# Many-Body Perturbation theory: Basic concepts and approximations


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FLASH it

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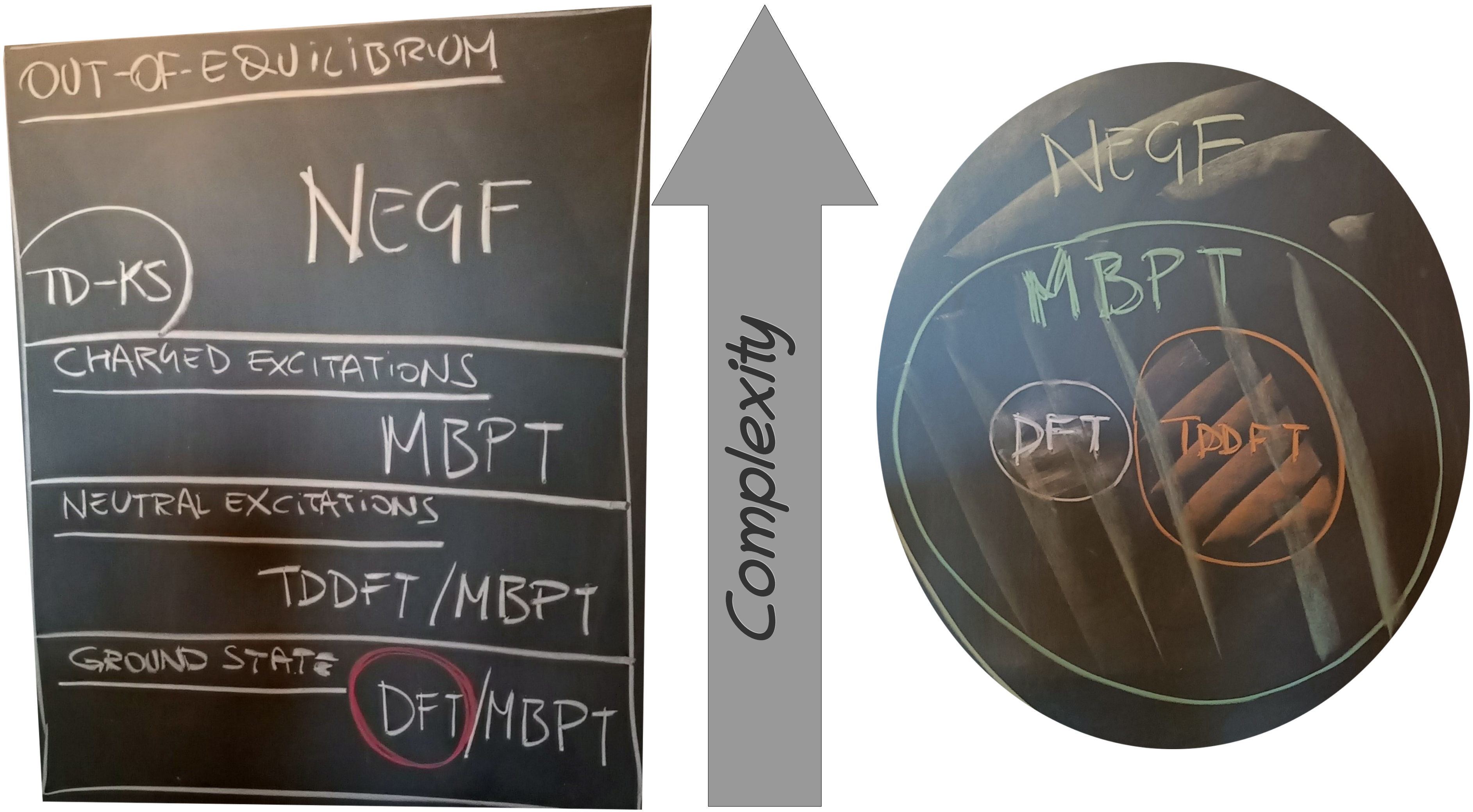
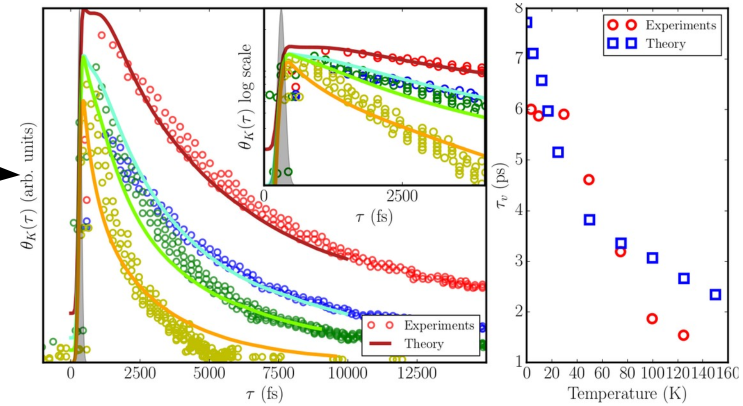
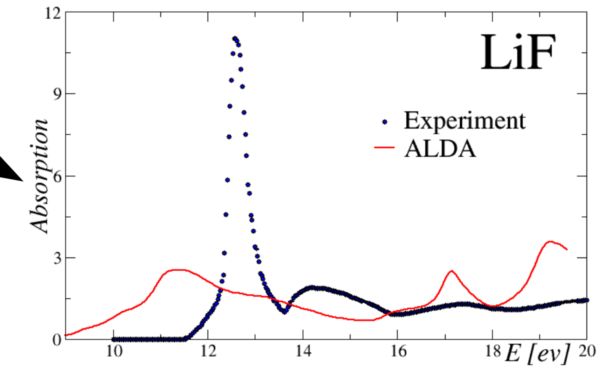
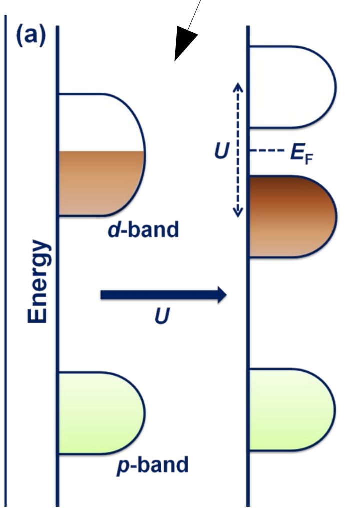
# Different physics, different approaches

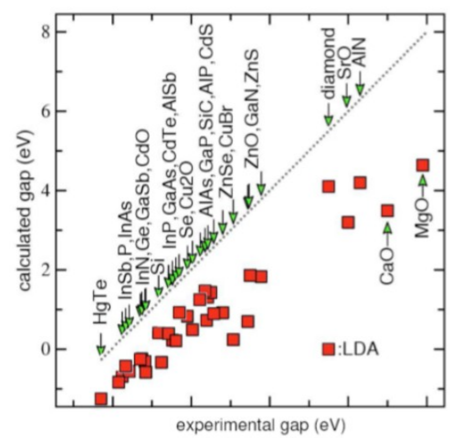


# Different physics, different approaches


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

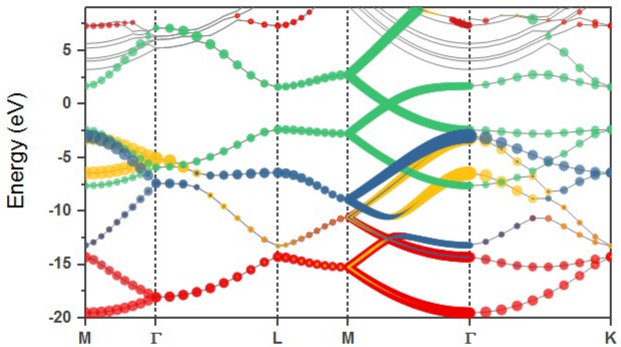
GaAs:
0.30 eV (LDA) vs 1.4 eV (expt)

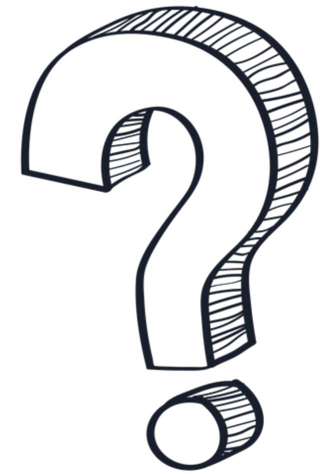
Adapted from M. van Schilfgaarde *et al.* PRL **96** (2006)

# The Many-Body problem

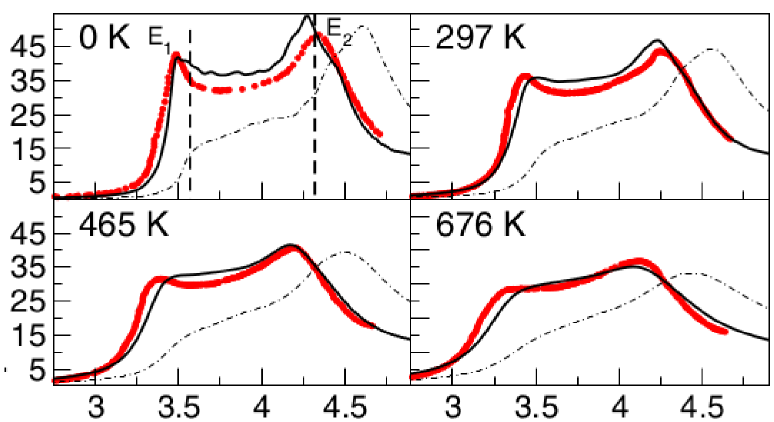
$$H = \sum_i h(x_i, p_i) + \frac{1}{2}\sum_{i \neq j} \left|x_i - x_j\right|^{-1}$$

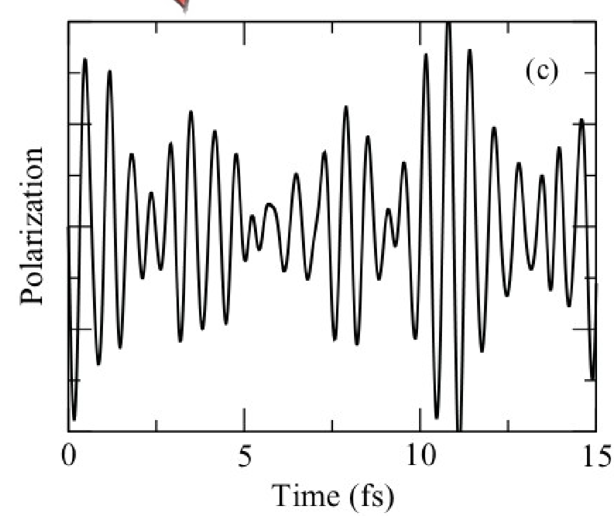
# The Many-Body Problem: a micro-macro connection



$$\hat{H} = \sum_i \hat{h}\left(x_i\right) + \frac{1}{2}\sum_{ij}{}' \frac{1}{|x_i - x_j|}$$



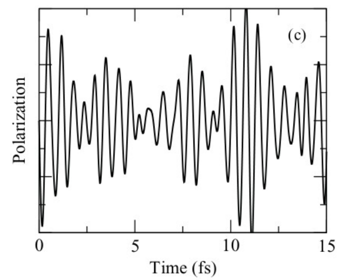



# A (very) hard job!

$$\langle N| = \overline{(|N\rangle)}$$

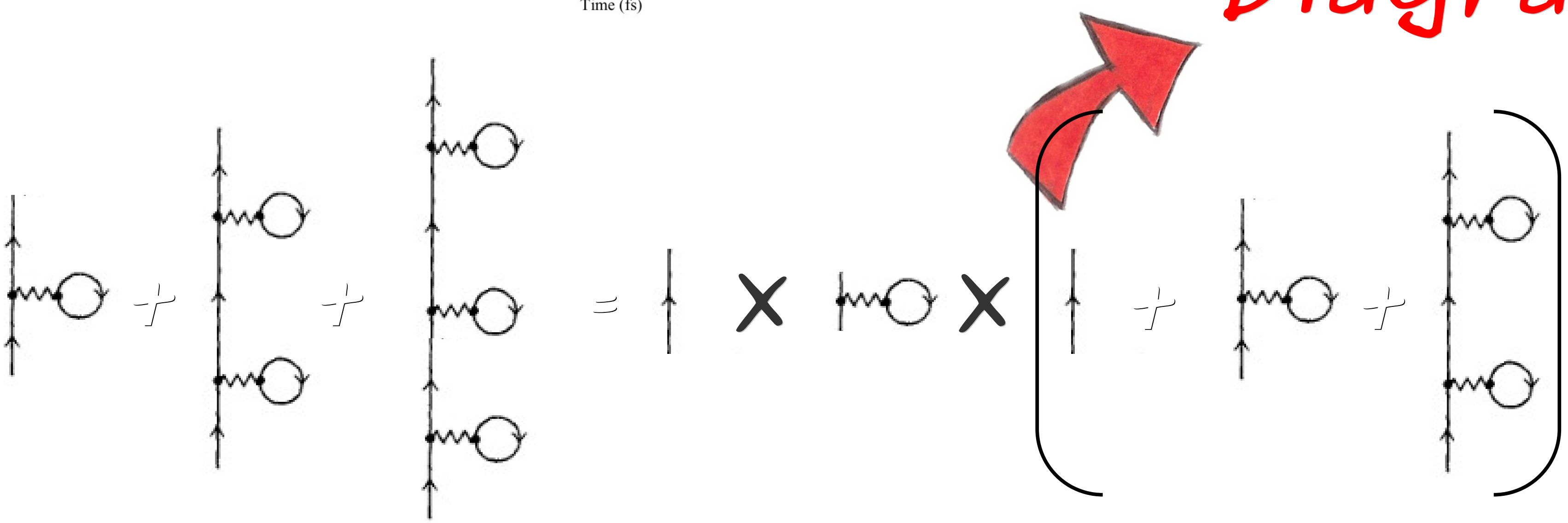
QM

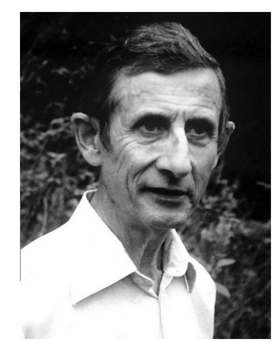
$$A = \langle N|\hat{A}|N\rangle$$



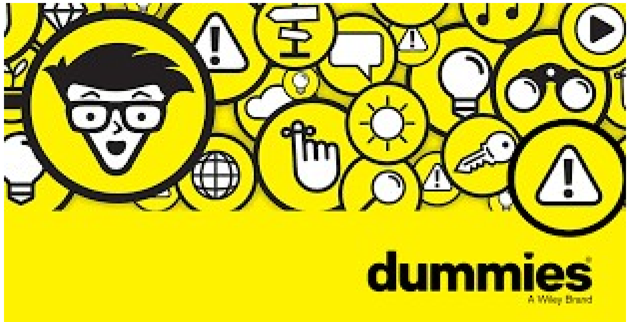

$$|N(t)\rangle = U(t, t_0)|N(t_0)\rangle$$

Diagrams

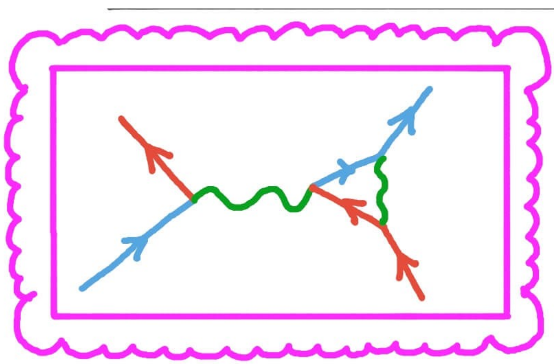




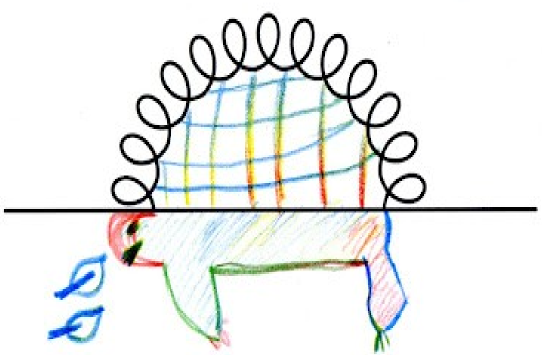
# Outline



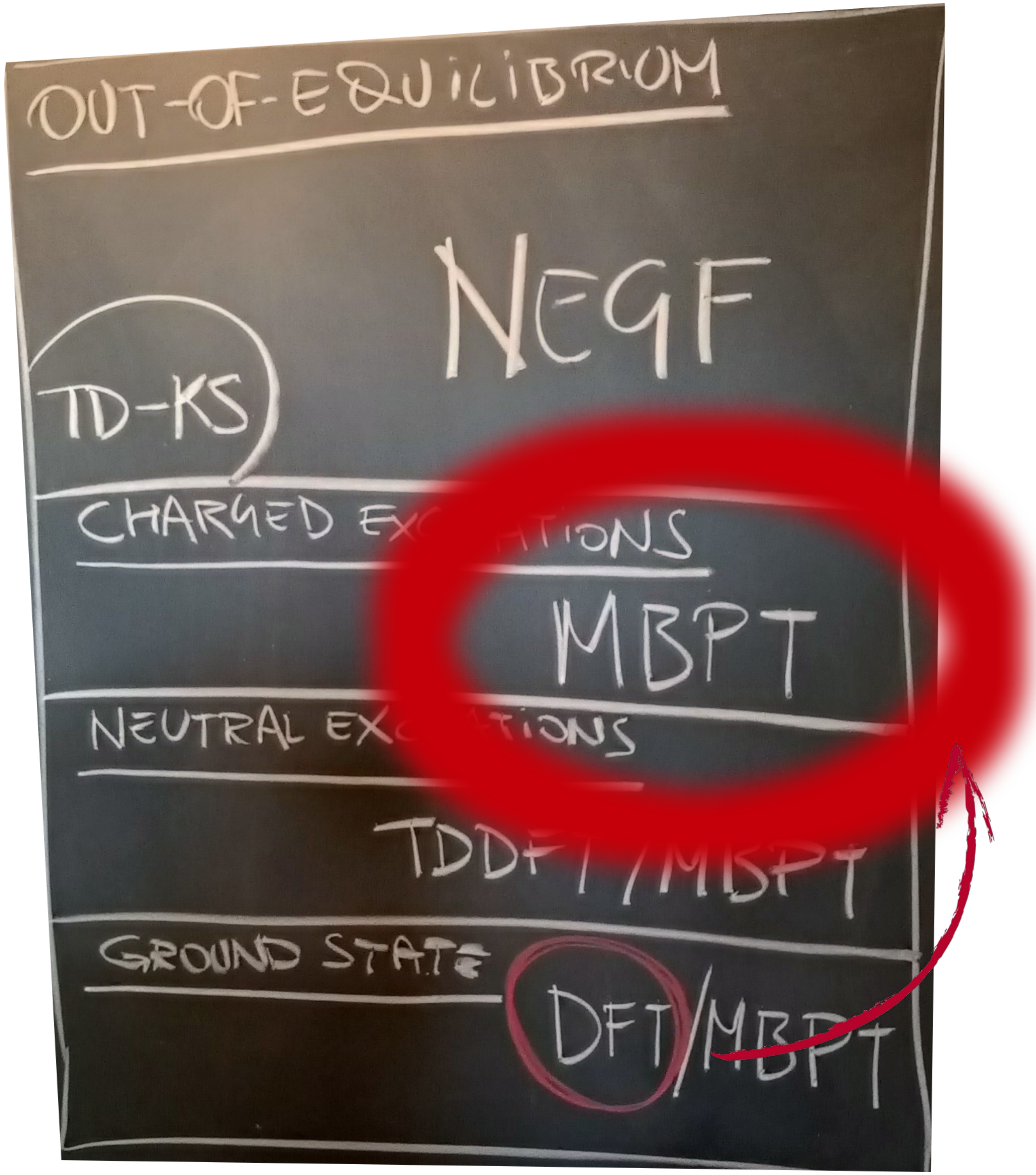

Many-Body Perturbation Theory for dummies



Feynman diagrams for dummies



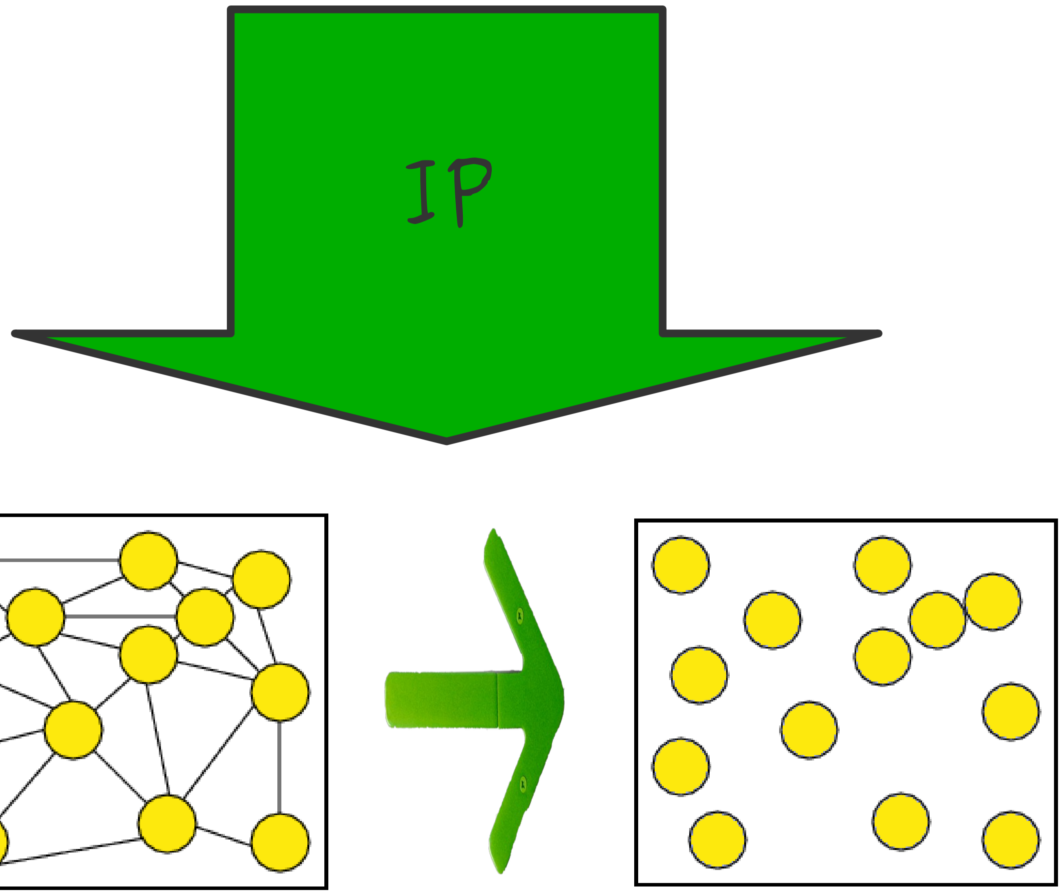
The “zoo” of MBPT approximations




# Many-Body Perturbation Theory for dummies

# The Many-Body problem

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

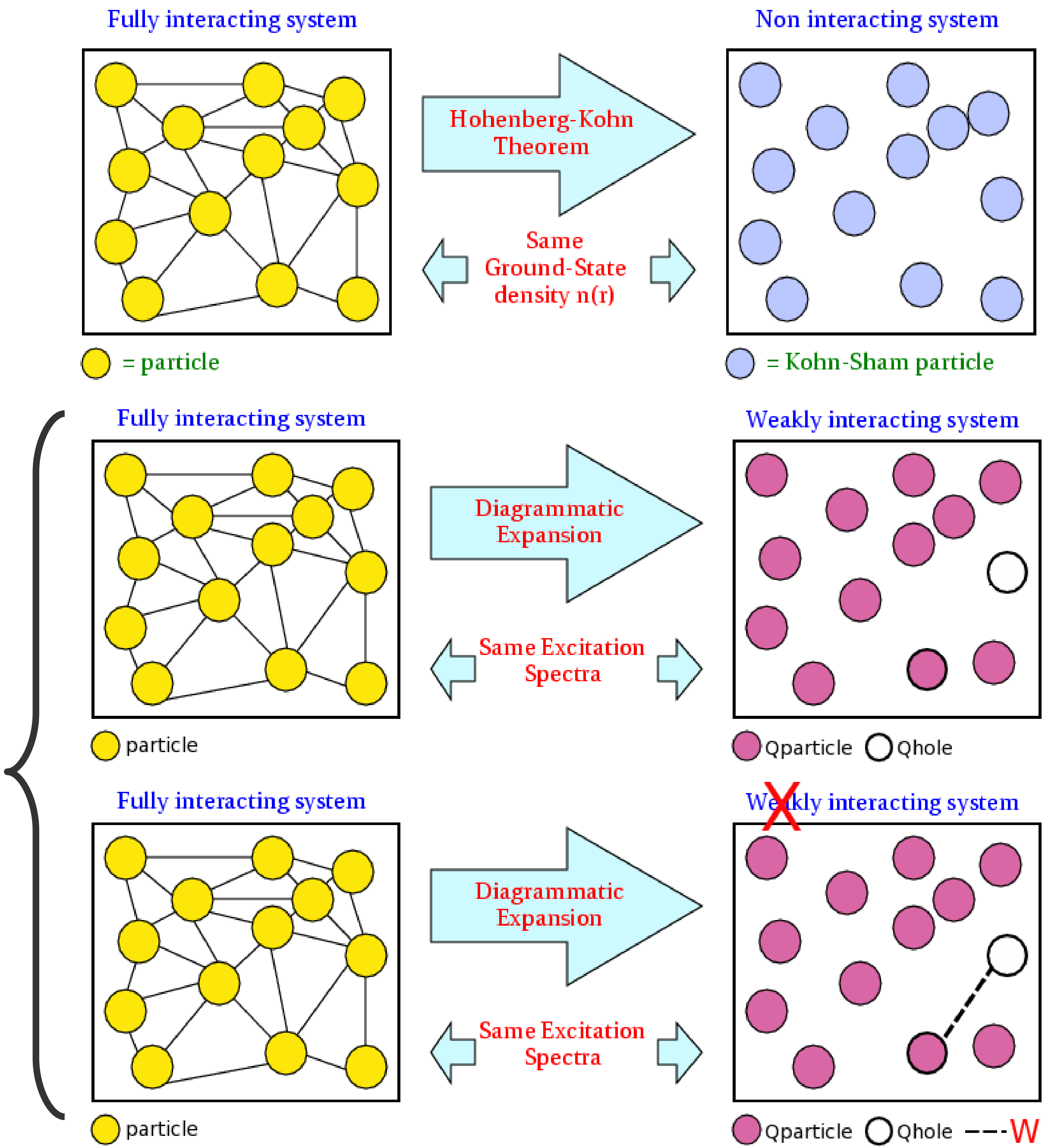



$$H \approx \sum_i h(x_i)$$

# The Many-Body problem

DFT

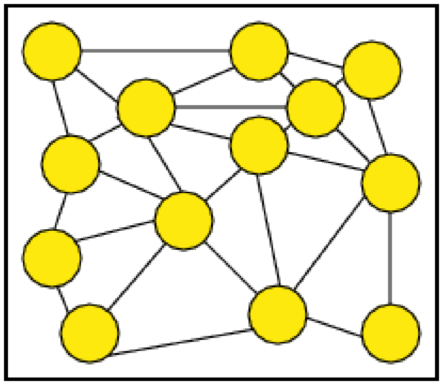
MBPT



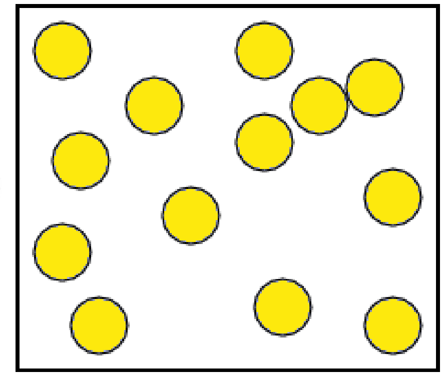
# The Many-Body problem: 1 particle approx

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

$$H = \sum_i h(x_i)$$



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



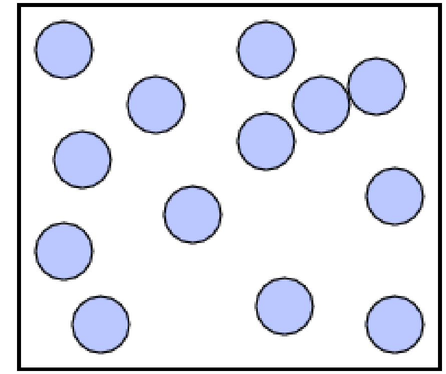
$$|N_0\rangle = \prod_{n\in filled} |n\rangle$$

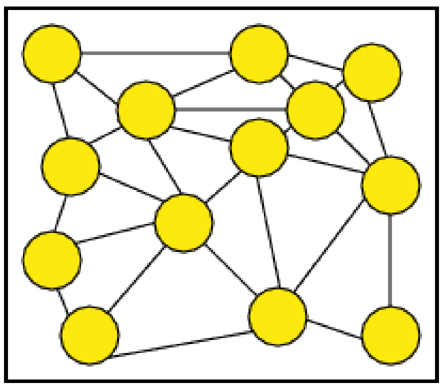
$$\langle N|\hat{A}|N\rangle \approx F_N[\{A_n\}]$$

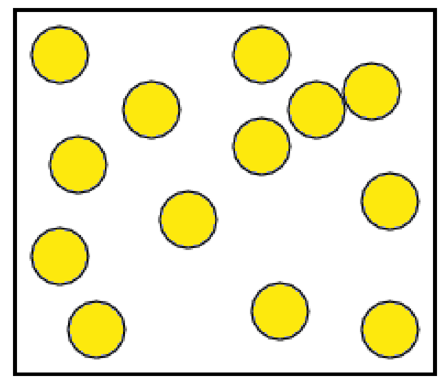
$$\langle N_0|\hat{H}\,|N_0\rangle = \sum_{n\in filled} \epsilon_n$$

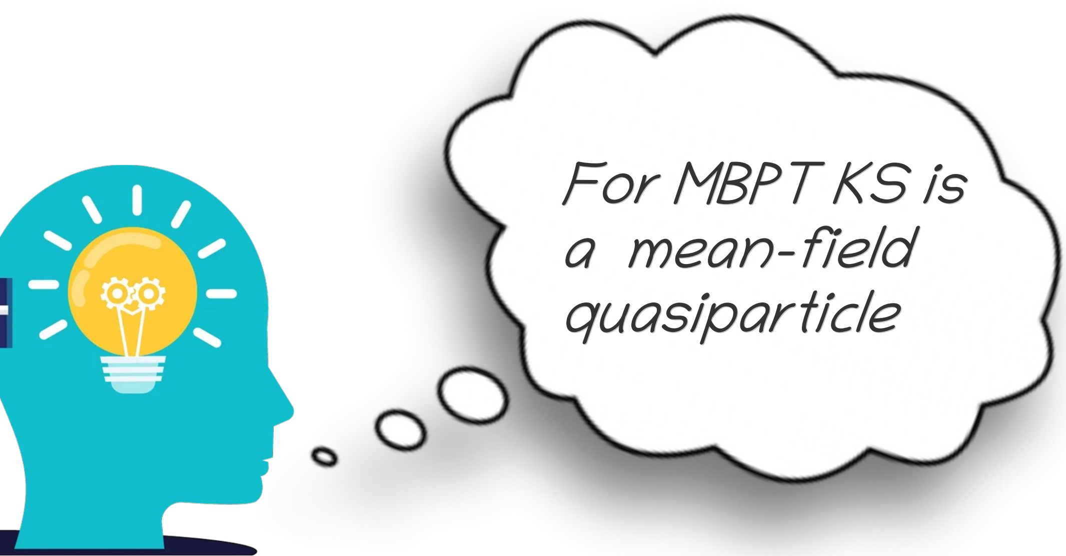
# Quasiparticles...

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

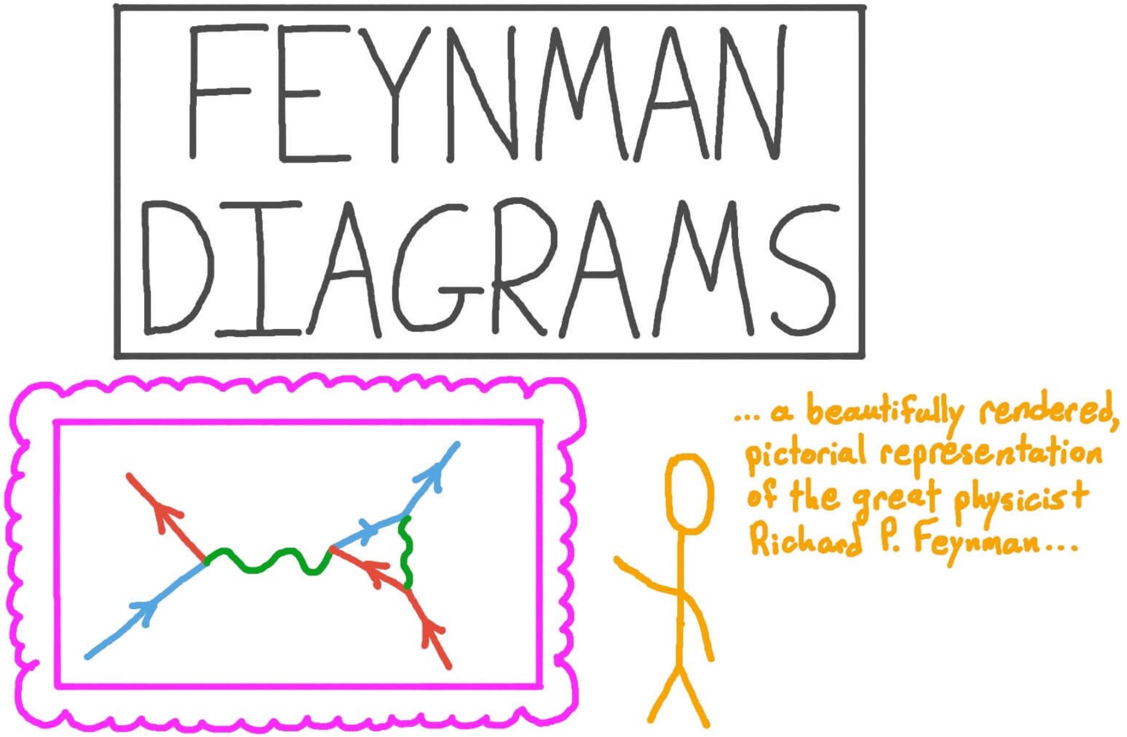







*The goal of the Many Body methods is to rewrite the fully interacting problem as an as much independent as possible counter-part*

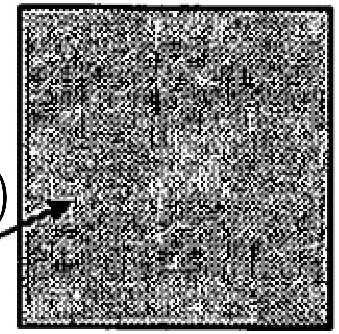



Feynmann diagrams for dummies

# The Coulomb interaction

$$\nabla^2 V(\mathbf{x},t) = 4\pi n(\mathbf{x},t)$$

n(**x**,t)

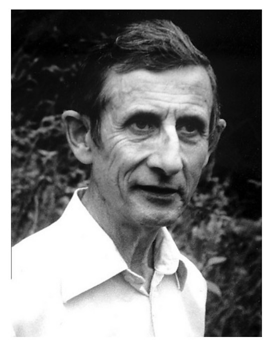


Let's add an external (oscillating) charge in the system

Poisson

$$V(\mathbf{r},t) = \int d\mathbf{r}' \frac{n(\mathbf{r}',t)}{\mathbf{r}-\mathbf{r}'}$$

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



$$\hat{n}(\mathbf{r}) = \hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r})$$

2nd quantization

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

# The time-dependent, interacting density (Kubo)

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

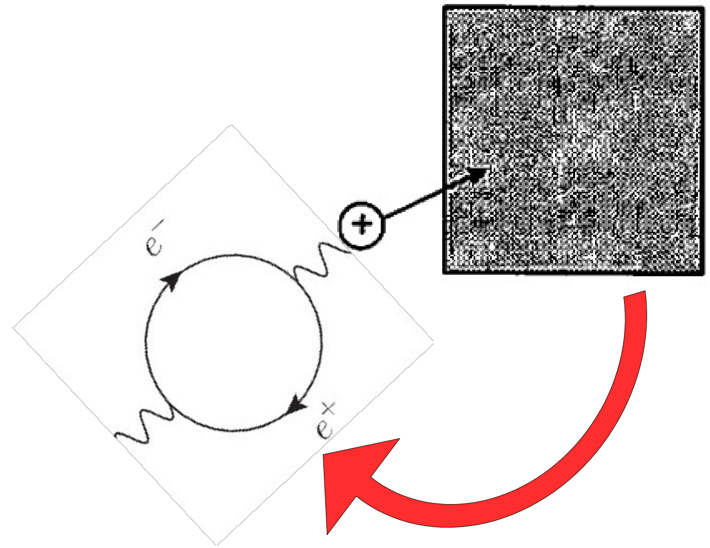
Ground State $\Psi(t) = \Psi_0$

Density Functional Theory

Semi-classical excitation

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

Kubo

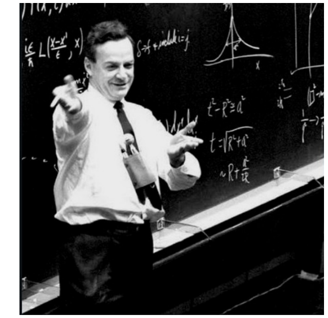


$$\mathrm{n}(\mathbf{r},\mathrm{t}) = \mathrm{n}_0(\mathbf{r}) + \int d\mathbf{r}' \int_0^t dt' \chi^R(\mathbf{r}t,\mathbf{r}'t') V(\mathbf{r}',t')$$

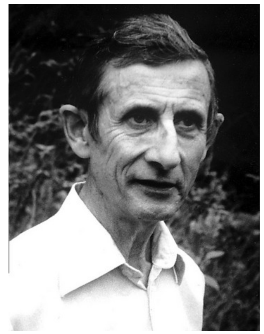
$$\chi(\mathbf{r}t,\mathbf{r}'t') = -i \left\langle \Psi \left| [\hat{n}(\mathbf{r},t), \hat{n}(\mathbf{r}',t')] \right| \Psi \right\rangle \theta(t-t')$$

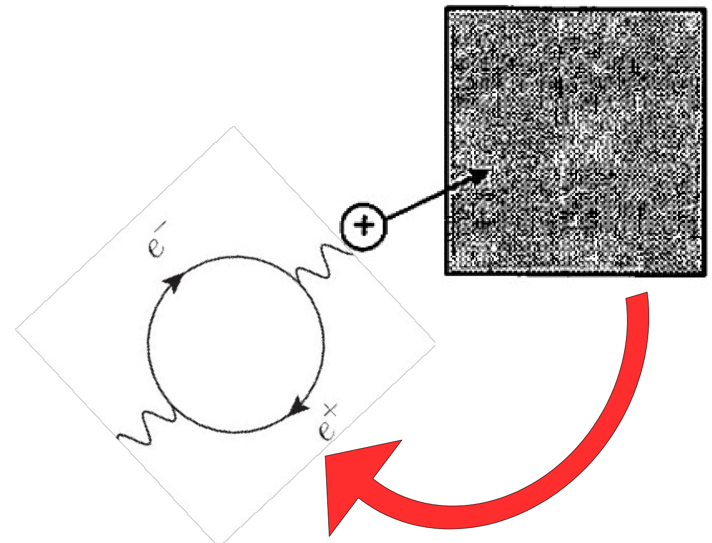
# The response (Green's) function

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



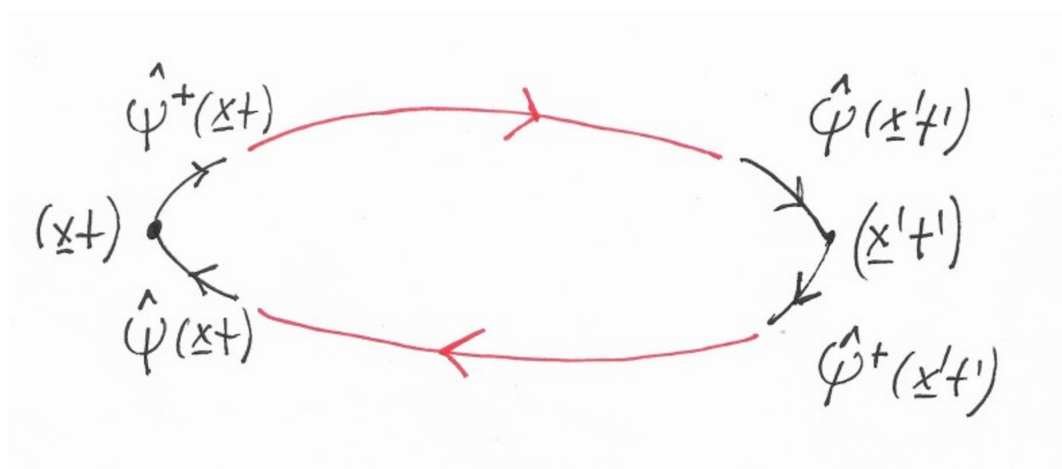
$$\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \hat{d}_{\mathbf{k}}$$






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

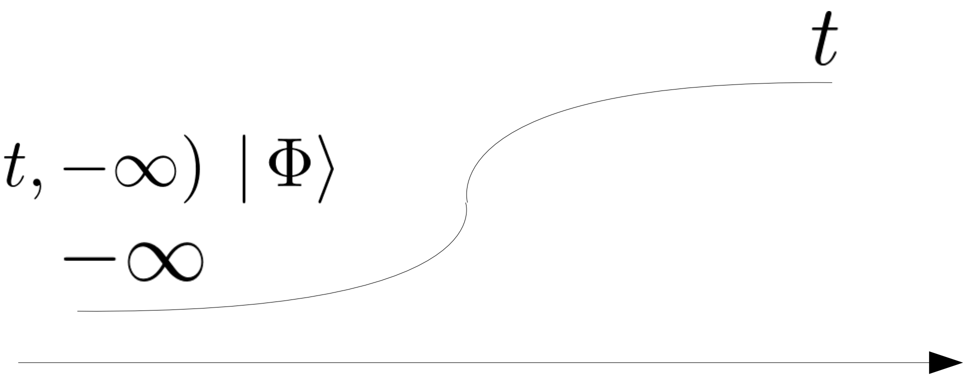
$$\langle \Psi | [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] | \Psi \rangle$$



# The time-dependent, interacting density

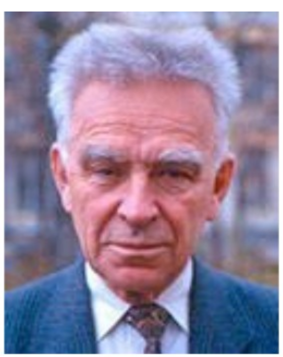
$$n(\mathbf{r},t) = \left\langle \Psi(t) \left| \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) \right| \Psi(t) \right\rangle$$

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




*Adiabatic Hypothesis*

$$\hat{U}(t) \equiv \hat{U}(t,-\infty)$$



$$n(\mathbf{r},t) = \sum_{\mathbf{k}\mathbf{k}'} \phi^*_{\mathbf{k}}(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r}) \left\langle \Psi(t) \left| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t)\hat{U}^\dagger(t)\hat{d}_{\mathbf{k}'} \right| \Psi(t) \right\rangle$$

# The evolution operator (scattering potential)

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

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

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

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

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

*Constrained time integrals*

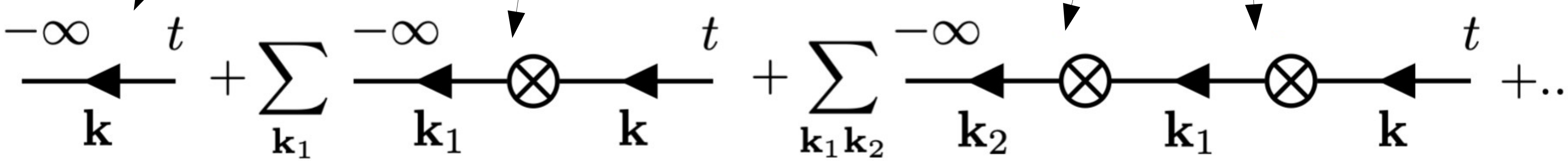
$$t > t_1 > t_2 > \cdots$$

# Half the dynamics...

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

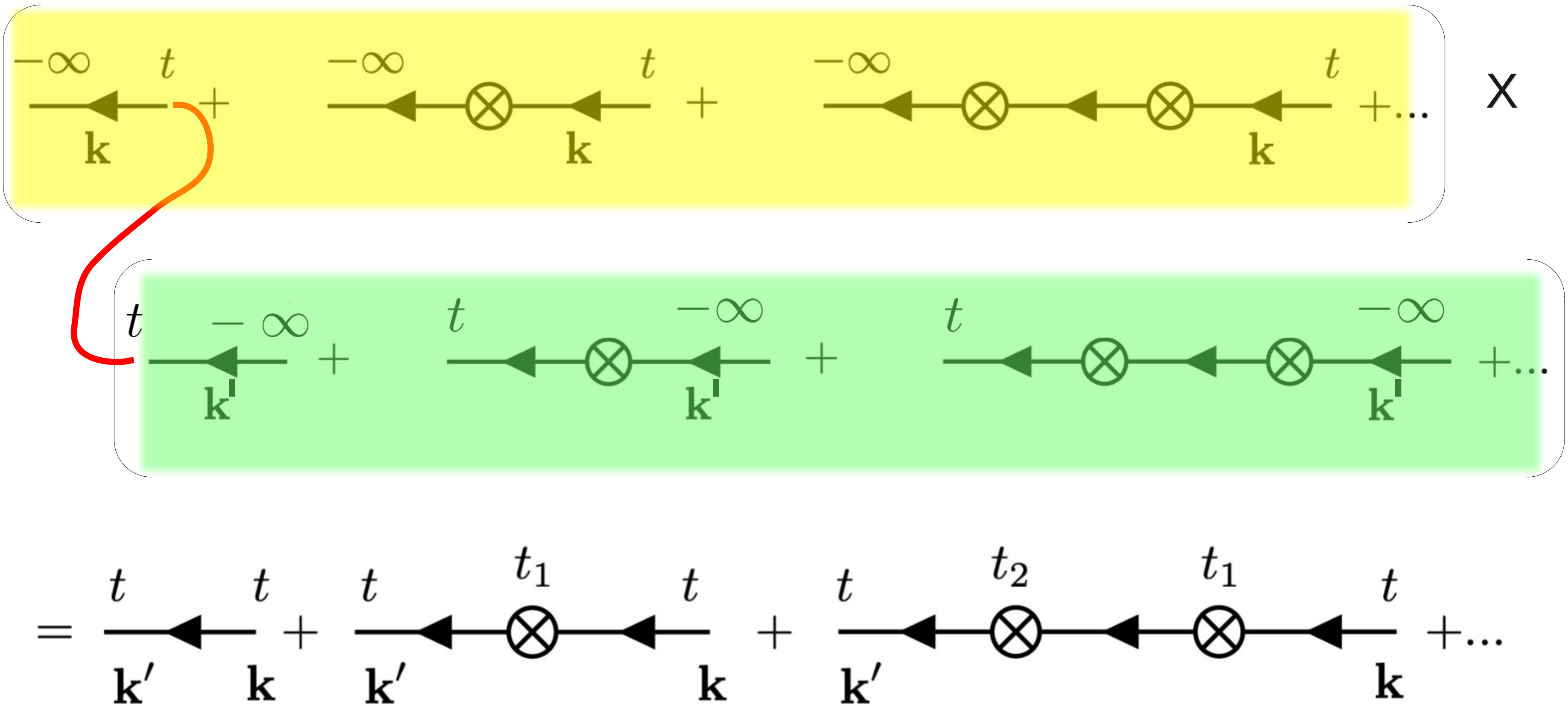
$$\hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}} \Big| \Psi(t) \Big\rangle = F^{\dagger}(t) \hat{U}^{\dagger}_{0}(t) \hat{d}^{\dagger}_{\mathbf{k}} \Big| \Psi(t) \Big\rangle$$

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

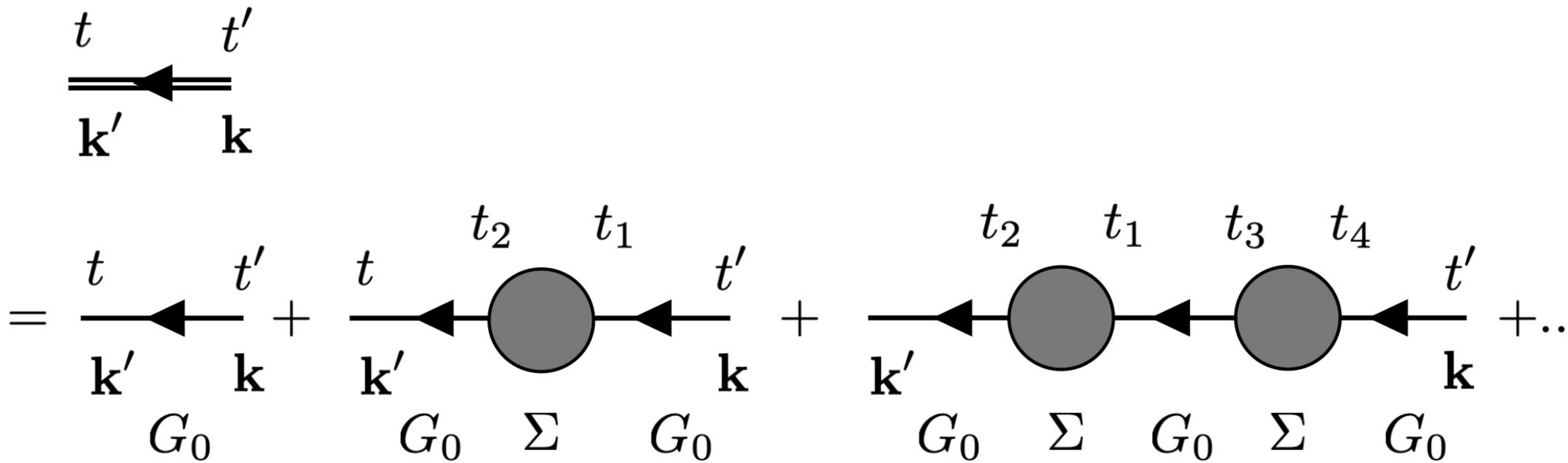


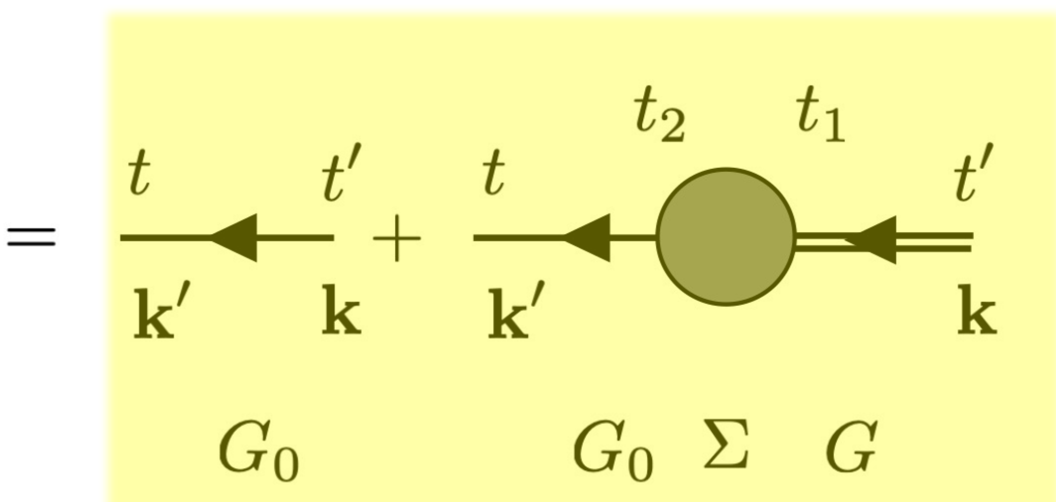
# Green's Functions

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

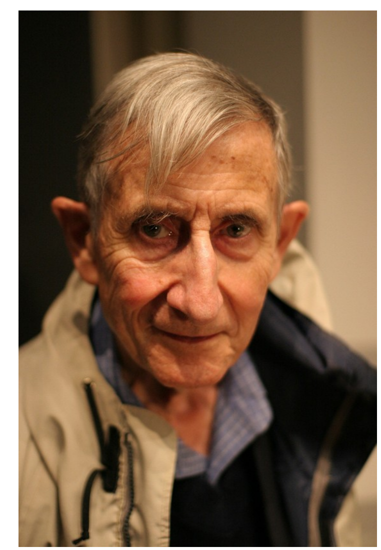


# The Dyson equation



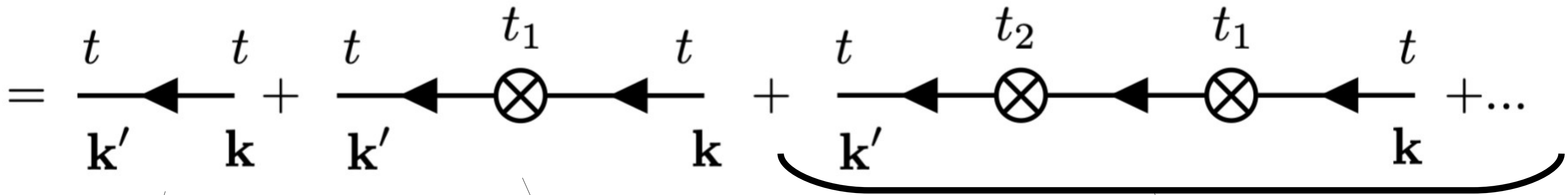




The Dyson Equation



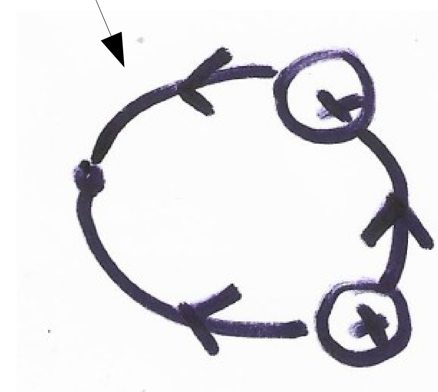
# Green's Functions: Kubo revisited

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




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

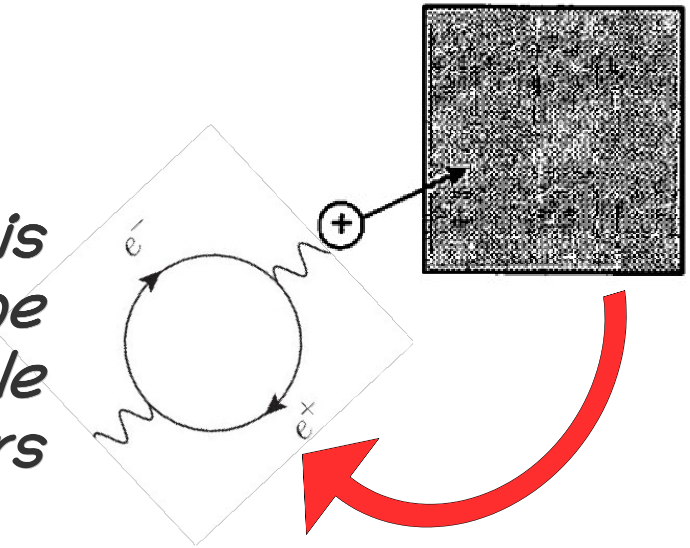
$\int d\mathbf{r}' \int_0^t dt' \chi^R\left(\mathbf{r}t, \mathbf{r}'t'\right) V\left(\mathbf{r}', t'\right)$

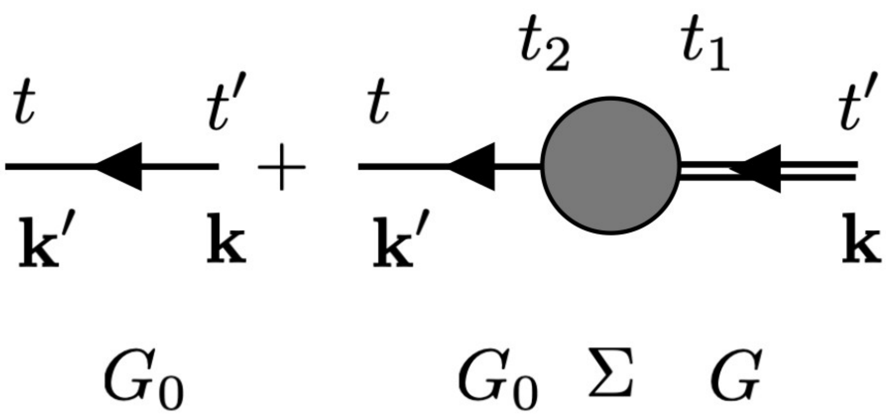


*Non-linear terms*

# Key messages

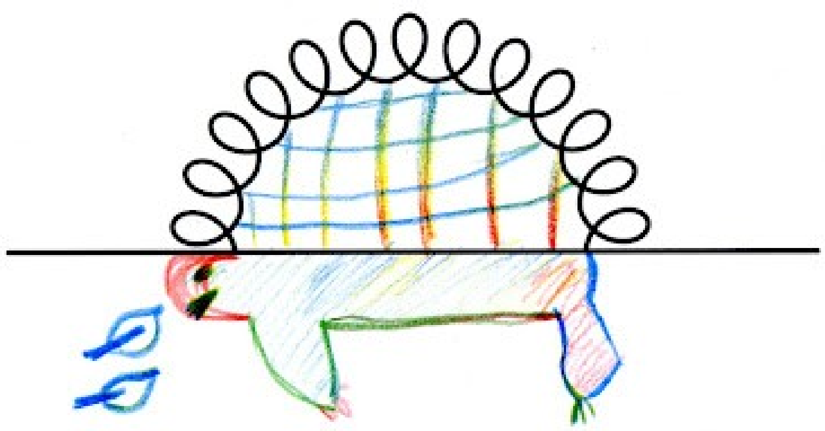
Basic MBPT process is screening trough the excitation of electron-hole (neutral) pairs




The very same process can be easily described by using a diagrammatic representation

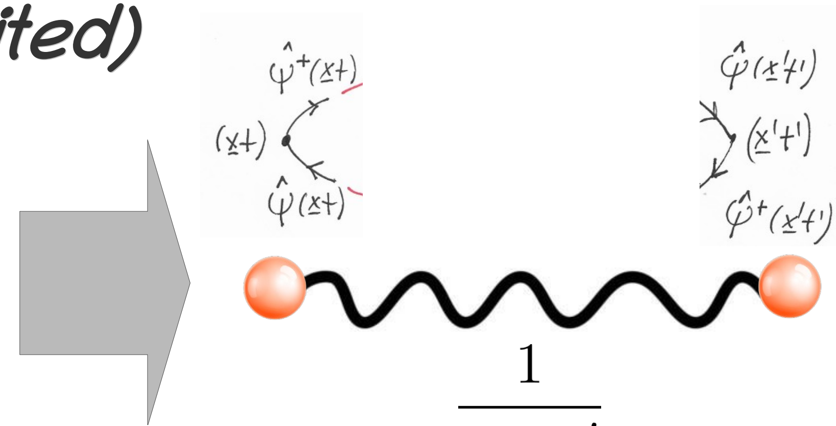
MBPT is (by far) more powerful when we move to more complicated interaction potentials



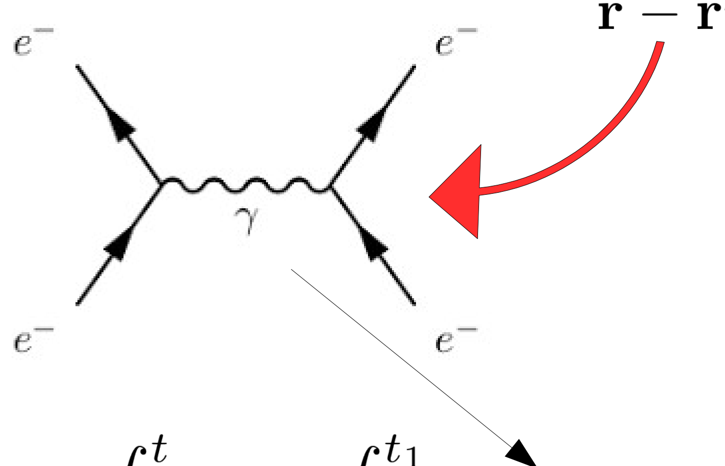
The "zoo" of MBPT approximations

# The Coulomb interaction (revisited)

$$V(\mathbf{r},t) = \int d\mathbf{r}' \frac{n(\mathbf{r}',t)}{\mathbf{r}-\mathbf{r}'}$$



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

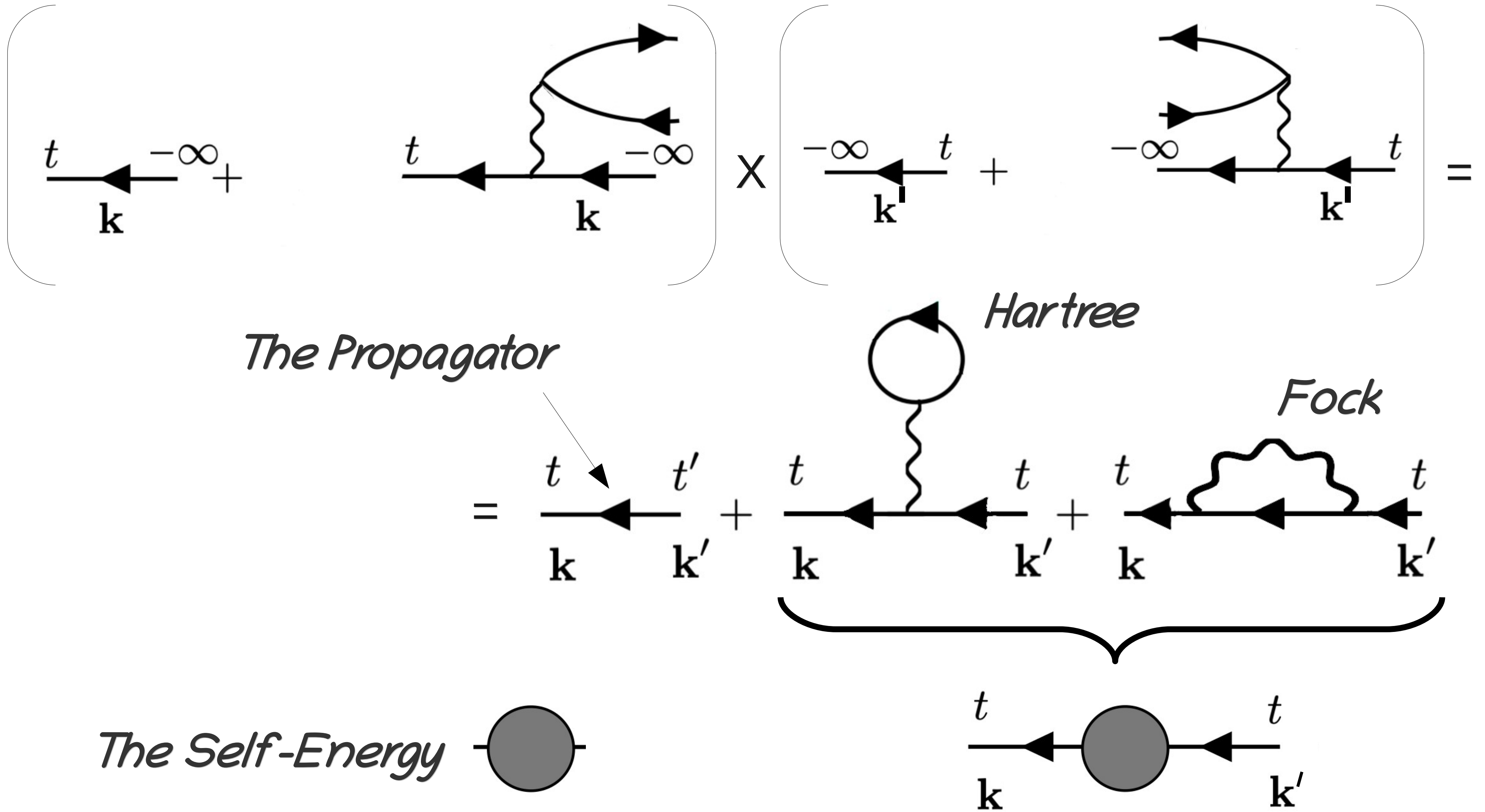



$$\hat{U}(t) = \hat{U}_0(t)\hat{F}(t)$$

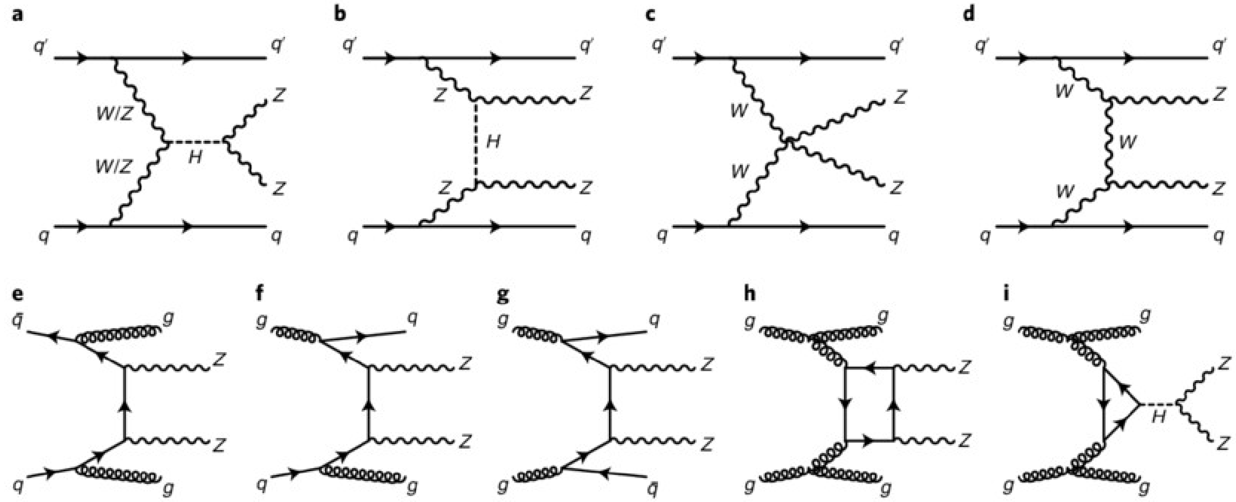
$$\hat{F}(t) = 1 - i\int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + (-i)^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \dots$$

# Feynman diagrams in the fully interacting case

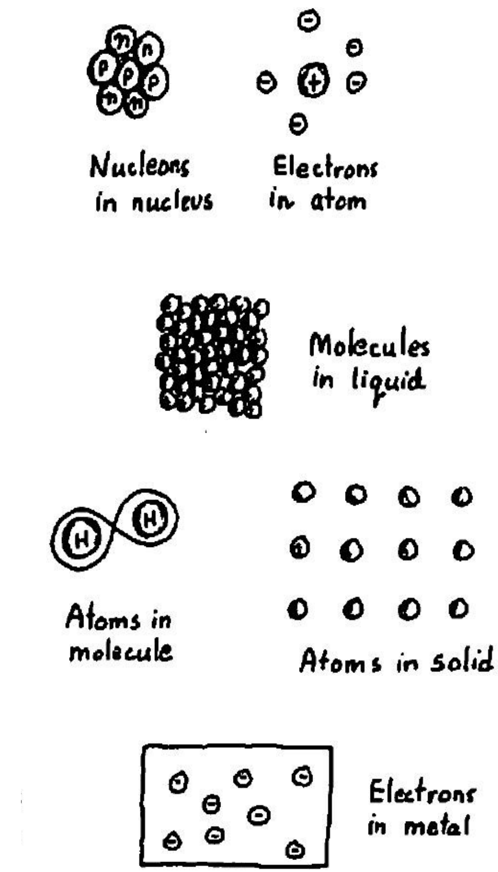
$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$



# Feynman diagrams in the fully interacting case




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



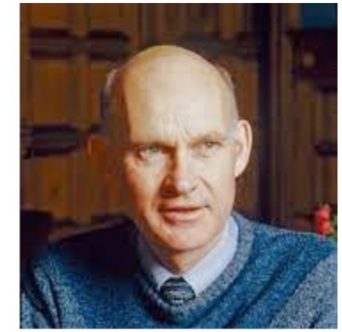

Short−range interactions ?

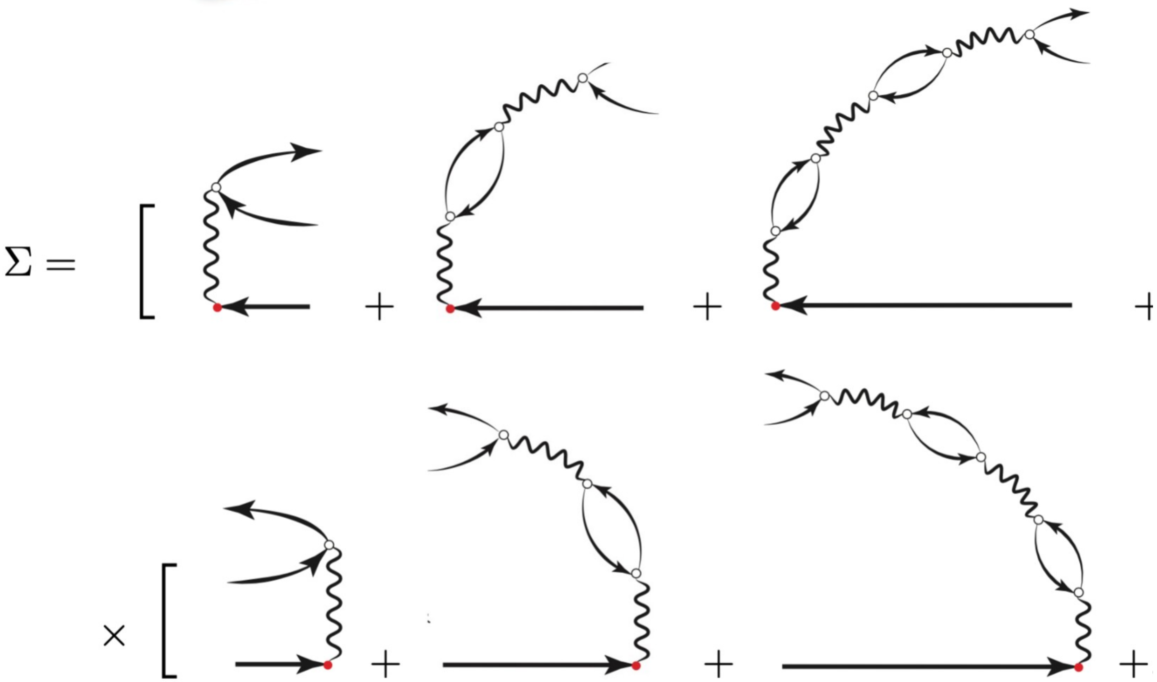
Low density regime ?

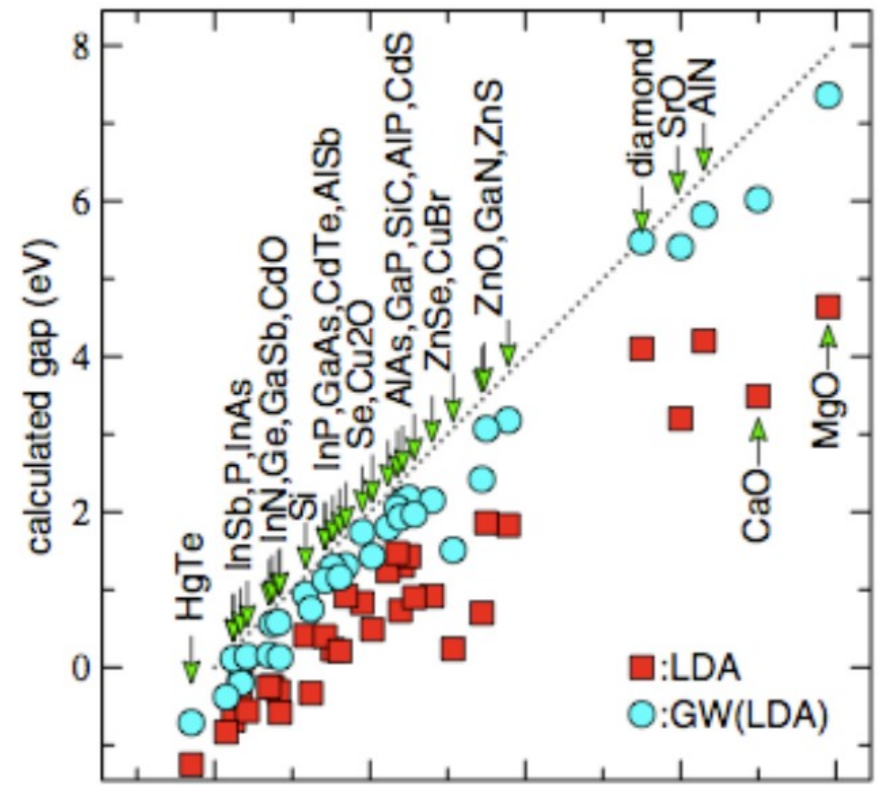
Conserving approximations

High density regime ?

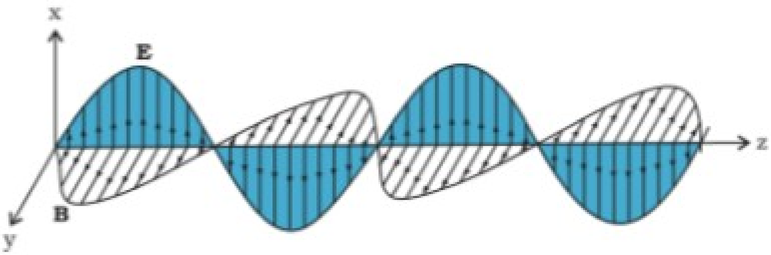
# The GW approximation

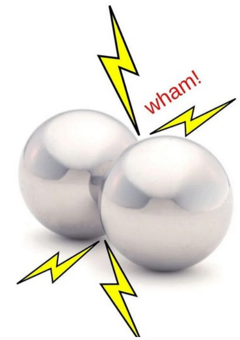





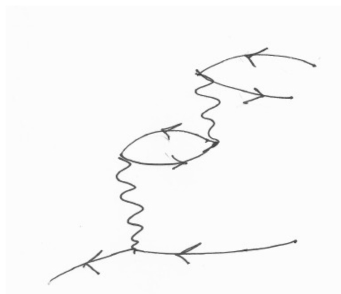



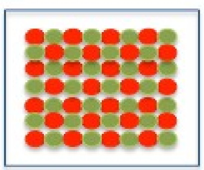
# The T-matrix approximation



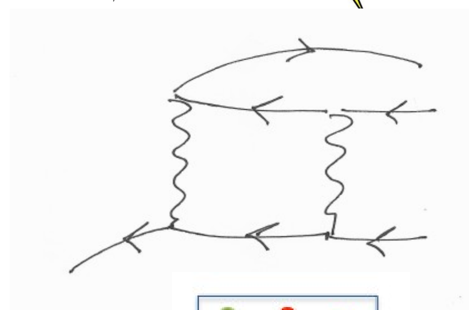



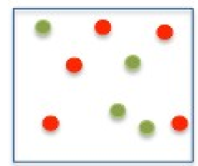

VIKTOR MIKHAĬLOVICH
GALITSKIĬ
(1924–1961)



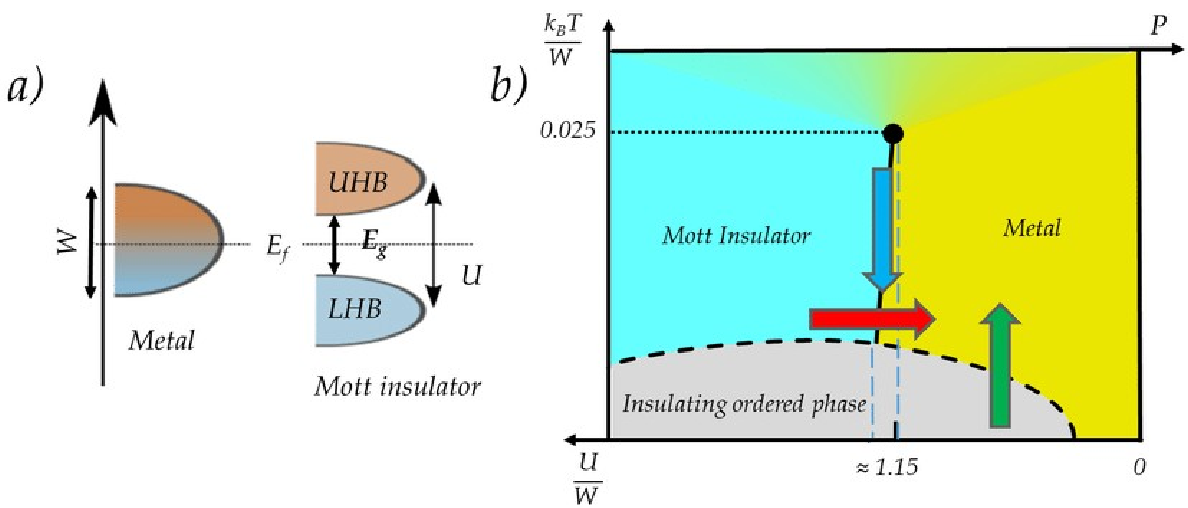


High Density



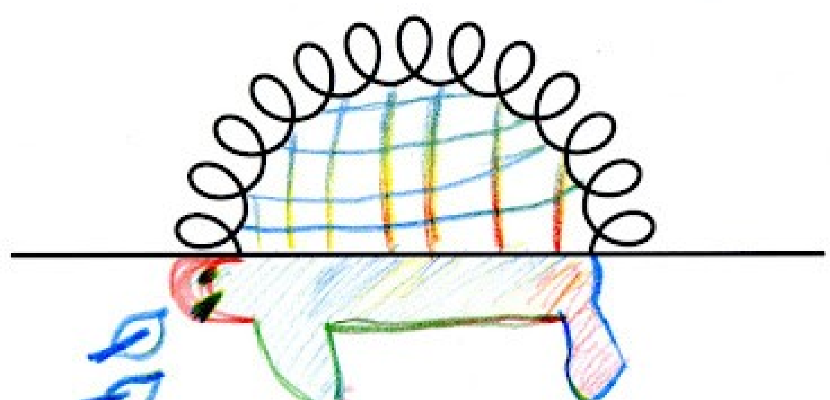


Low Density

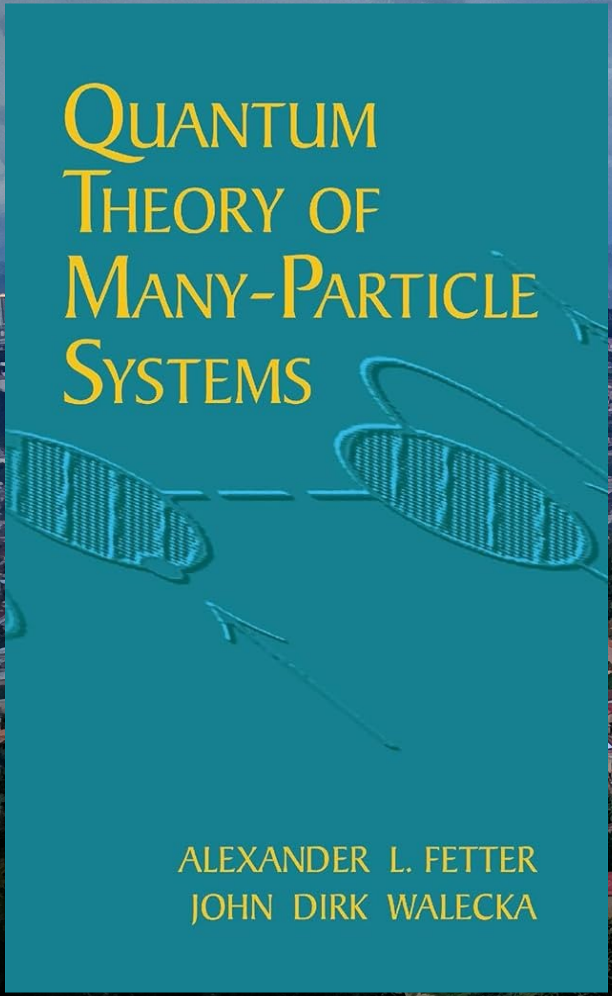


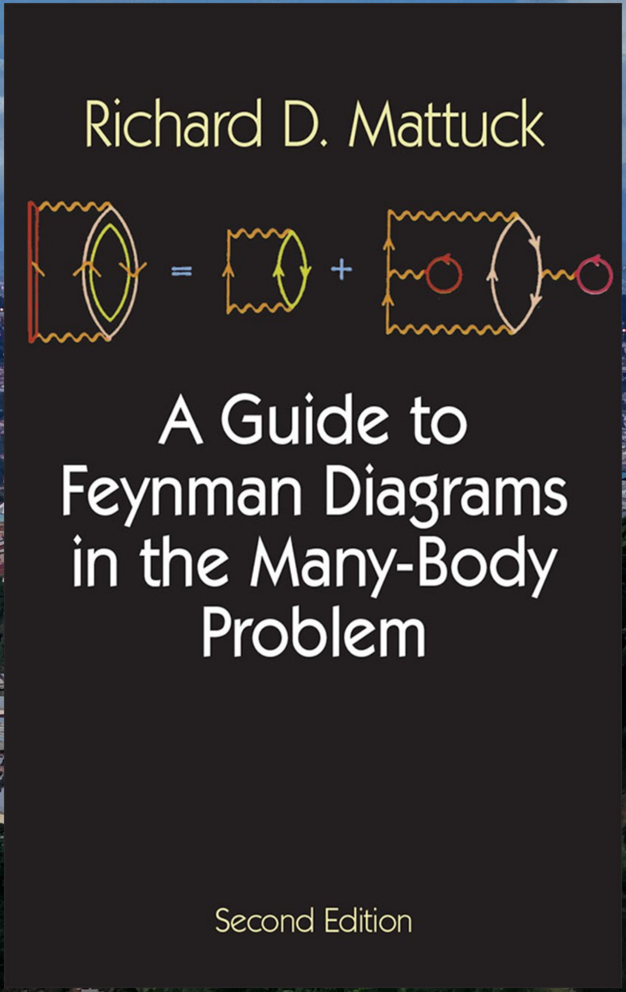
# Take-home messages

- MBPT is an exact **excited state** theory
- MBPT is based on Quantum Mechanics and 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


QUANTUM
THEORY OF
MANY-PARTICLE
SYSTEMS
ALEXANDER L. FETTER
JOHN DIRK WALECKA


Richard D. Mattuck
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+
A Guide to
Feynman Diagrams
in the Many-Body
Problem
Second Edition

# References

Yambo WIKI

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- Edu Home
- WWW Home
- Tutorials
- download
- Install
- Virtual Machines (Cloud, docker, VBox)
- Developers Corner

Read!

- Theory
- Lectures
- Cheatsheets
- Selected Readings
- Thesis

Learn! (Modular Tutorials)

- Overview
- Files Download
- First steps
- GW basics
- GW in parallel

# 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

wiki.yambo-code.eu