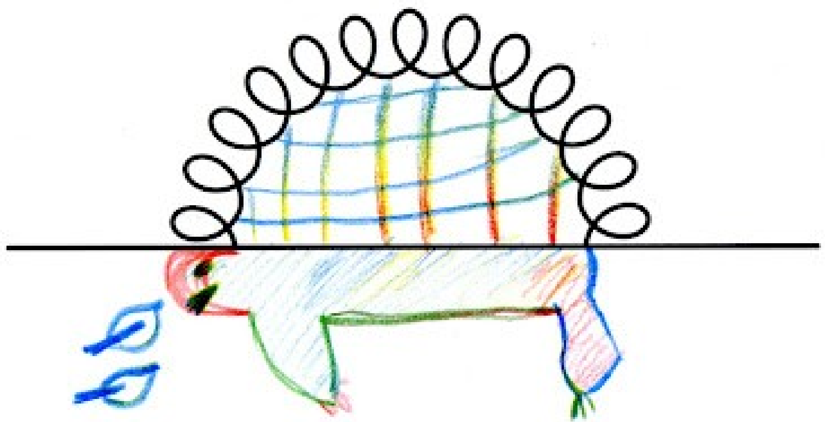
In MBPT the many-body problem is rewritten in terms as **pseudo-time** propagation under the action of a **slowly varying potential**



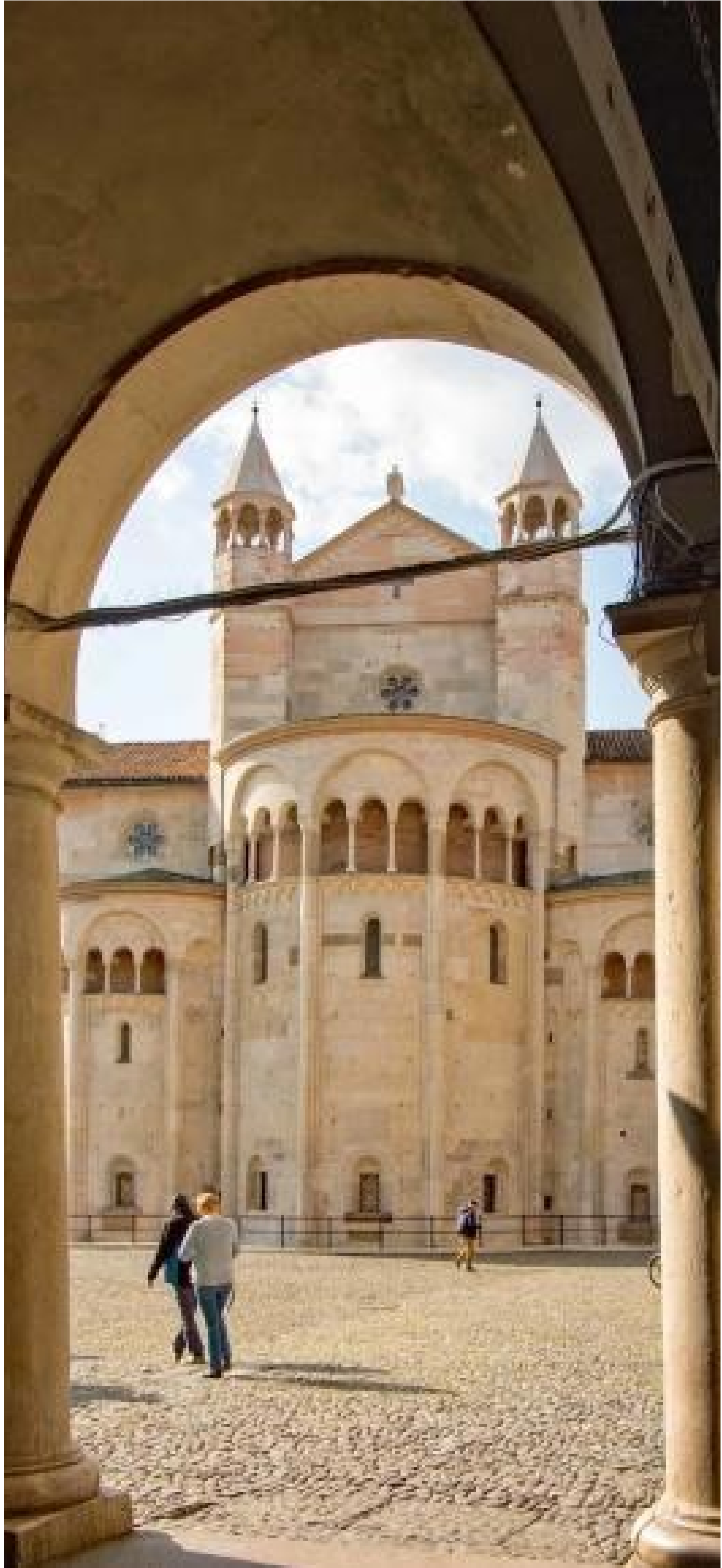




Diagrams allow to introduce a **geometric representation** of the dynamics

In MBPT **time does not correspond to real-time.** At finite temperatures, actually, it even becomes imaginary (Matsubara formalism)

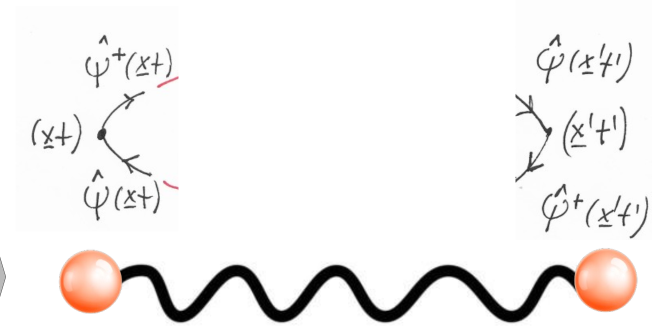


# The "zoo" of MBPT approximations

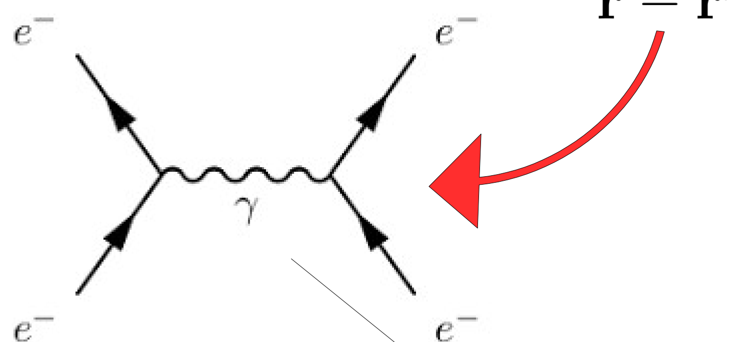


# The Coulomb interaction (revisited)

$$\hat{H}_{int}(t) = e^{\eta t} \int d\mathbf{r}\mathbf{r}' \frac{\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

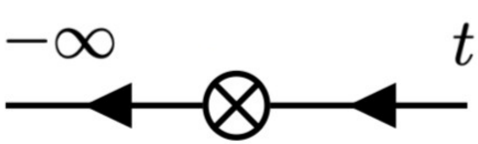


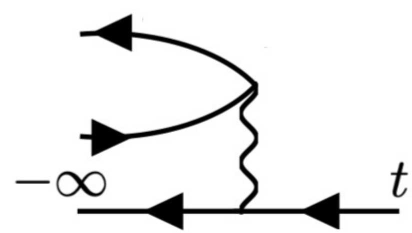

$$\frac{1}{\mathbf{r}-\mathbf{r}'}$$




$$\hat{U}(t) = \hat{U}_0(t)\hat{F}(t)$$

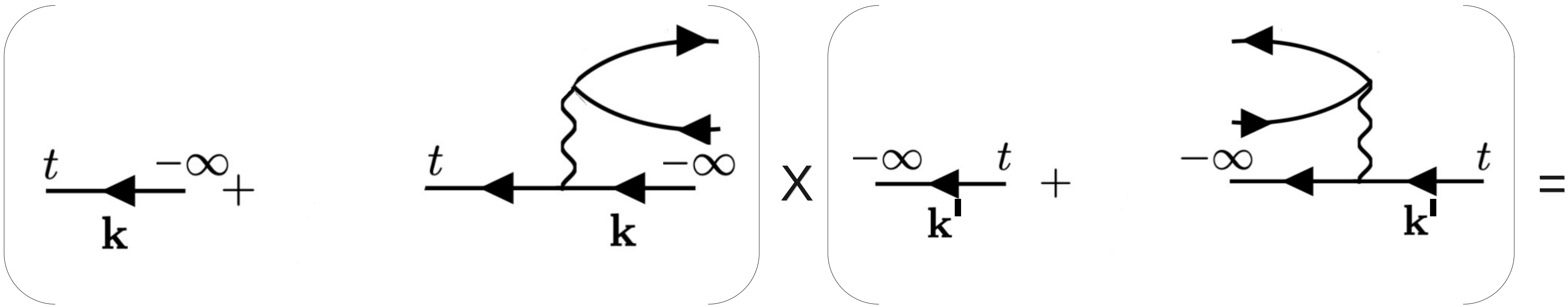
$$\hat{F}(t) = 1 - i\int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + (-i)^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \ldots$$

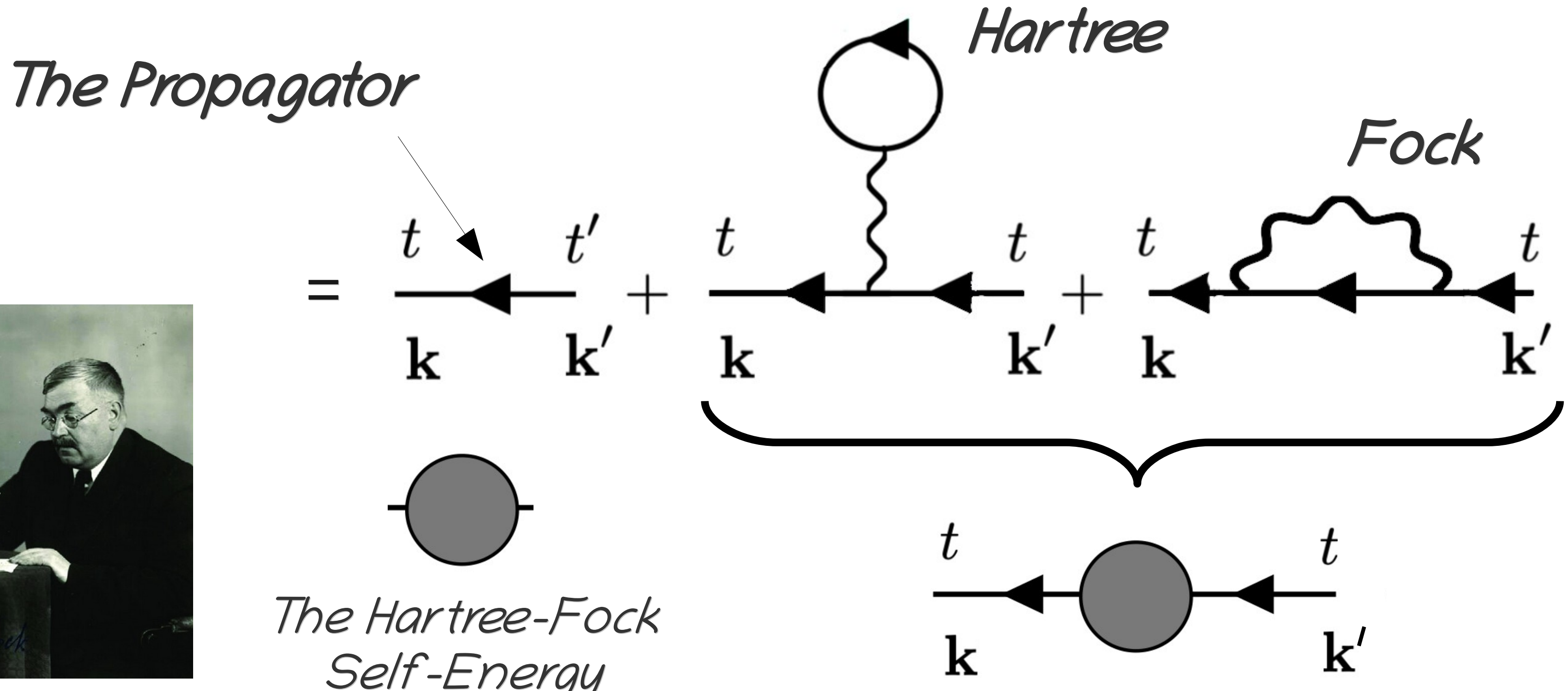


# Hartree-Fock (diagrammatic representation)

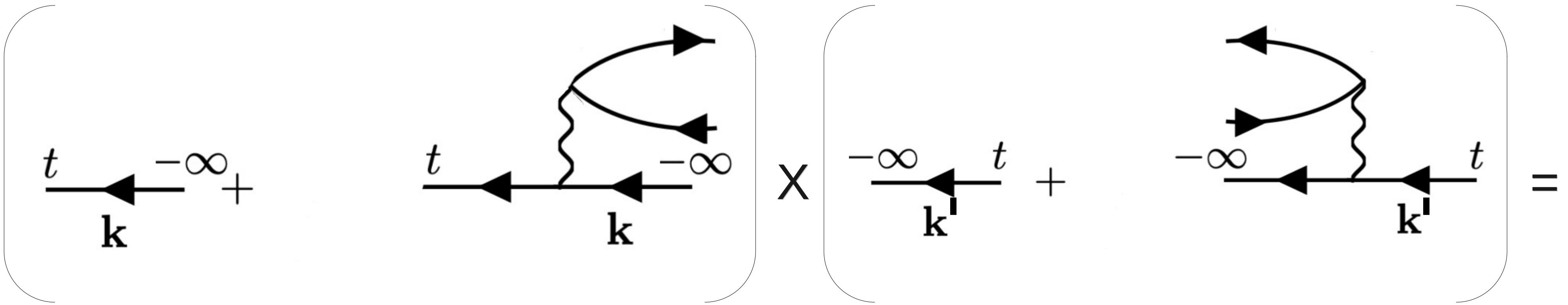
$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$

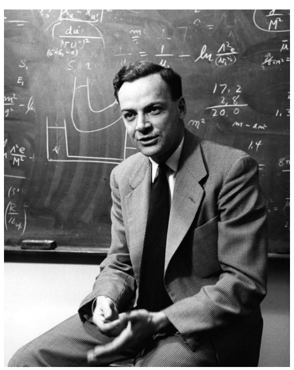


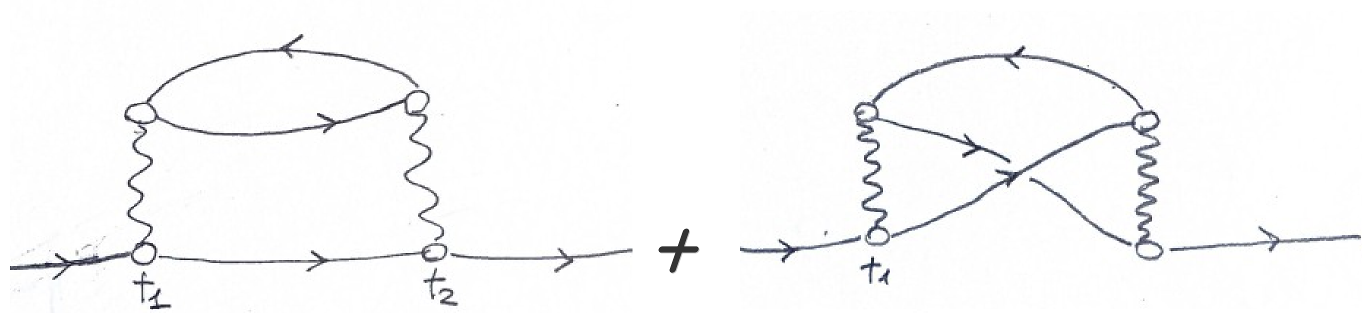

# Feynman diagrams in the fully interacting case

$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$



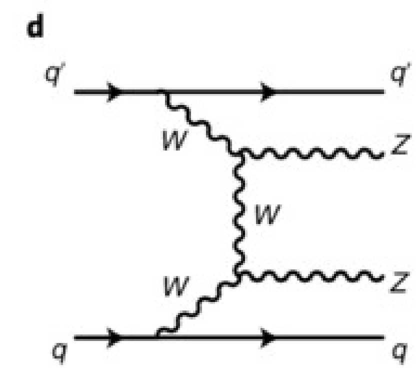



= (HF)+

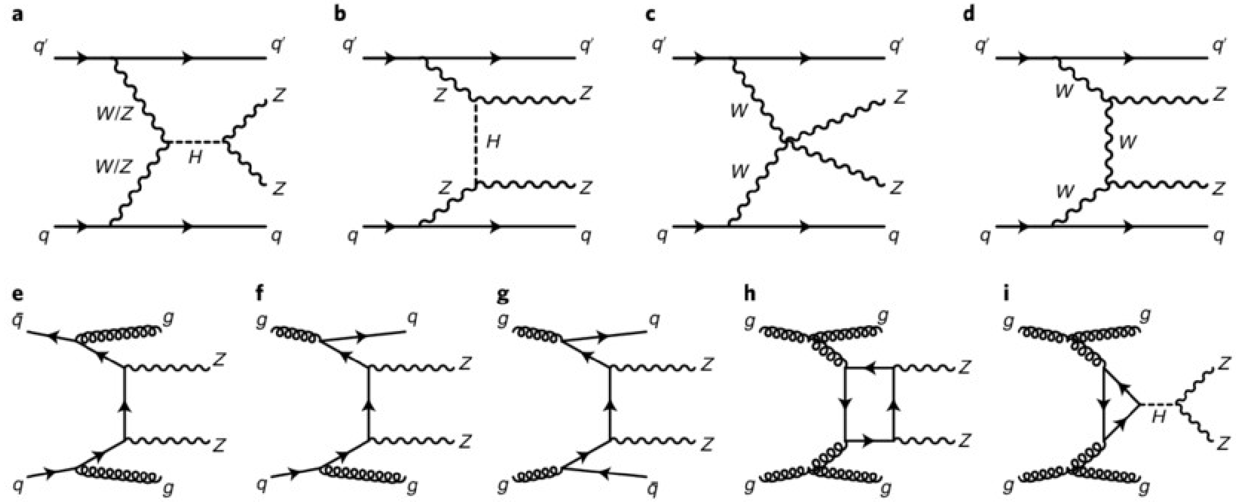



$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle$$

Diagrammatic Rules



# Feynman diagrams in the fully interacting case



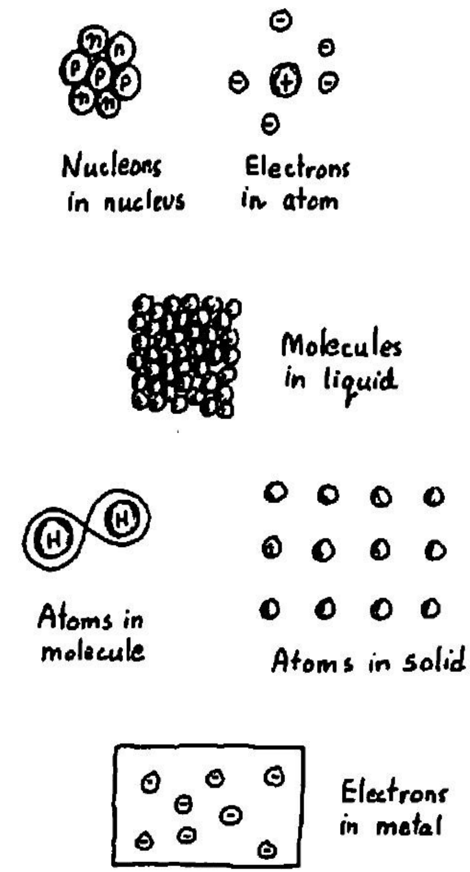

Use Physical arguments to choose specific classes of diagrams !!!

Short-range interactions ?

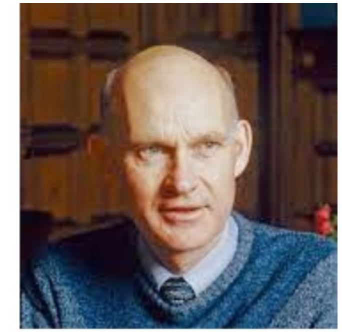
High density regime ?

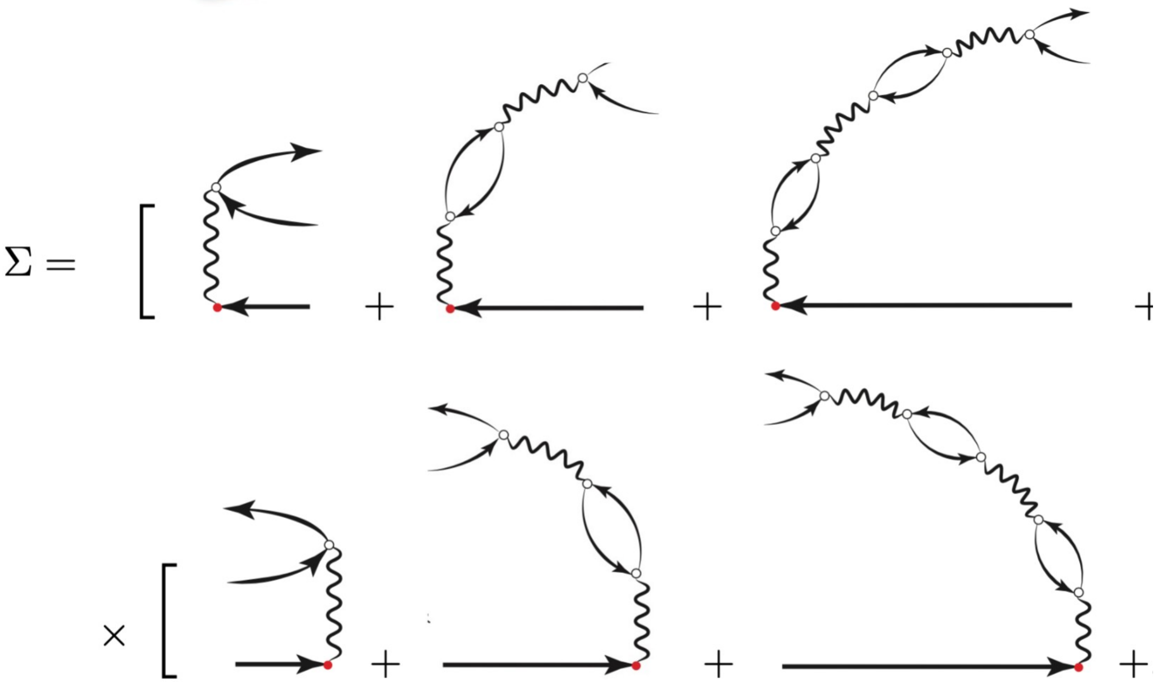
Low density regime ?

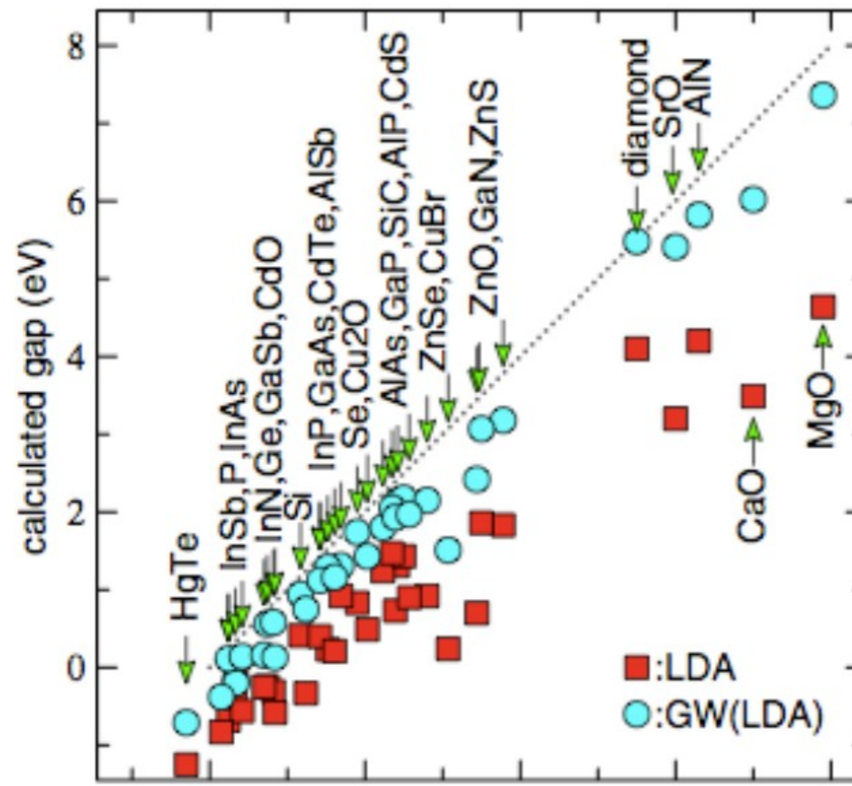
Conserving approximations



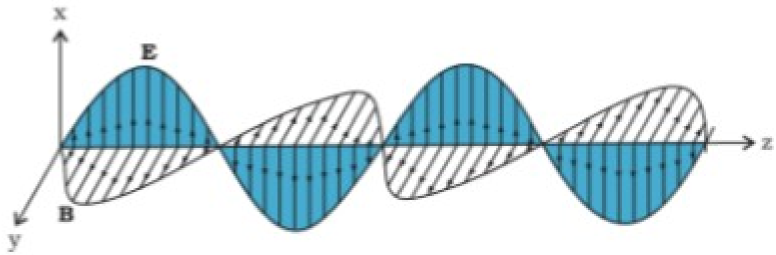
# The GW approximation

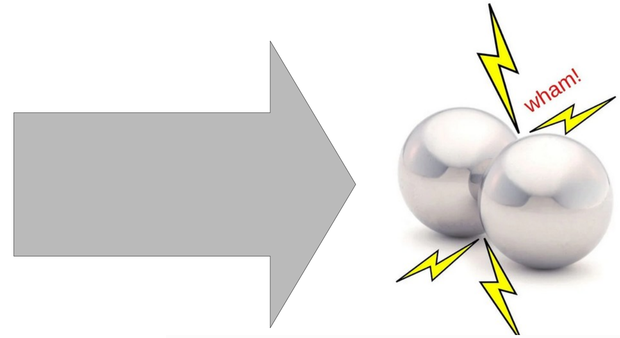





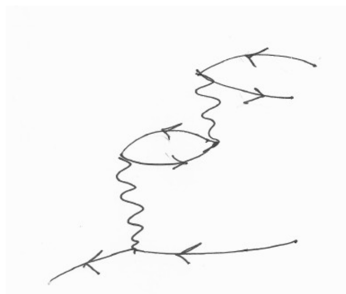



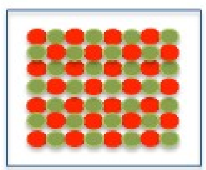
# The T-matrix approximation



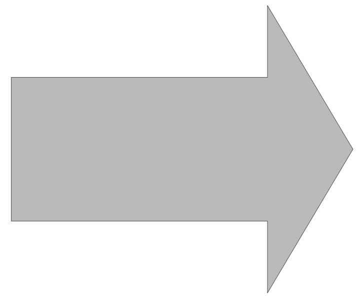



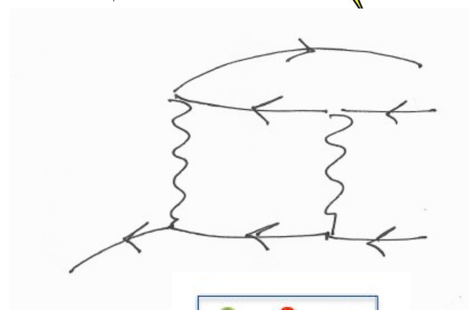

VIKTOR MIKHAĬLOVICH GALITSKIĬ
(1924–1981)

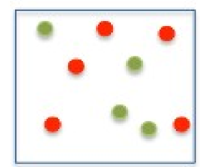




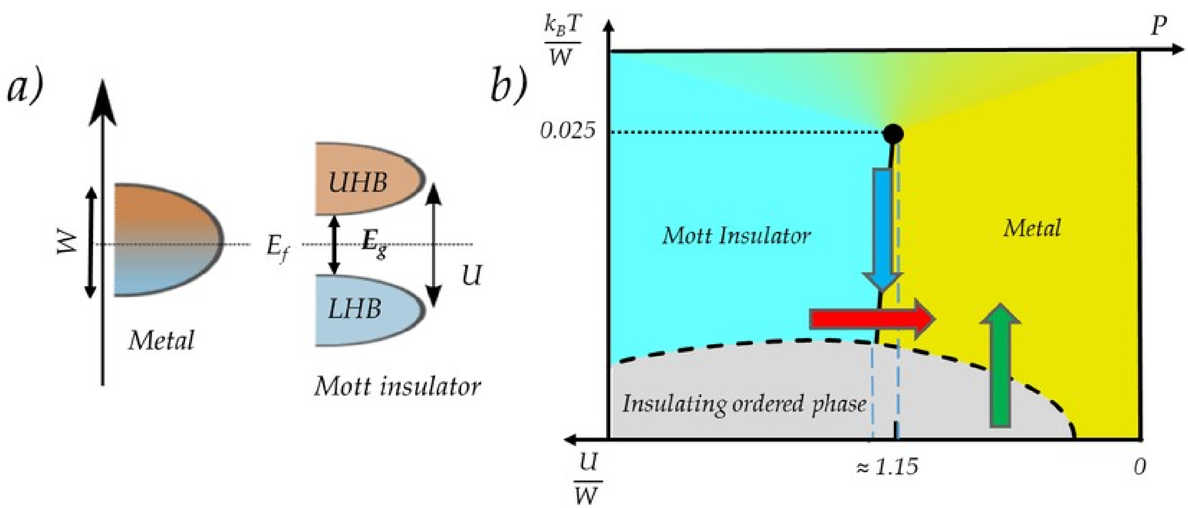
High Density







Low Density



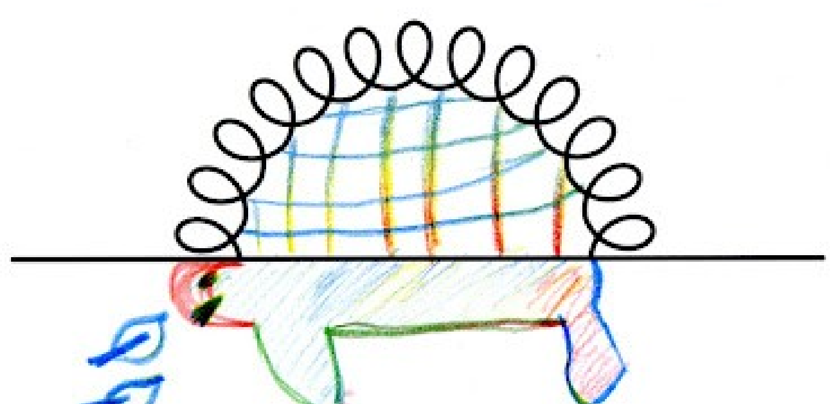
# Take-home messages

- MBPT is an exact **excited state** theory

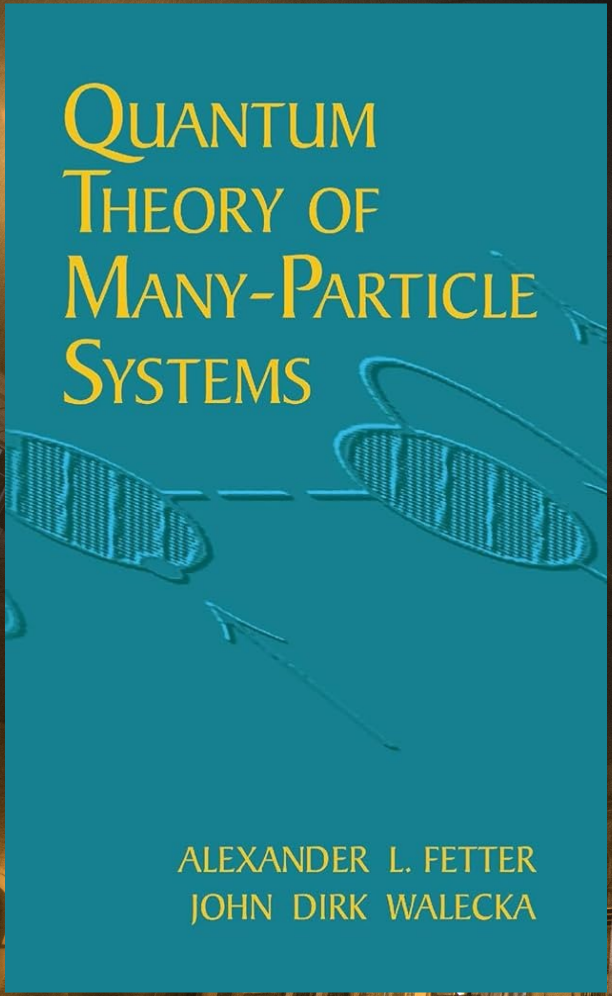
- MBPT can take into fully account **non-local processes (spatially and temporally)**

- From the MBPT perspective **DFT is a mean-field approximation**

- The price to pay is a theory: whose **complexity grows exponentially with the perturbative order**, based on the delicate assumption of validity of the perturbative expansion, bound to use well documented, but also rigid, approximations.



# References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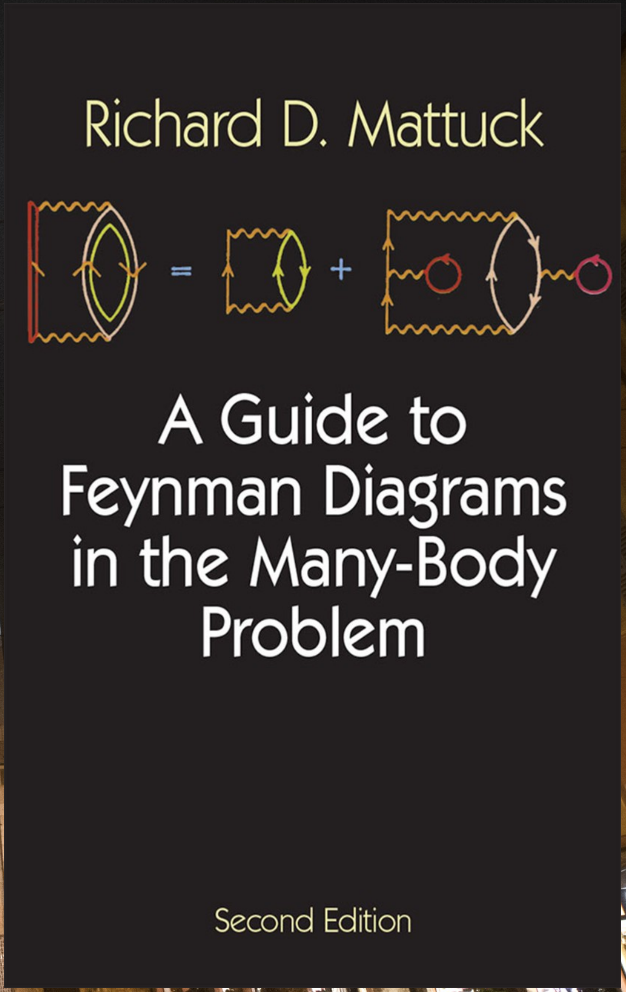
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Second Edition

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## Selected Readings

**Contents** [hide]



### General Theory

- Theoretical spectroscopy, M. Gatti
- Energy Loss Spectroscopy, F. Sottile

### Many-body Theory

- PhD lectures: MBPT and Yambo, L. Chiodo et al.
- Introduction to Many Body Physics, Piers Coleman
- Pedagogical introduction to equilibrium Green's functions: condensed matter examples with

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