

# Many-Body Perturbation theory: Basic concepts and approximations

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[www.yambo-code.eu](http://www.yambo-code.eu)



Istituto di Struttura  
della Materia

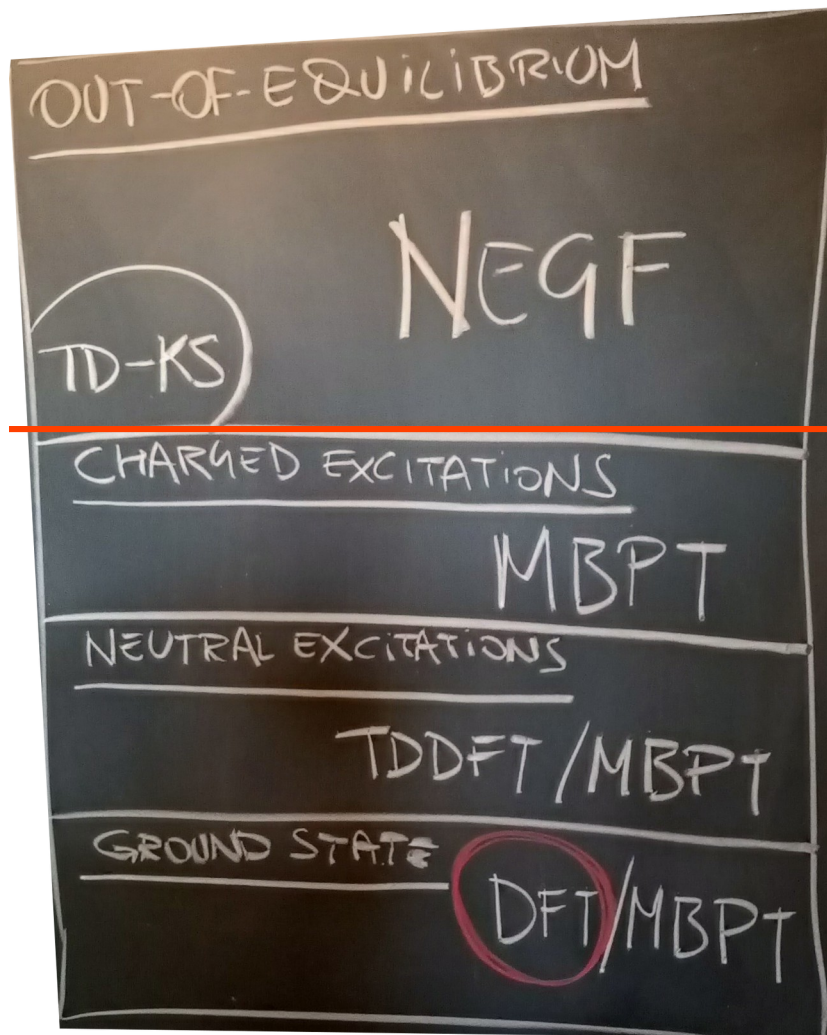
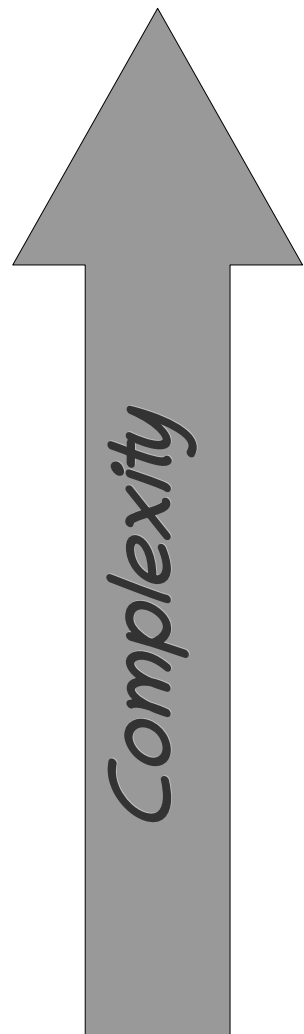


Ultrafast Science Laboratory of the  
Material Science Institute National Research Council  
(Monterotondo Stazione, Italy)

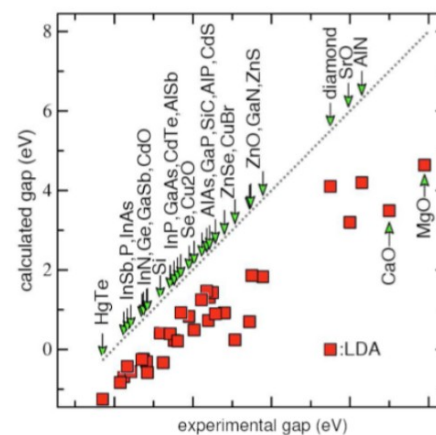
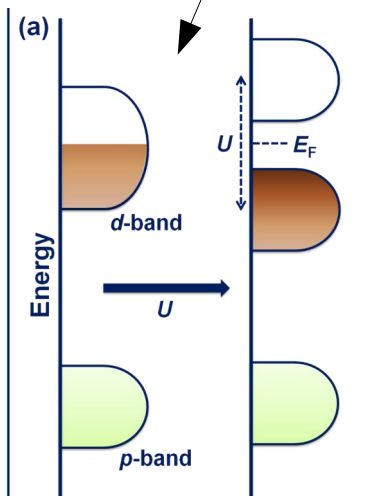
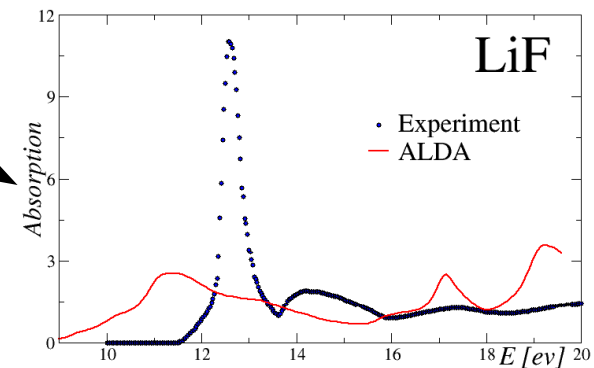
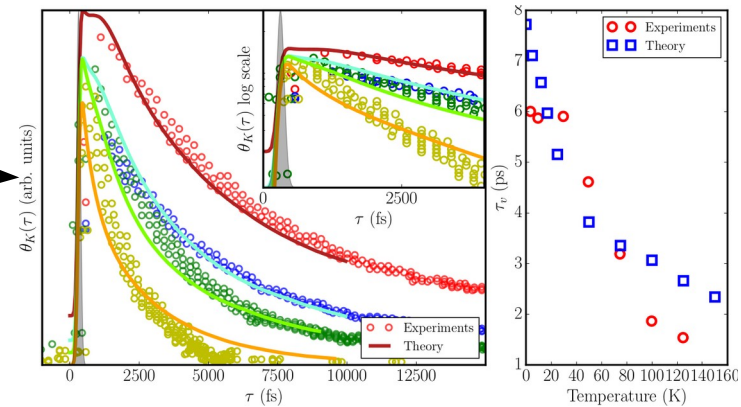
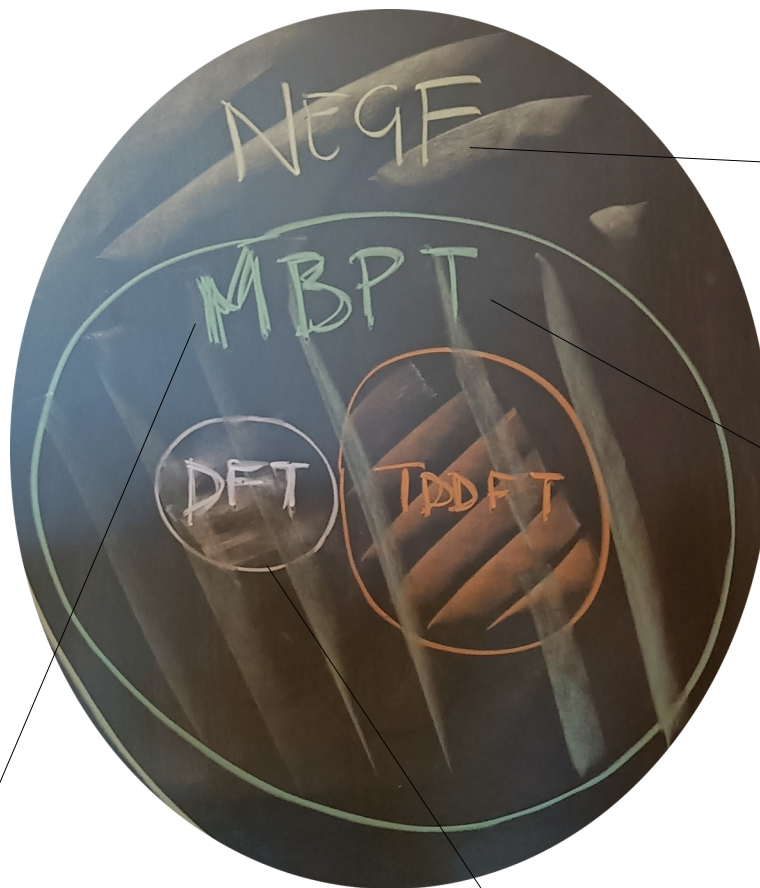
<http://www.yambo-code.eu/andrea>



# *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)

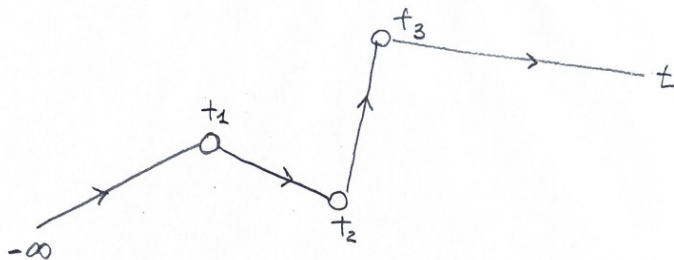
Adapted from M. van Schilfgaarde *et al.* PRL **96** (2006)

# Outline

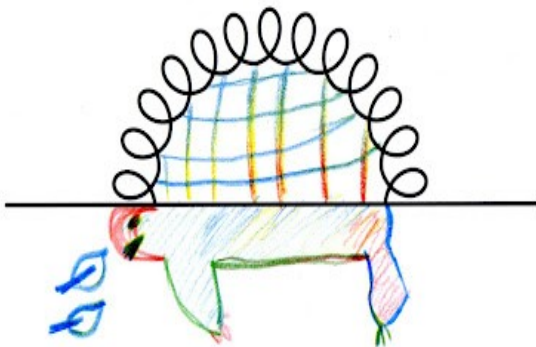
$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

The Hamiltonian

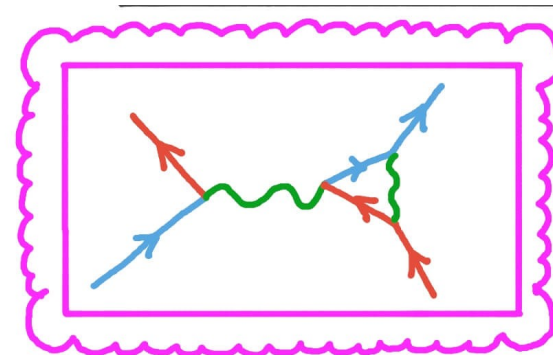
Many-Body Perturbation  
Theory for dummies



Lippmann-Schwinger propagators



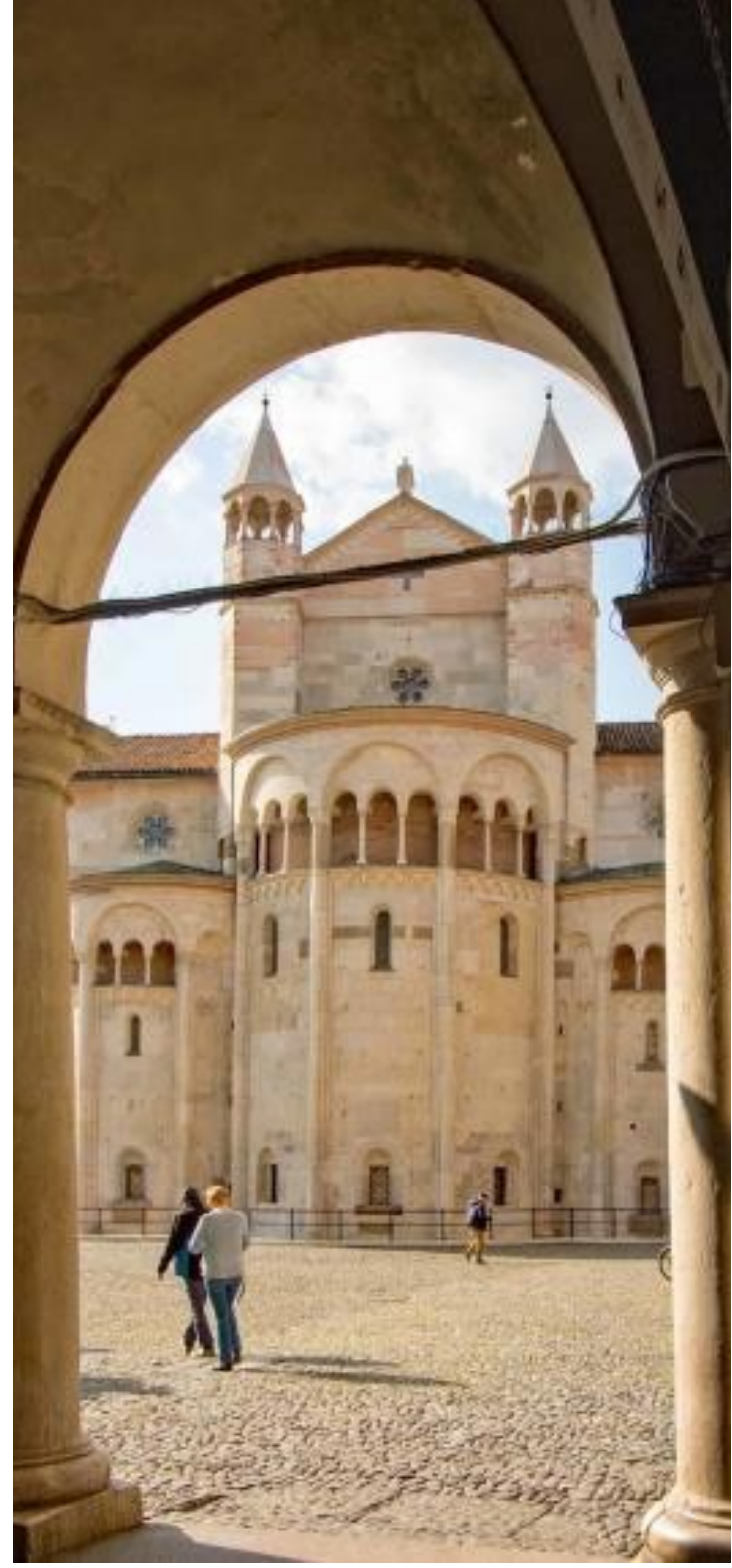
The “zoo” of MBPT approximations



Feynman diagrams for dummies



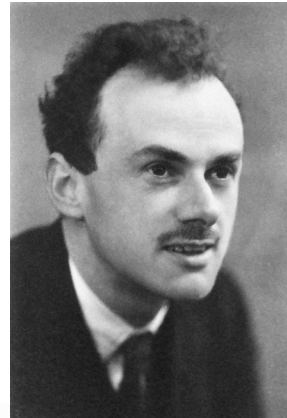
# From QED to MBPT and the role of Classical Mechanics



# The "Fermi" Hamiltonian



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



The radiation Gauge  
(E. Fermi, 1932)

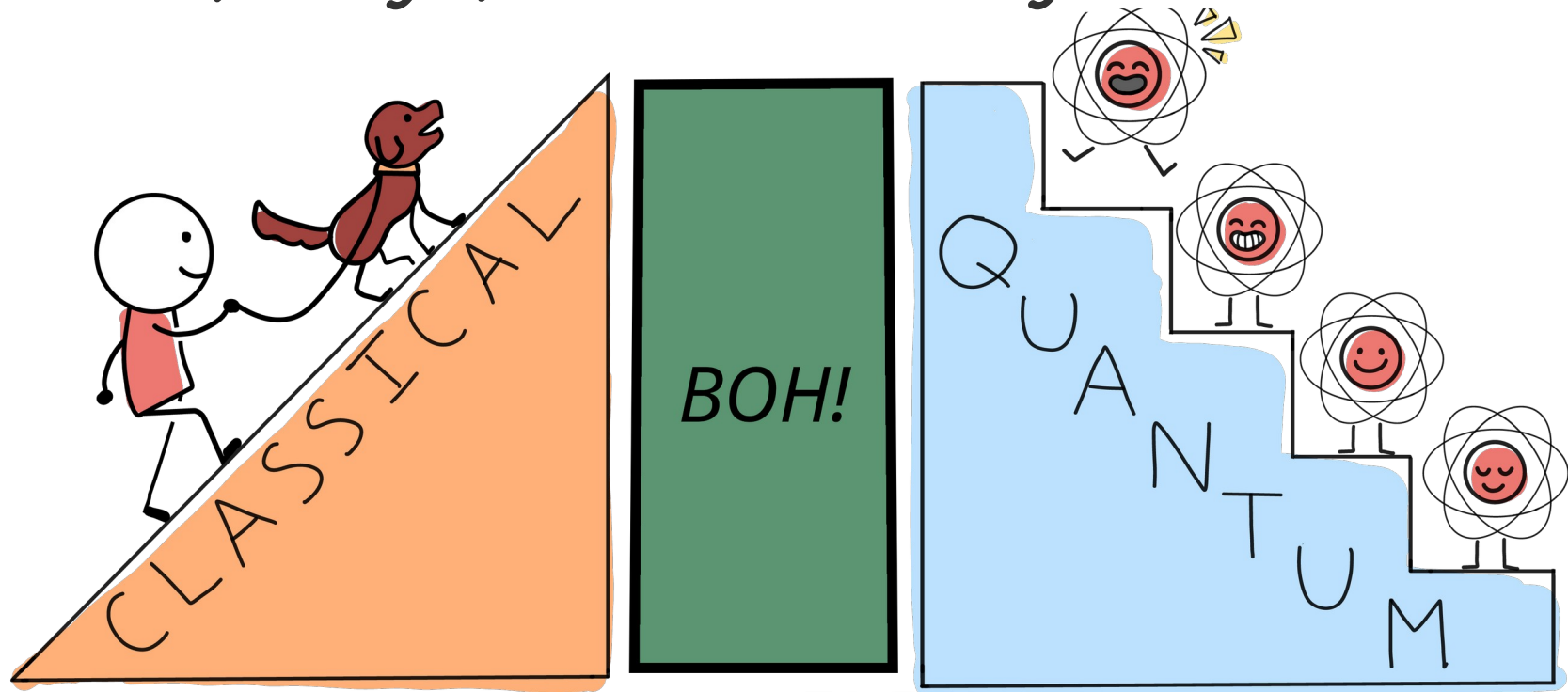
$$\nabla \cdot \hat{\mathbf{A}}(\mathbf{r}, t) = 0$$

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



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

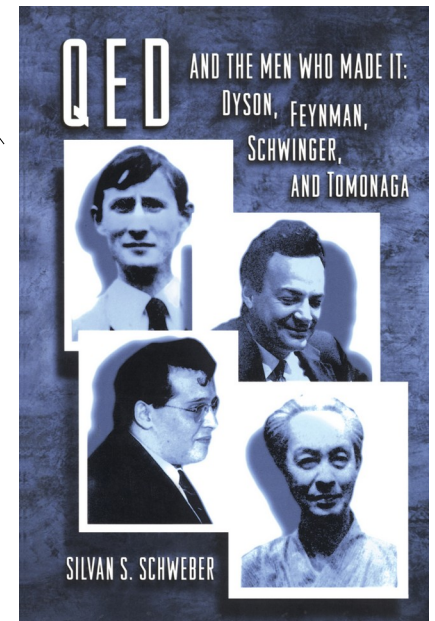
# Is MBPT a purely quantistic theory?



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



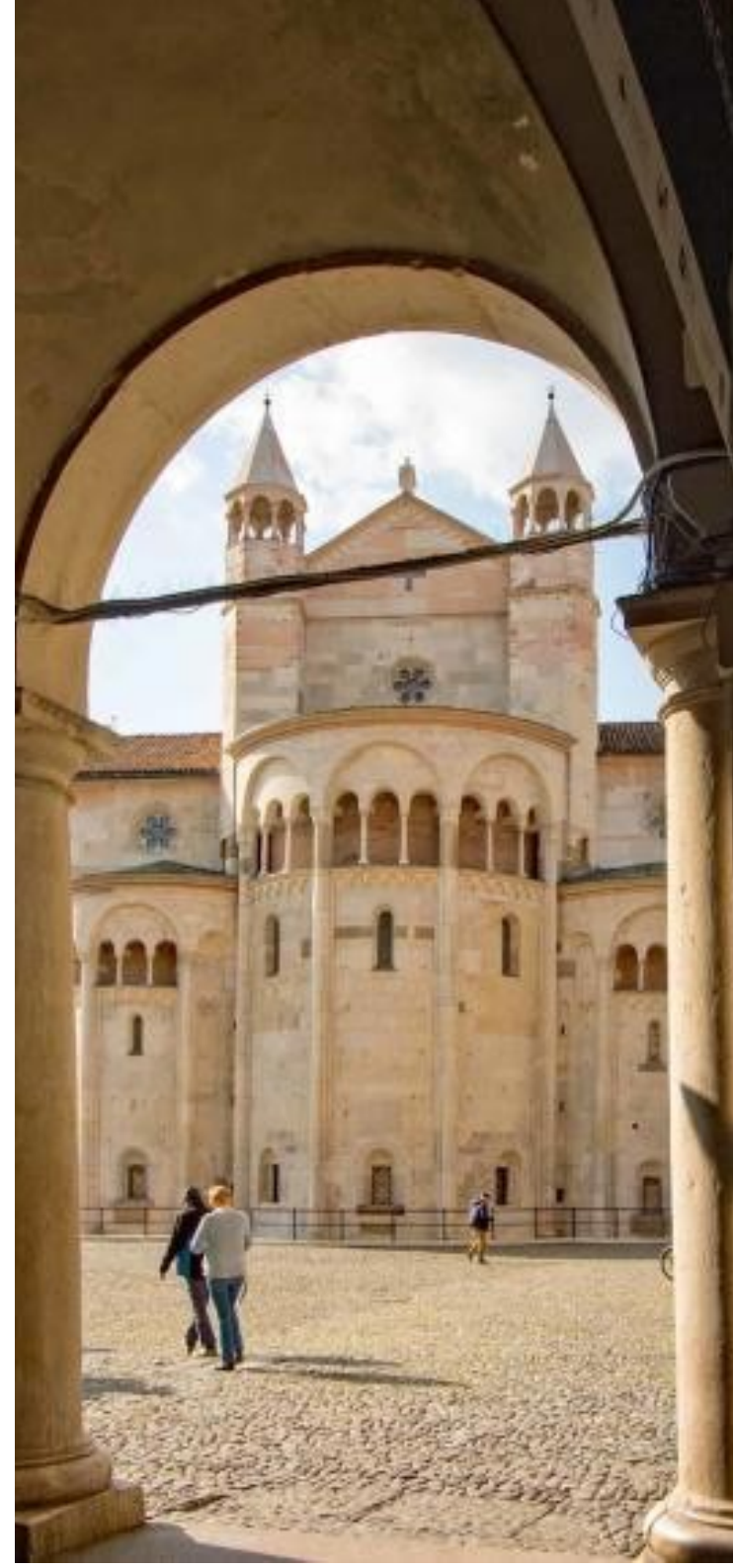
# MBPT





<u>OUT-OF-EQUILIBRIUM</u>	
TD-KS	NEGF
	CHARGED EXCITATIONS
	MBPT
	NEUTRAL EXCITATIONS
	TDDFT/MBPT
GROUND STATE	DFT/MBPT

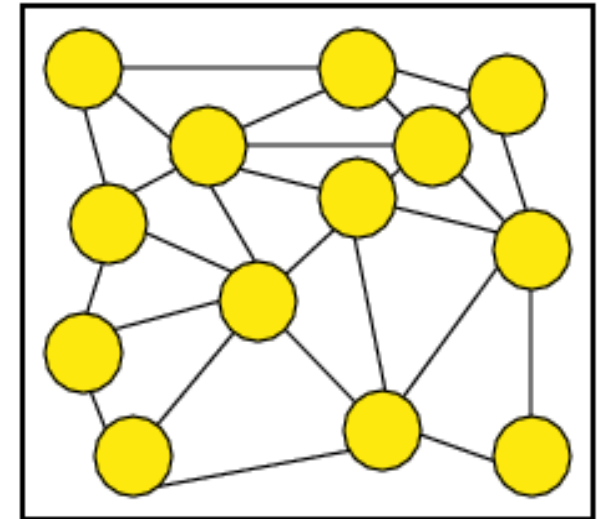
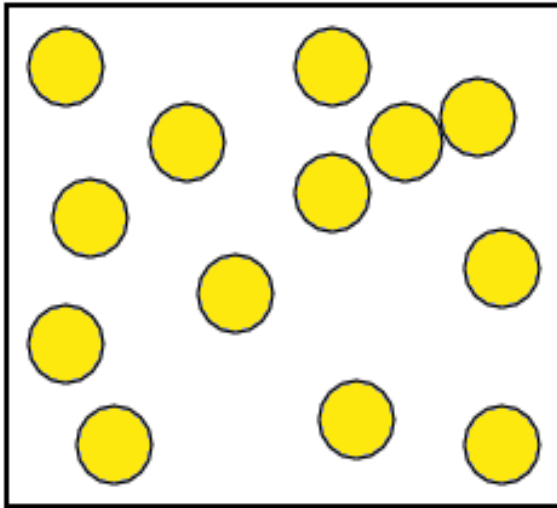
Many-Body Perturbation  
Theory for dummies





# *The Many-Body problem*

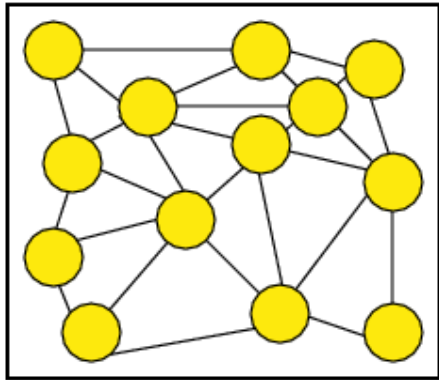
$$H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1}$$



# The Many-Body problem: 1 particle approx

$$H = \sum_i h(x_i) + \frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|} \quad \text{[Crossed out with a red X]}$$

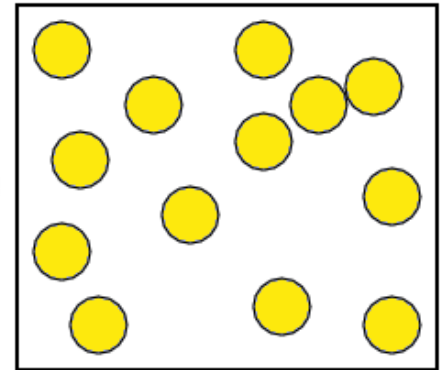
$$H = \sum_i h(x_i)$$



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



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



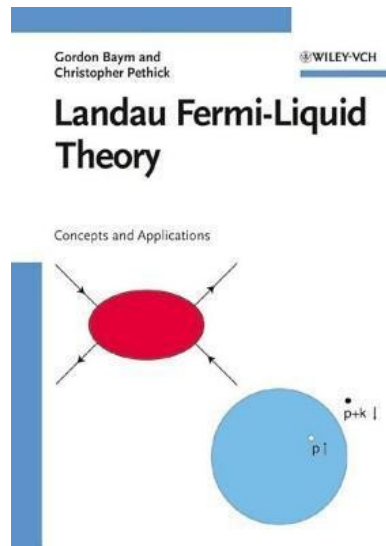
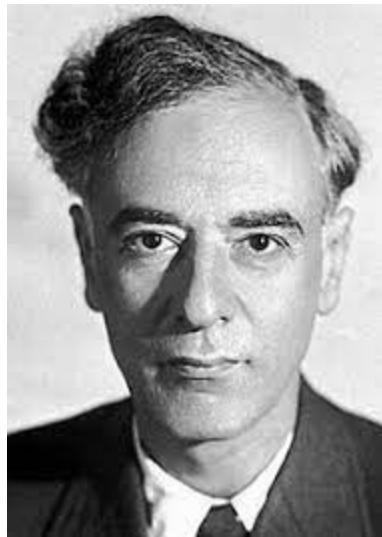
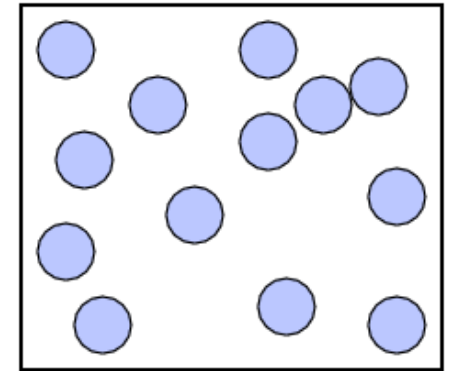
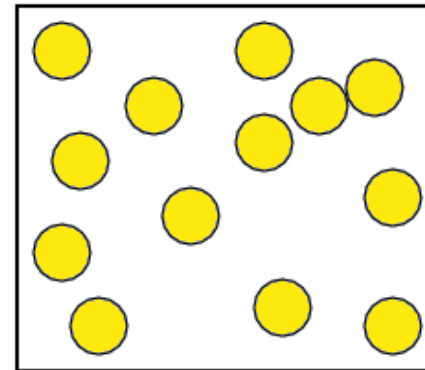
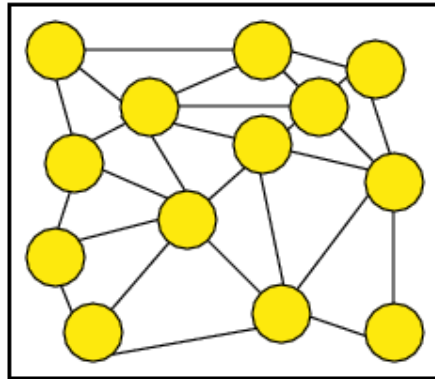
$$\langle N | \hat{A} | N \rangle \approx F_N [\{A_n\}]$$

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



# Quasiparticles...

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

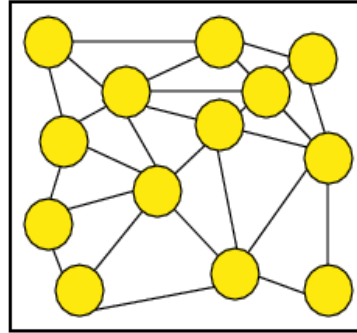


*The goal of the Many Body methods is to rewrite the fully interacting problem as an as much independent as possible counter-part*

# Mean-Field and beyond

DFT

Fully interacting system

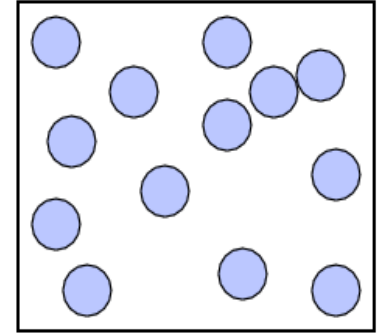


● = particle

Hohenberg-Kohn  
Theorem

Same  
Ground-State  
density  $n(r)$

Non interacting system

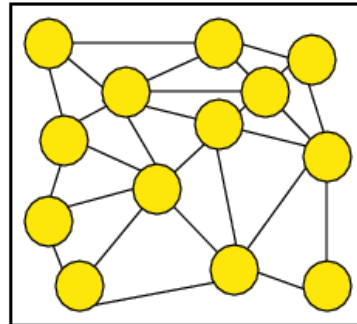


● = Kohn-Sham particle

For MBPT KS is  
a mean-field  
quasiparticle

MBPT

Fully interacting system

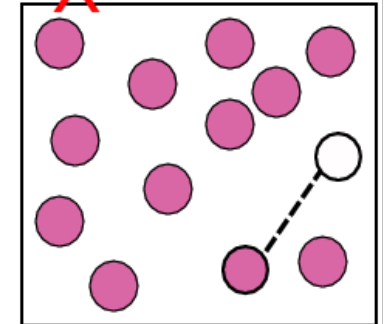


● particle

Diagrammatic  
Expansion

Same Excitation  
Spectra

~~Weakly~~ interacting system



● Qparticle ○ Qhole --- W







*Schrödinger equation*

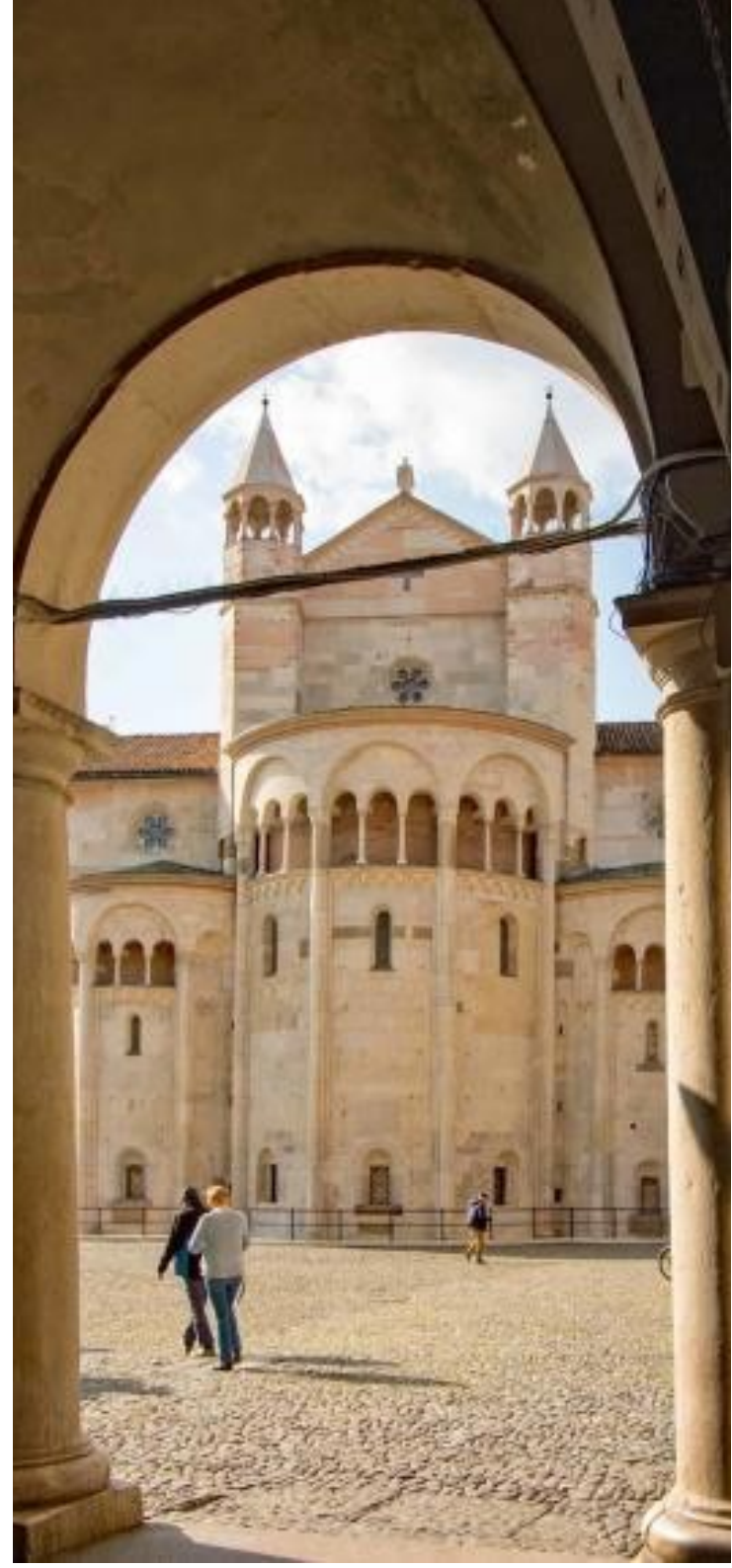
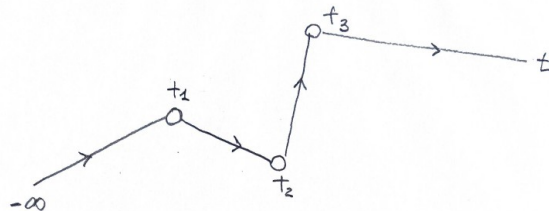
$$\left( i\hbar\partial_t - \hat{H}_0 \right) |\psi(t)\rangle = \hat{V}|\psi(t)\rangle$$

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

*Feynman path  
integral  
approach (CM  
trajectories)*



Lippmann-Schwinger  
(quantum) propagation



# Lippmann-Schwinger propagators

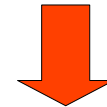


$$(i\hbar\partial_t - \hat{H}_0) |\psi(t)\rangle = e^{\eta t} \hat{V} |\psi(t)\rangle$$

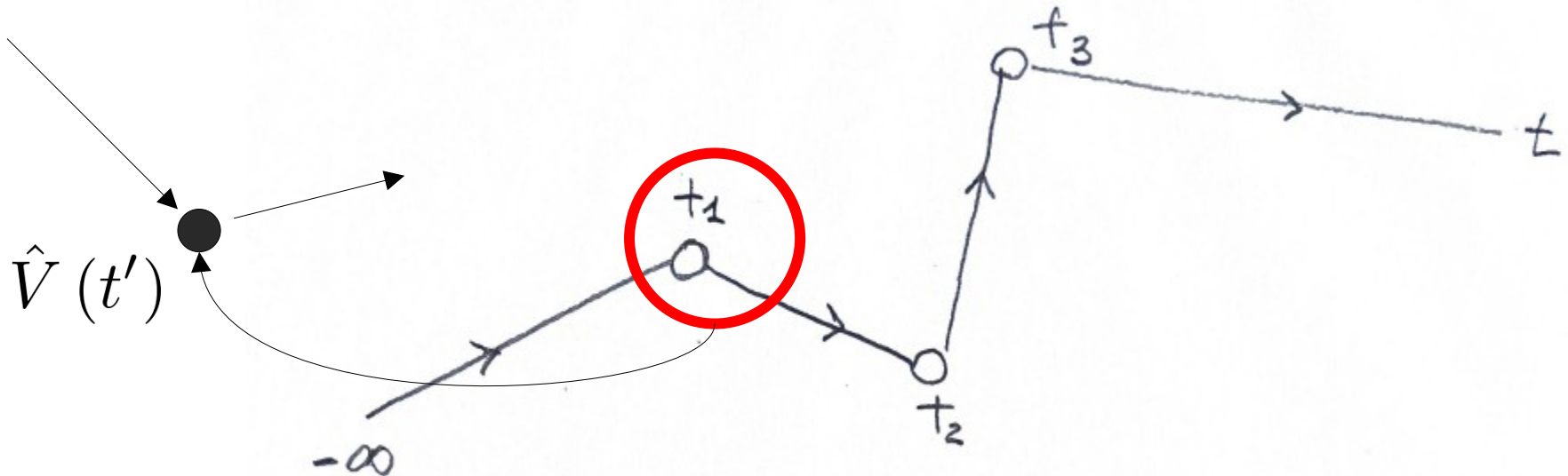
*Schrödinger equation*

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

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

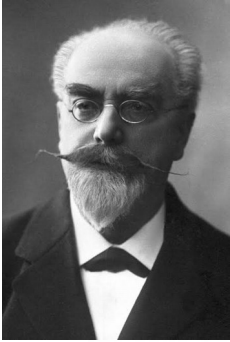


$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty} \hat{G}_0(t, t') \hat{V}(t') |\psi(t')\rangle dt'$$

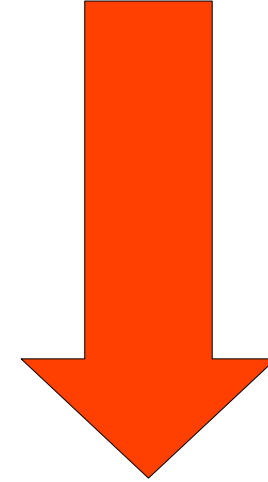
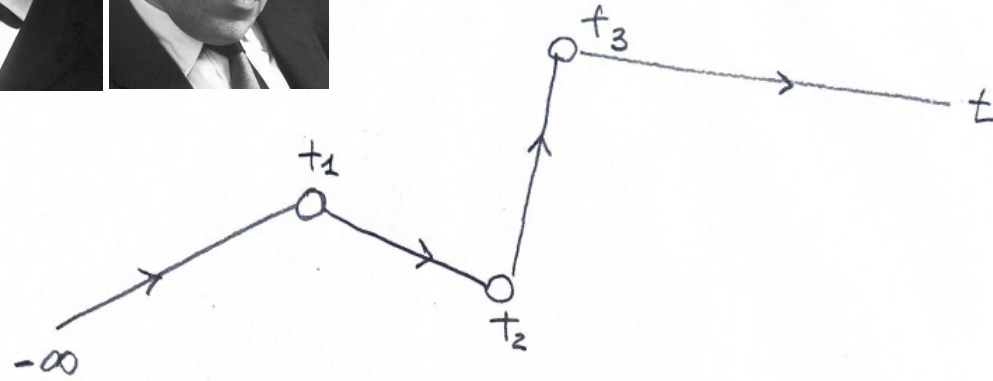




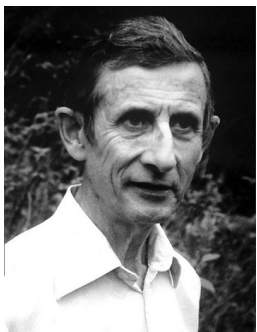
# Lippmann-Schwinger propagators



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

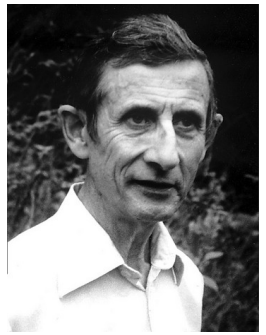


$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty} \hat{G}_0(t, t') \hat{V}(t') |\psi(-\infty)\rangle dt' + \\ + \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \hat{G}_0(t, t_1) \hat{V}(t_1) \hat{G}_0(t_1, t_2) \hat{V}(t_2) |\psi(-\infty)\rangle + \dots$$

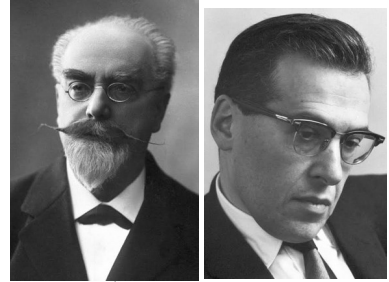


$$G_0 \hat{V} + G_0 \hat{V} G_0 \hat{V} + \dots = G \hat{V}$$

# Lippmann-Schwinger propagators

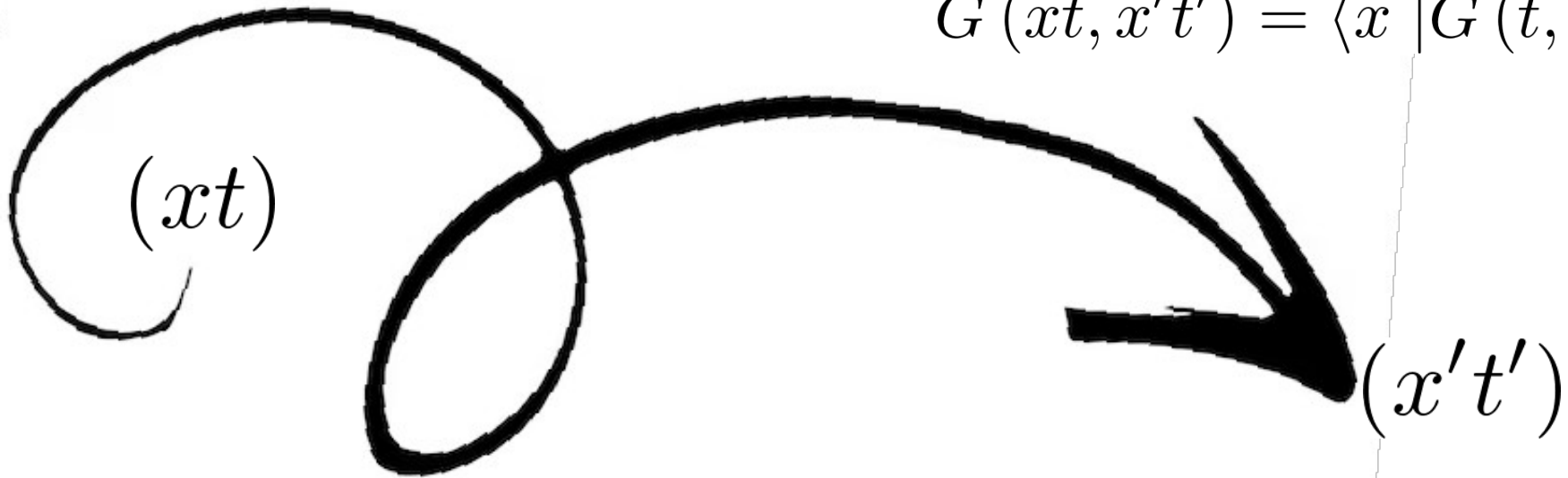


$$\hat{G}(t, t') = \hat{G}_0(t, t') + \int_{-\infty}^{\infty} \hat{G}_0(t, t_1) \hat{V}(t_1) \hat{G}(t_1, t')$$



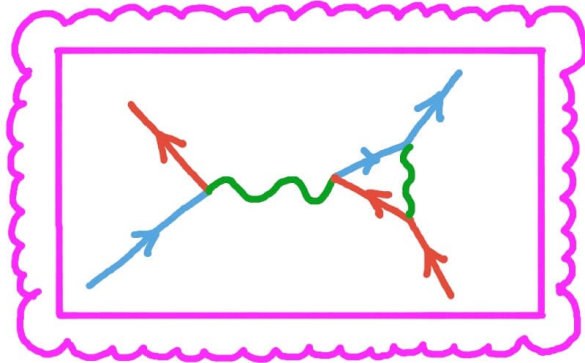
$$|\psi(t)\rangle = |\psi(-\infty)\rangle + \int_{-\infty}^{\infty} \hat{G}(t, t') \hat{V}(t') |\psi(-\infty)\rangle dt'$$

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



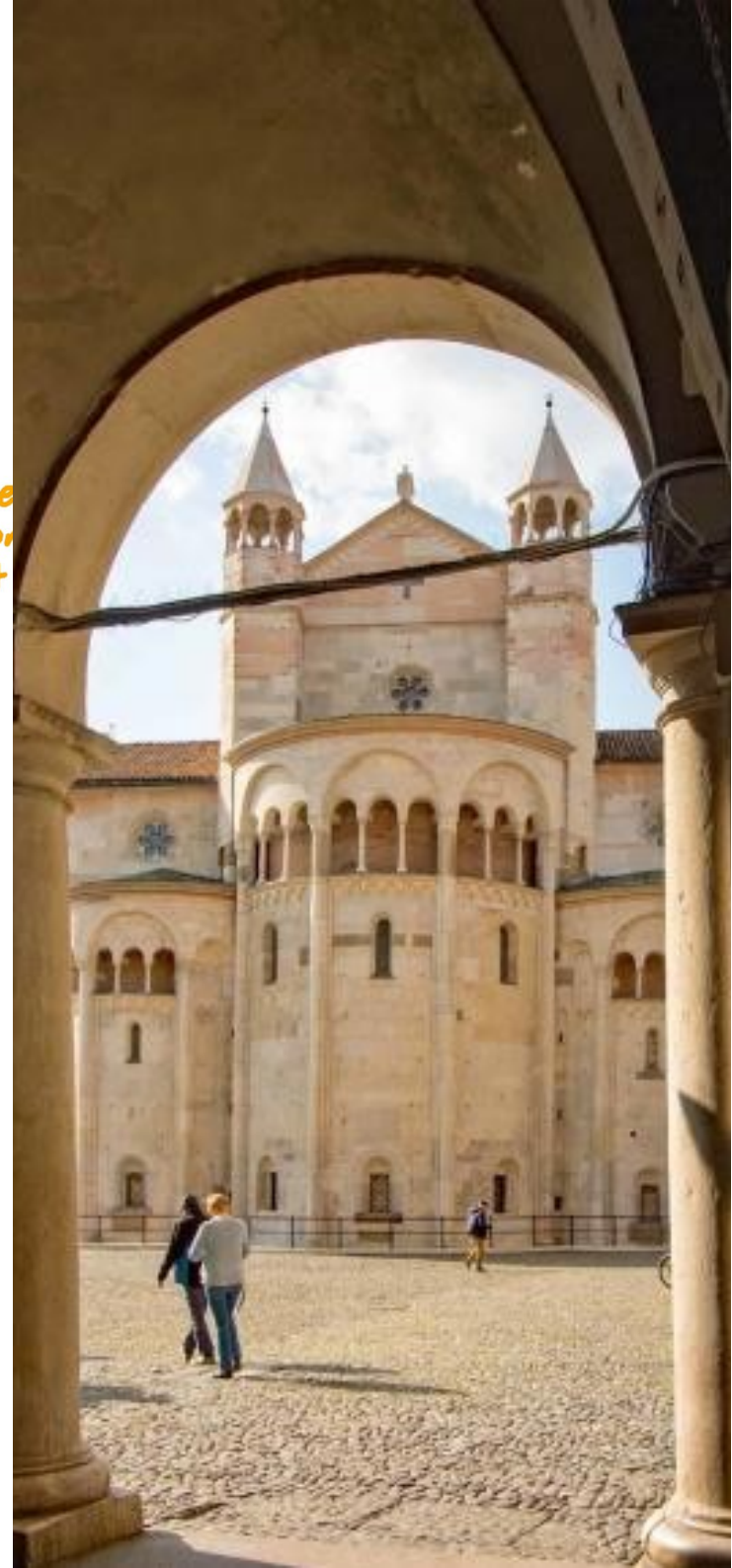
$$|x\rangle = \hat{\psi}^\dagger(x) |vacuum\rangle \quad \longrightarrow \quad G(xt, x't') = \langle \hat{\psi}^\dagger(xt) \hat{\psi}(x't') \rangle$$

# FEYNMAN DIAGRAMS



... a beautifully rendered  
pictorial representation  
of the great physicist  
Richard P. Feynman...

Feynmann diagrams for  
dummies





# The time-dependent, interacting density (Kubo)

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

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

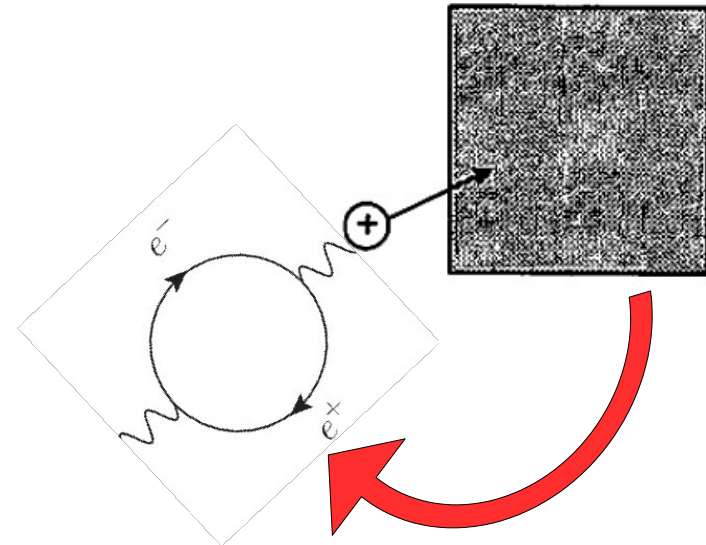


*Density Functional Theory*

Semi-classical **WEAK**  
excitation

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

Kubo

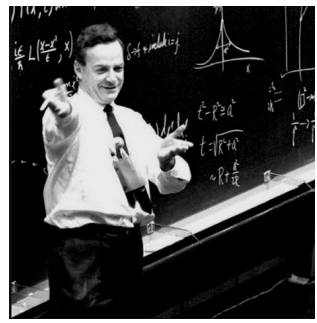


$$n(\mathbf{r}, t) = n_0(\mathbf{r}) + \int d\mathbf{r}' \int_0^t dt' \chi^R(\mathbf{r}t, \mathbf{r}'t') V(\mathbf{r}', t')$$

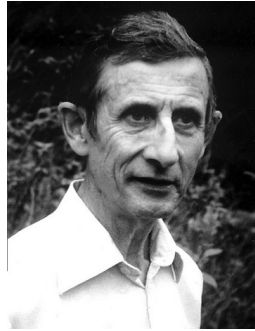
$$\chi(\mathbf{r}t, \mathbf{r}'t') = -i \langle \Psi | [\hat{n}(\mathbf{r}, t), \hat{n}(\mathbf{r}', t')] | \Psi \rangle \theta(t - t')$$

# The response (Green's) function

$$n(\mathbf{r}, t) = n_0(\mathbf{r}) + \int d\mathbf{r}' \int_0^t dt' \underbrace{\chi^R(\mathbf{r}t, \mathbf{r}'t')} V(\mathbf{r}', t')$$



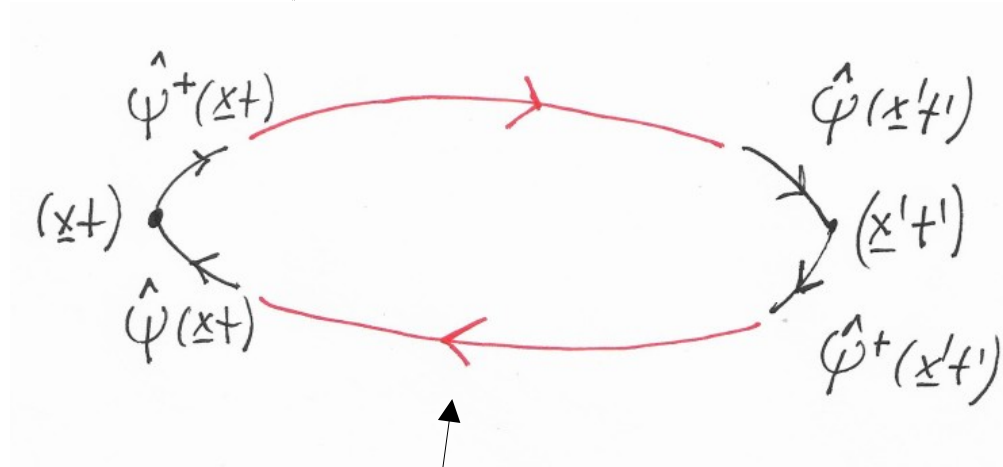
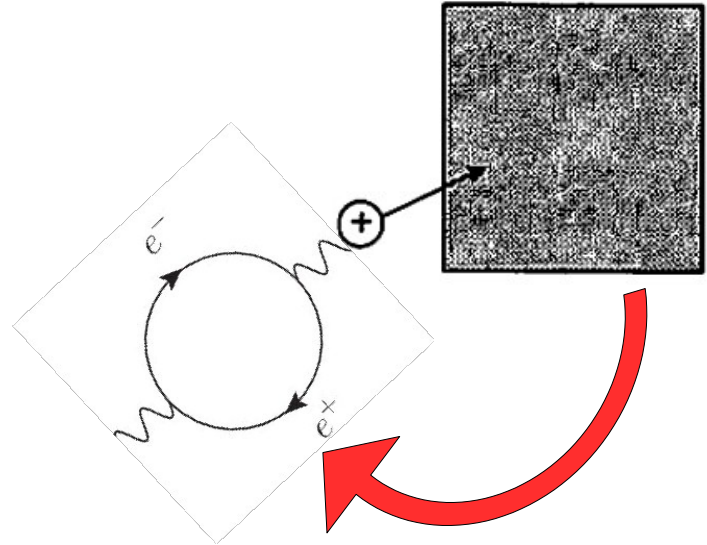
$$\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \hat{d}_{\mathbf{k}}$$



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

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

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

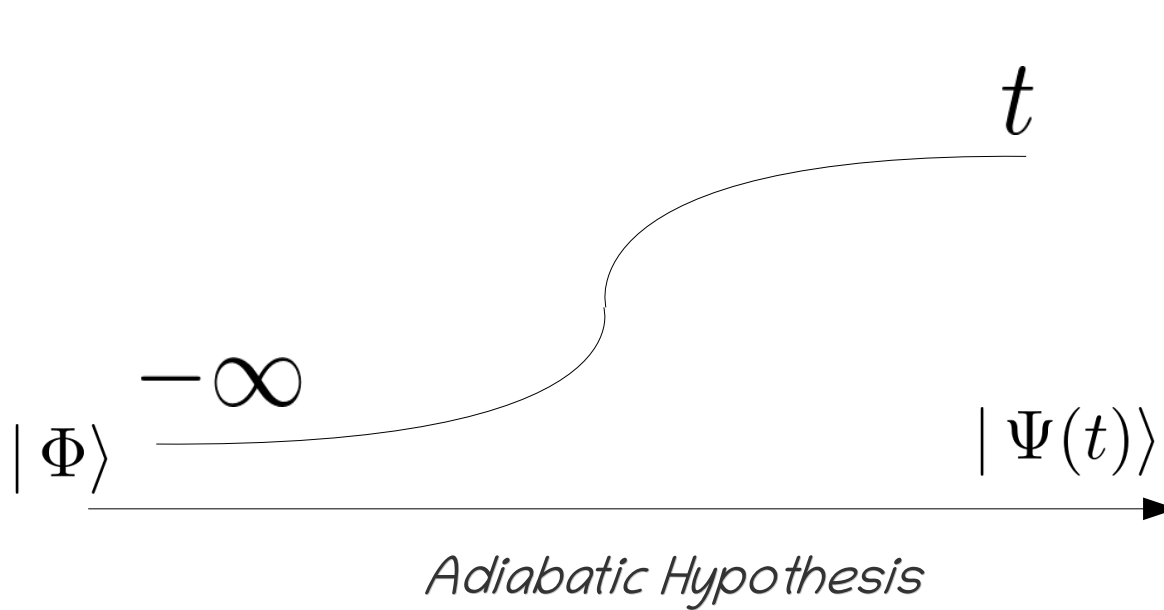


$$G(xt, x't') G(x't', xt)$$

# *The adiabatic ansatz*

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

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



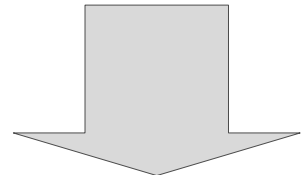
Gell-Mann  
Low  
Theorem

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

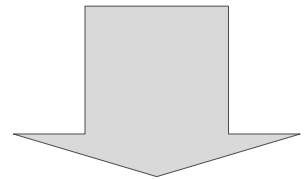


# *The evolution operator (scattering potential)*

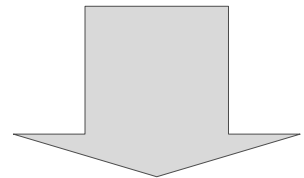
$$\hat{H}(t) = \hat{H}_0 + \underbrace{\hat{V}(t)}$$


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

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



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



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

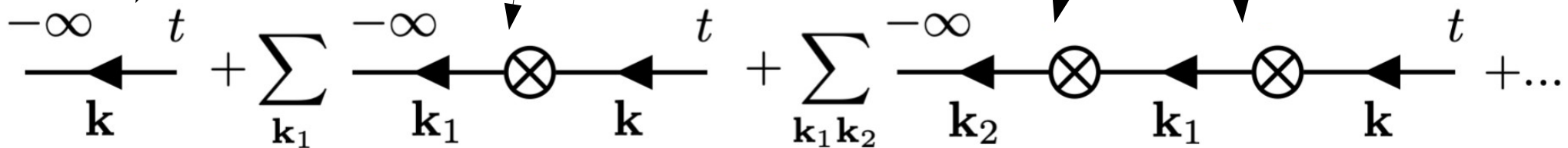
*Constrained time integrals*  
 $t > t_1 > t_2 > \dots$

# Half the dynamics...

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

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

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



# The Dyson equation



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

$$\left( \begin{array}{c} t \xrightarrow{\mathbf{k}'} \xleftarrow{-\infty} + t \xleftarrow{\mathbf{k}'} \otimes \xleftarrow{-\infty} + t \xleftarrow{\mathbf{k}'} \otimes \xleftarrow{\mathbf{k}'} \otimes \xleftarrow{-\infty} + \dots \end{array} \right) \times$$

$$\left( \begin{array}{c} \xleftarrow{\mathbf{k}} \xleftarrow{-\infty} + \xleftarrow{\mathbf{k}} \otimes \xleftarrow{-\infty} + \xleftarrow{\mathbf{k}} \otimes \xleftarrow{\mathbf{k}} \otimes \xleftarrow{-\infty} + \dots \end{array} \right)$$

$$= \begin{array}{c} t \xleftarrow{\mathbf{k}'} \xleftarrow{\mathbf{k}} + t \xleftarrow{\mathbf{k}'} \otimes \xleftarrow{t_1} \left( t \xleftarrow{\mathbf{k}} + t \xleftarrow{\mathbf{k}'} \otimes \xleftarrow{t_2} \otimes \xleftarrow{t_1} \xleftarrow{\mathbf{k}} + \dots \right) \end{array}$$

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



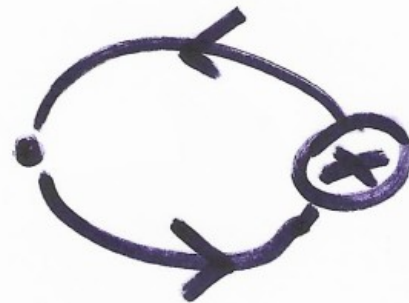
# Green's Functions: Kubo revisited

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

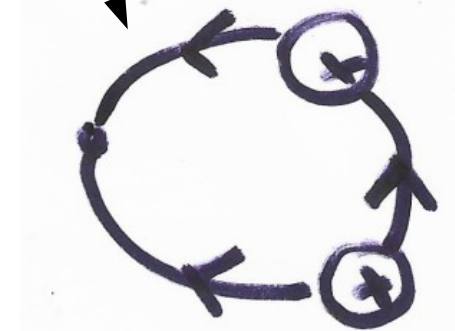
$$= \underbrace{\text{---} \xleftarrow{t} \text{---} \xleftarrow{t} \text{---}}_{\mathbf{k}' \quad \mathbf{k}} + \text{---} \xleftarrow{t} \text{---} \bigotimes_{t_1} \text{---} \xleftarrow{t} \text{---} \text{---} \xleftarrow{t} \text{---} \bigotimes_{t_2} \text{---} \xleftarrow{t} \text{---} \bigotimes_{t_1} \text{---} \xleftarrow{t} \text{---} \text{---} \xleftarrow{t} \text{---} \text{---} + \dots$$



$n_0(\mathbf{r})$



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



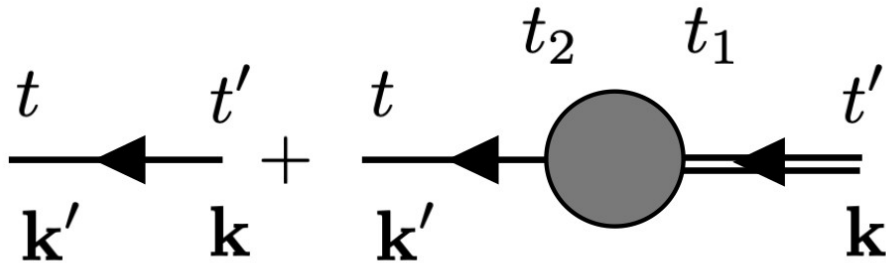
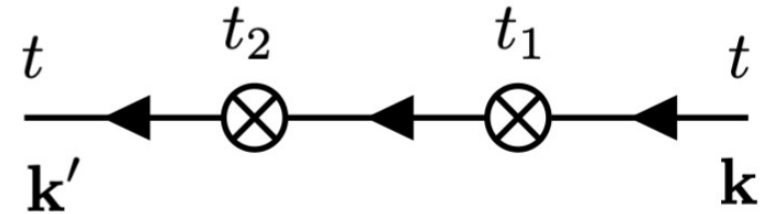
*Non-linear terms*

# Key messages



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

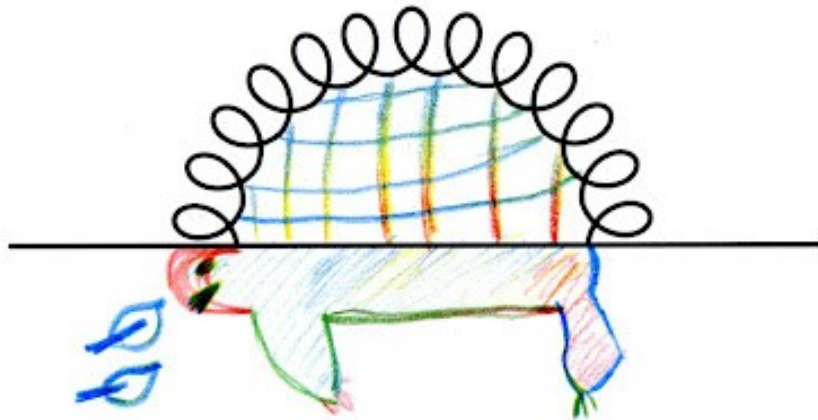
In MBPT the many-body problem is rewritten in terms as pseudo-time propagation under the action of a slowly varying potential



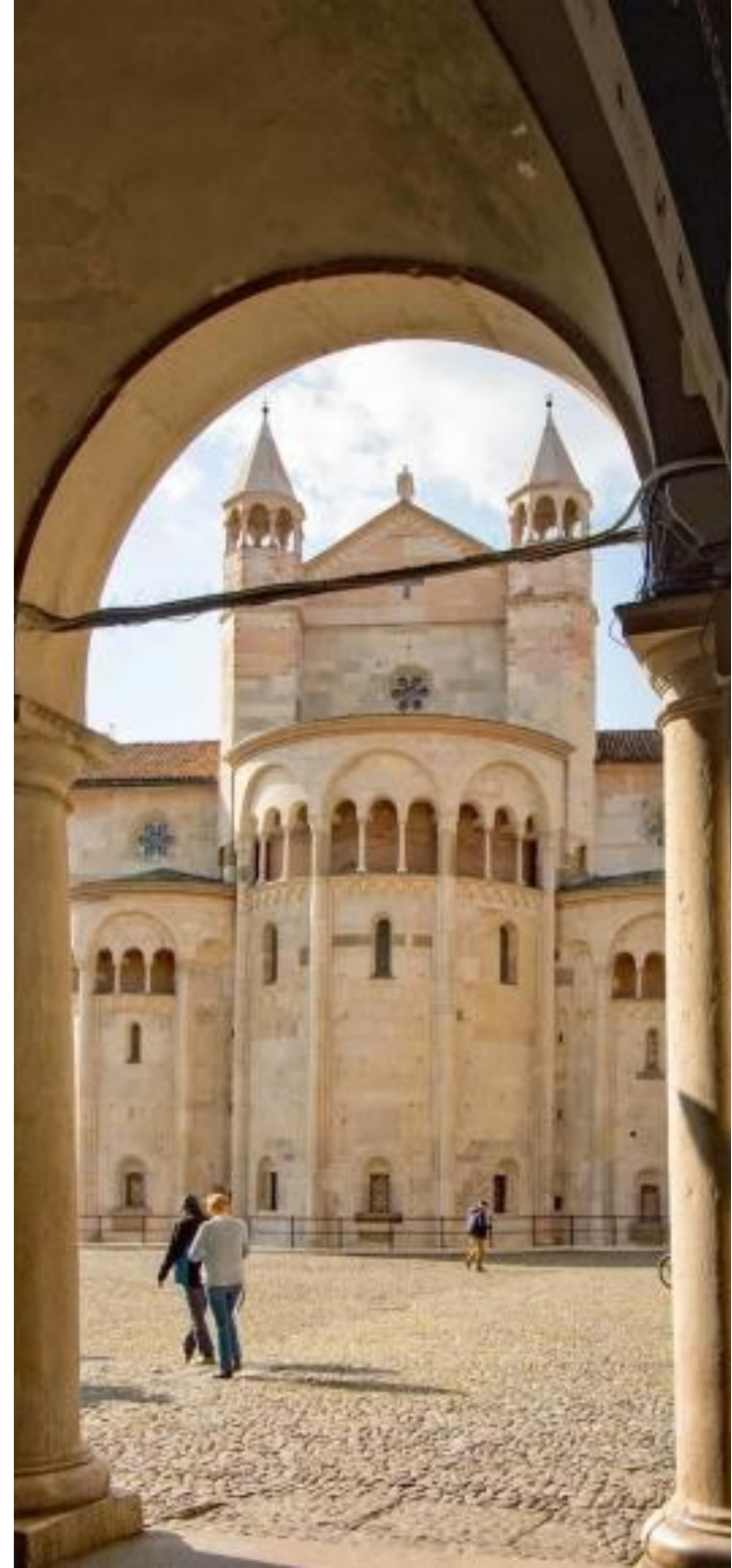
Diagrams allow to introduce a geometric representation of the dynamics

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





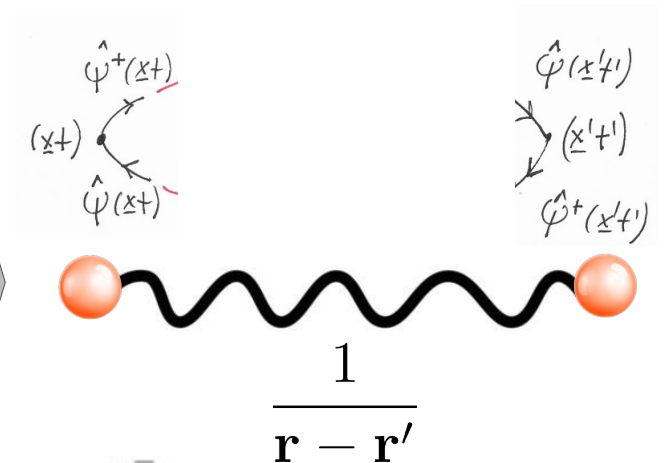
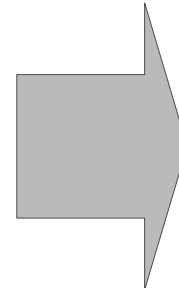
The “zoo” of MBPT  
approximations





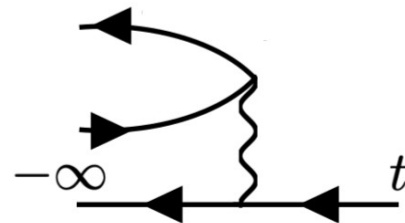
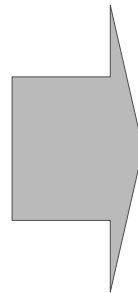
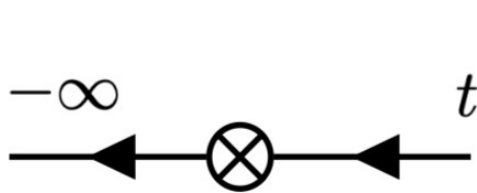
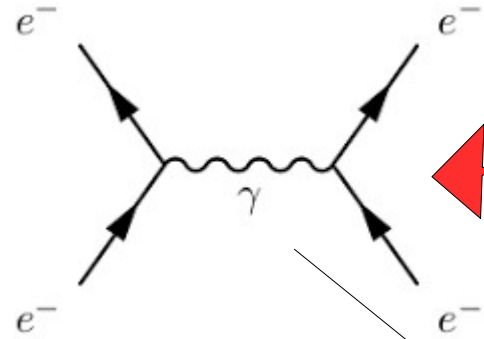
# The Coulomb interaction (revisited)

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



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

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



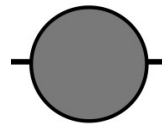
# Hartree-Fock (diagrammatic representation)

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

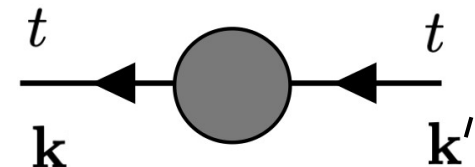
$$\left( \begin{array}{c} t \quad -\infty \quad + \\ \leftarrow \quad \leftarrow \quad \leftarrow \\ \mathbf{k} \end{array} \right) \times \left( \begin{array}{c} t \quad -\infty \\ \leftarrow \quad \leftarrow \\ \mathbf{k} \end{array} \right) \times \left( \begin{array}{c} -\infty \quad t \\ \leftarrow \quad \leftarrow \\ \mathbf{k}' \end{array} \right) + \left( \begin{array}{c} -\infty \quad t \\ \leftarrow \quad \leftarrow \\ \mathbf{k}' \end{array} \right) =$$

*The Propagator*

$$= \begin{array}{c} t \quad t' \\ \leftarrow \quad \leftarrow \\ \mathbf{k} \quad \mathbf{k}' \end{array} + \underbrace{\begin{array}{c} \text{Hartree} \\ \begin{array}{c} t \quad t \\ \leftarrow \quad \leftarrow \\ \mathbf{k} \quad \mathbf{k}' \end{array} \end{array} + \begin{array}{c} \text{Fock} \\ \begin{array}{c} t \quad t \\ \leftarrow \quad \leftarrow \\ \mathbf{k} \quad \mathbf{k}' \end{array} \end{array}}$$



*The Hartree-Fock  
Self-Energy*



# Feynman diagrams in the fully interacting case

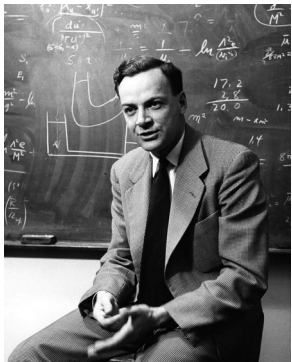
$$\langle \Psi(t) | \hat{d}_{\mathbf{k}}^\dagger \hat{U}(t) \hat{U}^\dagger(t) \hat{d}_{\mathbf{k}'}^\dagger | \Psi(t) \rangle =$$

$$\left( \text{Diagram 1} \right) \times \left( \text{Diagram 2} + \text{Diagram 3} \right) =$$

Diagram 1: A horizontal line with an arrow pointing left, labeled  $t$  at the left end and  $-\infty$  at the right end. Below the line is the label  $\mathbf{k}$ .

Diagram 2: A horizontal line with an arrow pointing left, labeled  $t$  at the left end and  $-\infty$  at the right end. Below the line is the label  $\mathbf{k}$ . A wavy line (photon) connects this diagram to Diagram 3.

Diagram 3: A horizontal line with an arrow pointing left, labeled  $-\infty$  at the left end and  $t$  at the right end. Below the line is the label  $\mathbf{k}'$ .



$$= (HF) + \text{Diagram 4} + \text{Diagram 5}$$

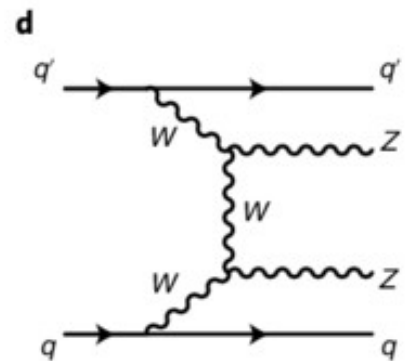
Diagram 4: A diagram showing two vertices,  $t_1$  and  $t_2$ , connected by a horizontal line with an arrow pointing right. A wavy line (photon) connects  $t_1$  to  $t_2$ . A loop of two arrows connects  $t_1$  and  $t_2$ .

Diagram 5: A diagram showing two vertices,  $t_1$  and  $t_2$ , connected by a horizontal line with an arrow pointing right. A wavy line (photon) connects  $t_1$  to  $t_2$ . A loop of two arrows connects  $t_1$  and  $t_2$ , with a crossing in the middle.



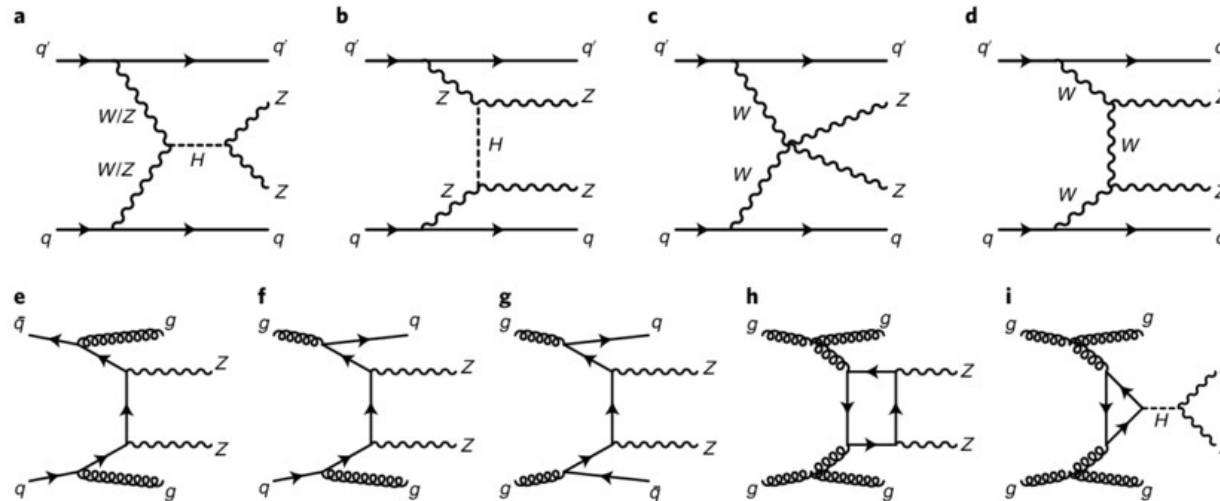
$$\langle \Psi(t) | \hat{d}_{\mathbf{k}}^\dagger \hat{U}(t) \hat{U}^\dagger(t) \hat{d}_{\mathbf{k}'}^\dagger | \Psi(t) \rangle$$

Diagrammatic Rules

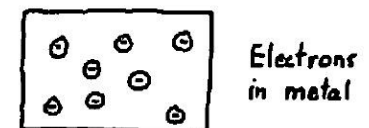
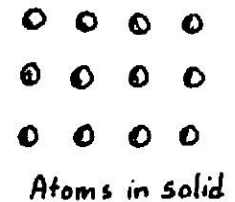
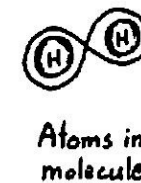
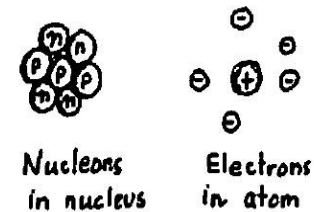




# Feynman diagrams in the fully interacting case



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



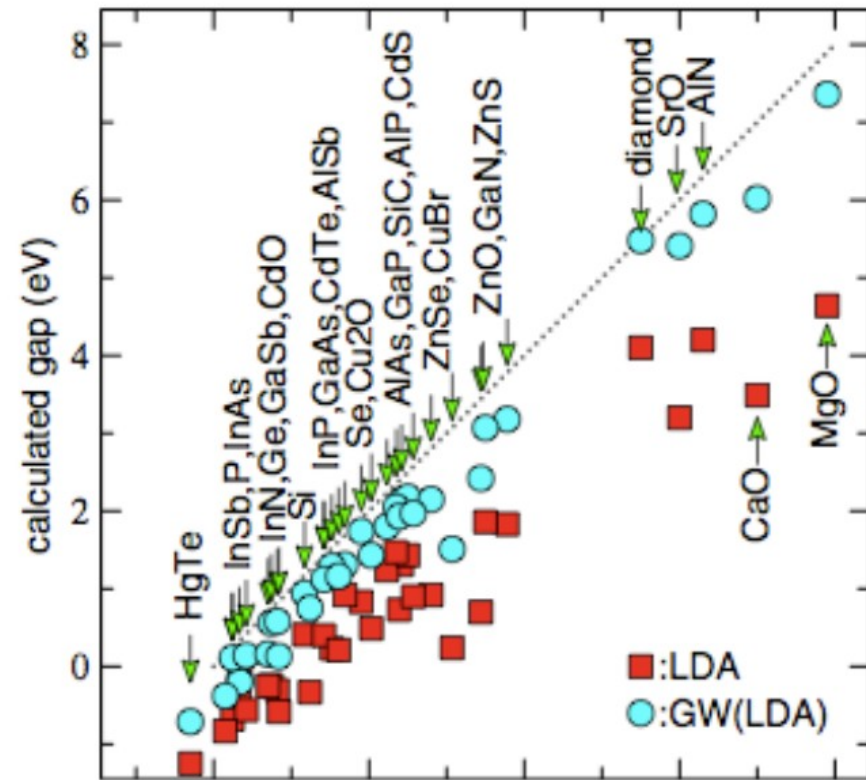
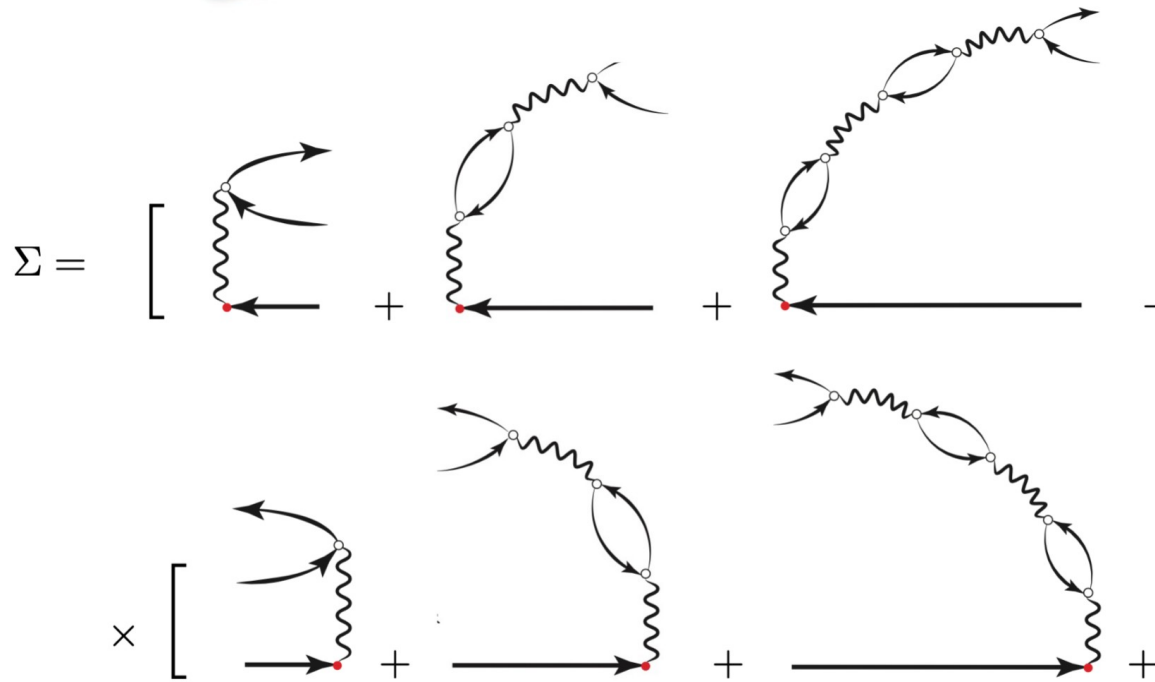
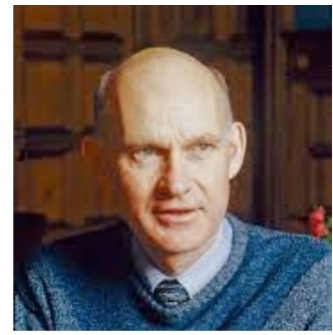
Short-range interactions ?

High density regime ?

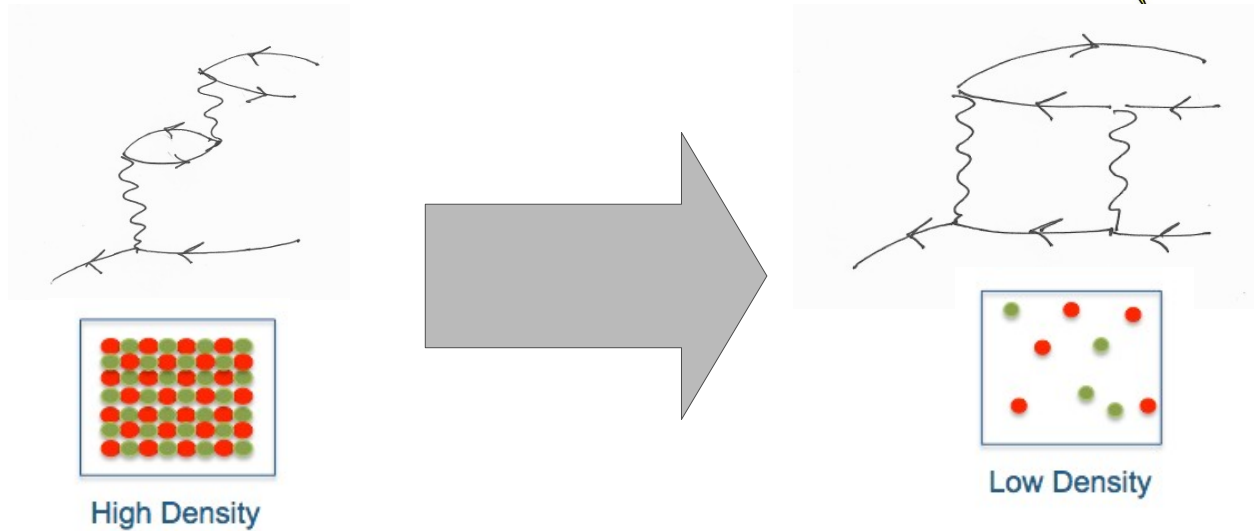
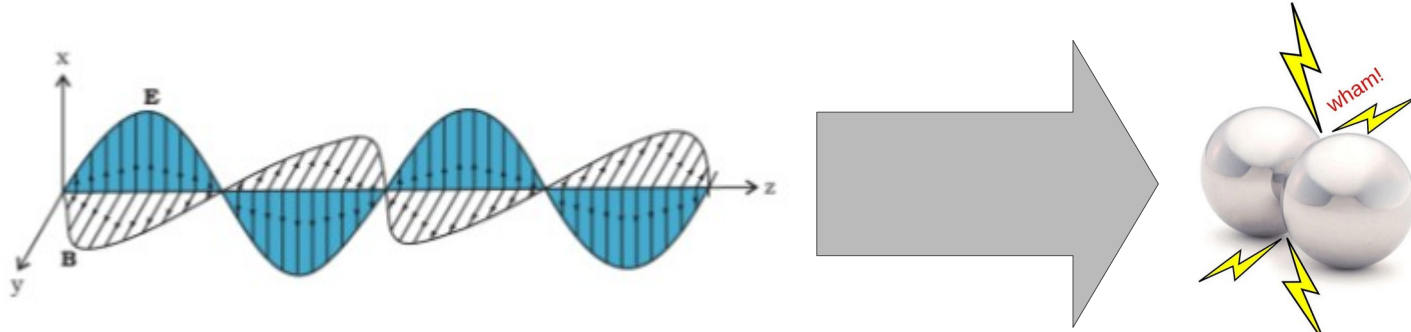
Low density regime ?

Conserving approximations

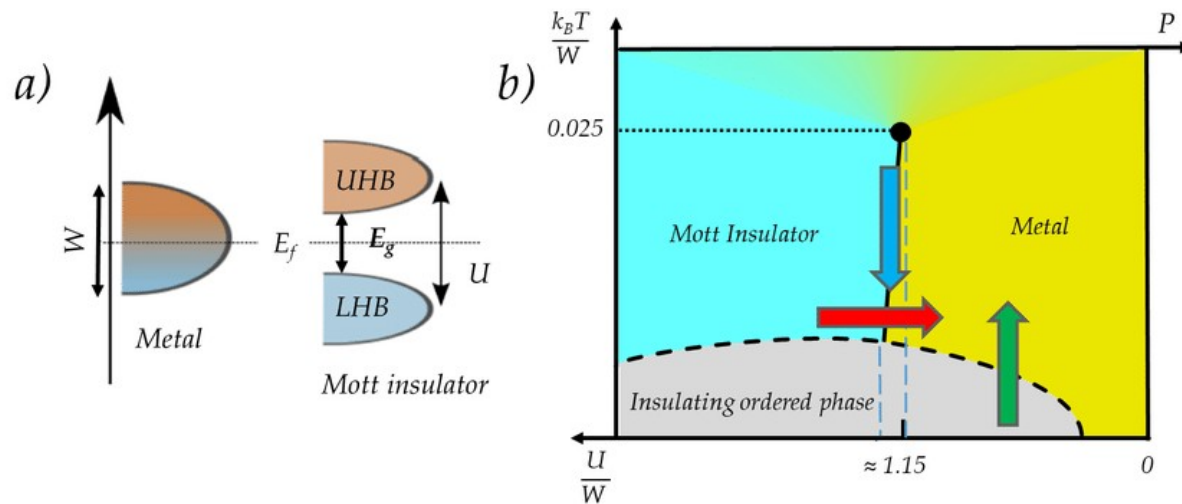
# The GW approximation



# The $T$ -matrix approximation

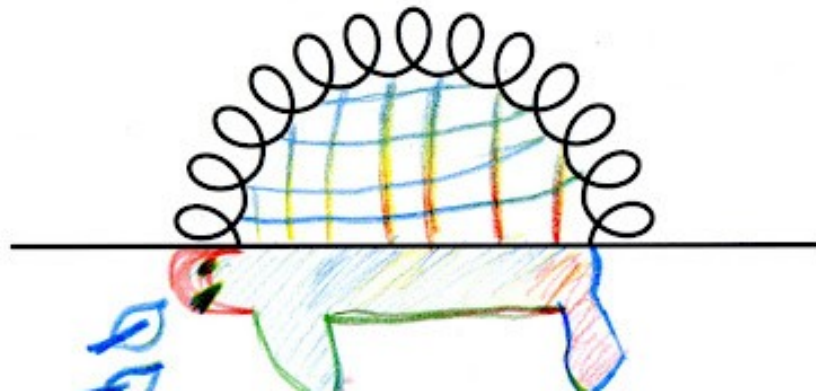


VIKTOR MIKHAĬLOVICH  
GALITSKIĬ  
(1924–1981)



# 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.



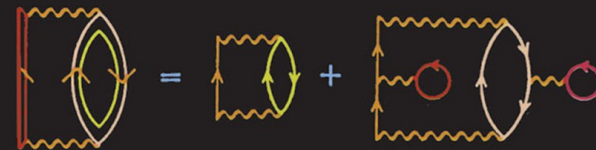


# References

## QUANTUM THEORY OF MANY-PARTICLE SYSTEMS

ALEXANDER L. FETTER  
JOHN DIRK WALECKA

Richard D. Mattuck




## A Guide to Feynman Diagrams in the Many-Body Problem

Second Edition



# References



Yambo.WIKI

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

Read!

- Theory
- Lectures
- Cheatsheets
- Selected Readings
- Thesis

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

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- 2 [Many-body Theory](#)
- 3 [The GW method](#)
- 4 [Density Functional Theory](#)
- 5 [TDDFT](#)
- 6 [Non-equilibrium Green's function](#)
- 7 [Theoretical Spectroscopy](#)
- 8 [Computer Programming](#)

### 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](#)