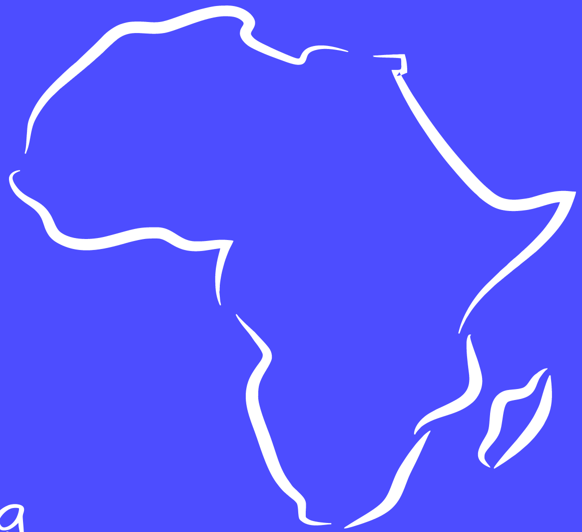
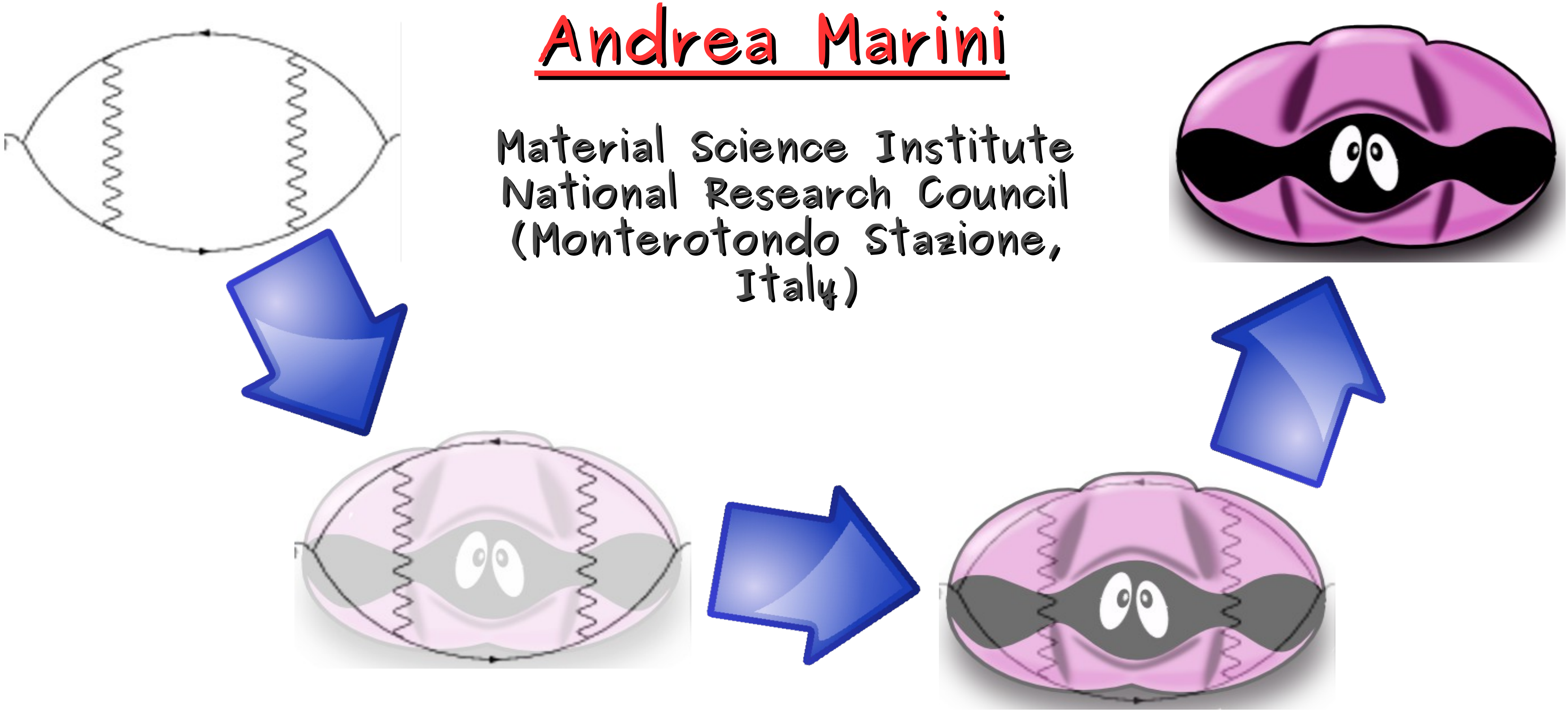
Introduction to the Many-Body problem (I)



ASESMA 2015, Johannesburg

Andrea Marini

Material Science Institute
National Research Council
(Monterotondo Stazione, Italy)



Why so many bodies ?

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

- Ket, bra and operators
- Static perturbation Theory
- Example: The Zeeman Effect
- Interaction Representation
- Time-dependent perturbation Theory
- Example: Interaction with the radiation field
- Hartree-Fock via Perturbation Theory
- Hartree-Fock via Variational approache
- Hartee-Fock drawbacks: correlation

Outline

A (very) hard job!

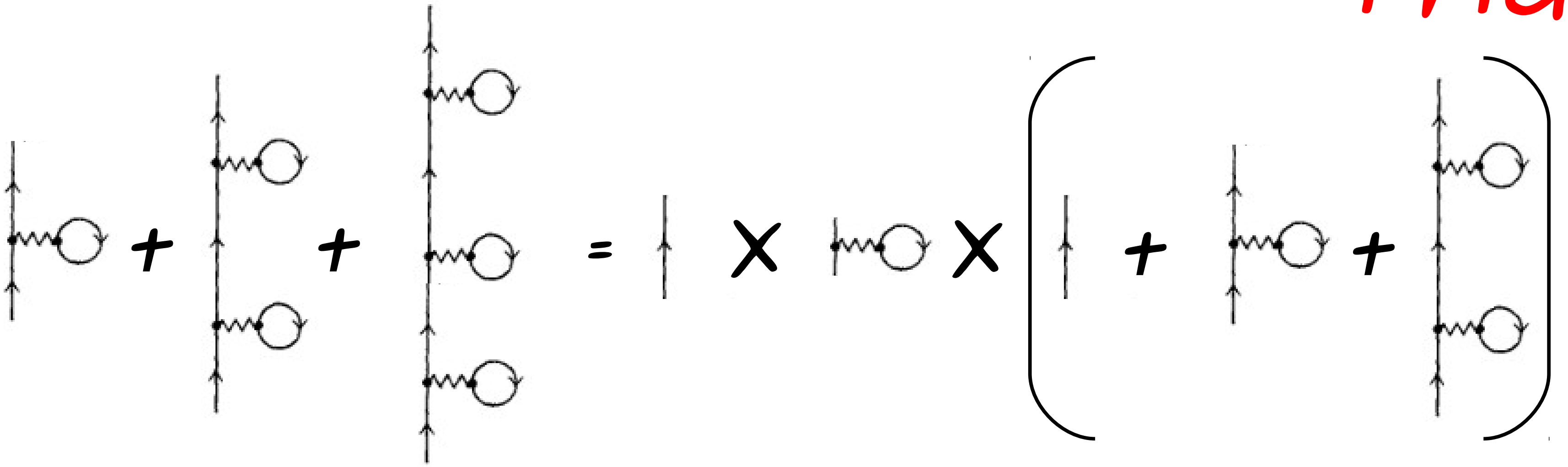
$$\langle n| = \overline{\left(|n\rangle\right)}$$

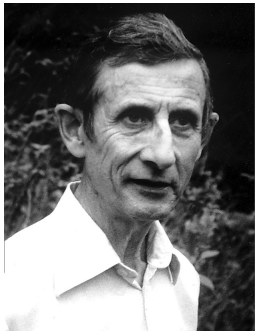
Today

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

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

Friday





Bra's, ket's and operators

Bra, Ket and operators (I)

A ket represents a physical state (atomic configuration, Bloch level,…) and it contains ALL we need to know about the state

"Ket"

$$|n\rangle$$

"Bra"

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

$$\langle n|m\rangle$$

$$\langle n|n\rangle = |n|$$

$$\sum_n |n\rangle\langle n| = 1$$

$$\vdots$$

Any observable is represented by an operator acting in the space of kets

$$\hat{A}|n\rangle = |n'\rangle$$

Bra, Ket and operators (II)

A space of kets can represent a basis to represent any mixed state belonging to the same space

$$|\Psi\rangle = \sum_n \Psi_n |n\rangle$$

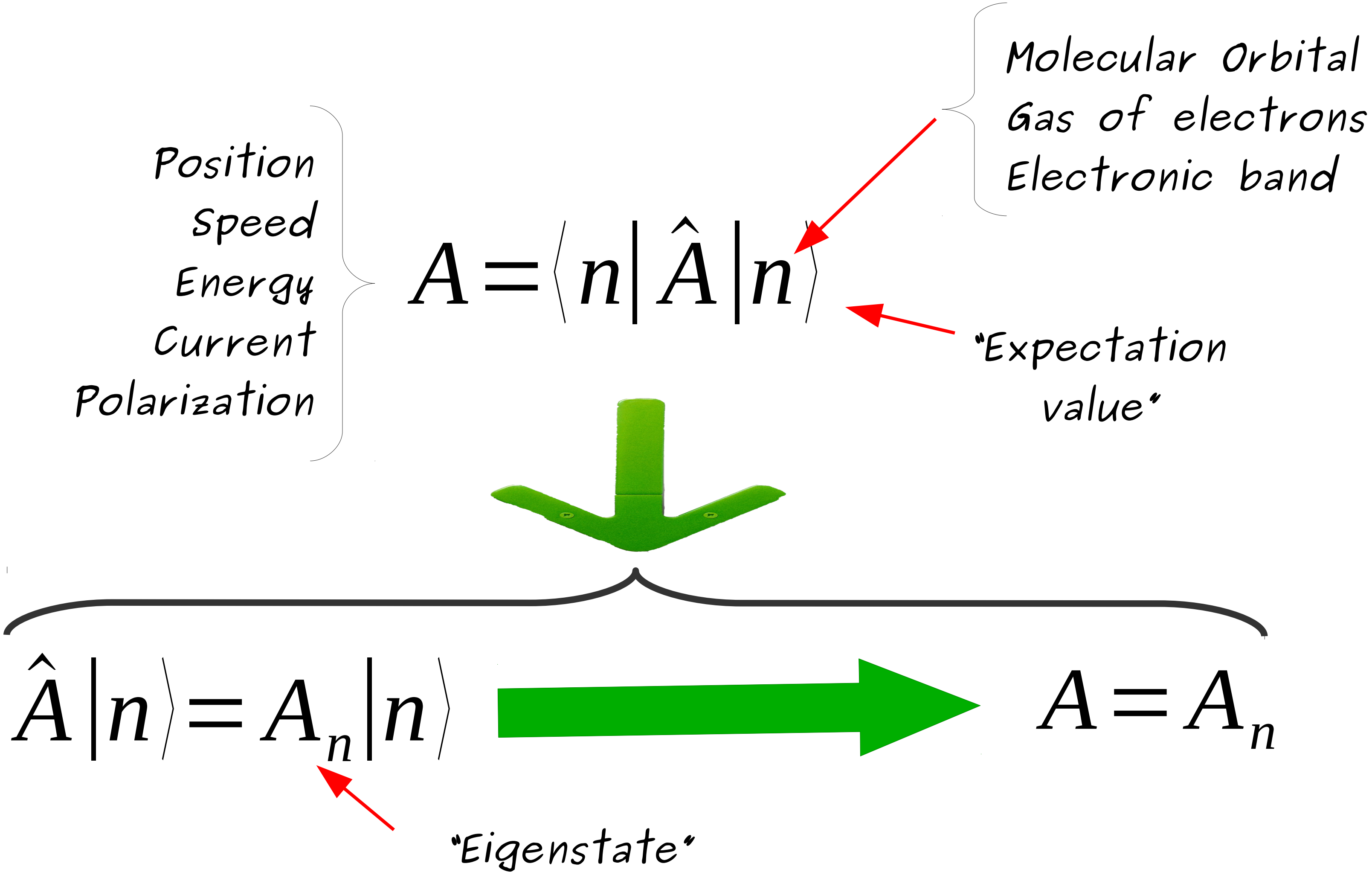
$$\langle m|n\rangle = \delta_{mn}$$

$$\Rightarrow$$

$$\langle m|\Psi\rangle = \Psi_m$$

$$\sum_n |n\rangle\langle n| = 1 \quad \Rightarrow \quad \hat{O} = \sum_{n,m} |n\rangle\langle n|O|m\rangle\langle m|$$

Observables and eigenstates



Position
Speed
Energy
Current
Polarization

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

Molecular Orbital
Gas of electrons
Electronic band

"Expectation value"

$$\hat{A}|n\rangle = A_n|n\rangle \longrightarrow A = A_n$$

"Eigenstate"

Schördinger and Heisenberg representations

$$|\Psi(t_0)\rangle \xrightarrow{\text{Time Evolution}} |\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$$

$$i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle$$ Schördinger equation

Time-Independent H

$$|\Psi_s(t)\rangle = \mathrm{e}^{-i\hat{H}(t-t_0)}|\Psi(t_0)\rangle \qquad U(t,t_0) = e^{-iH(t-t_0)}$$

States (Schördinger)

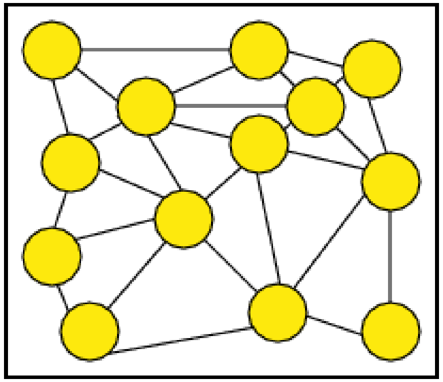
$$|\Psi_H(t)\rangle = \mathrm{e}^{i\hat{H}t}|\Psi_s(t)\rangle \qquad \hat{O}_H(t) = \mathrm{e}^{i\hat{H}t}\hat{O}\,\mathrm{e}^{-i\hat{H}t}$$

Operators (Heisenberg)

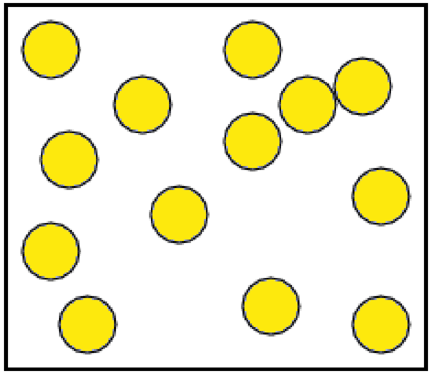
Independent Particle Approximation

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

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



$$|\Psi\rangle\approx\prod_n|n\rangle$$



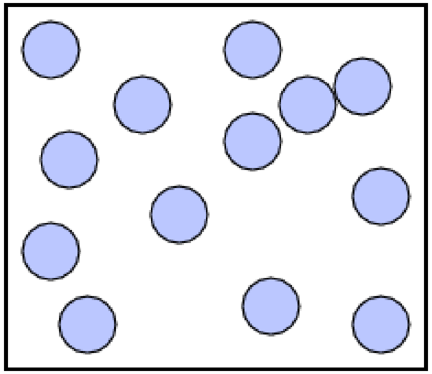
$$\hat{h}|n\rangle=\epsilon_n|n\rangle$$

$$|n(t)\rangle=e^{i\epsilon_n(t-t_0)}|n(t_0)\rangle$$

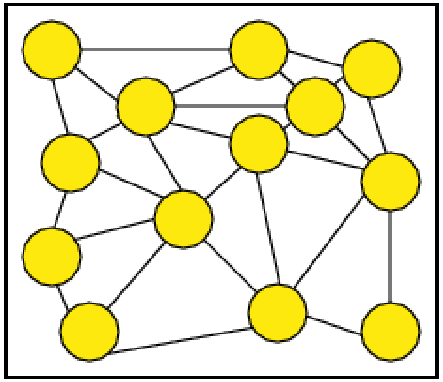
Independent-Particl
e Energy

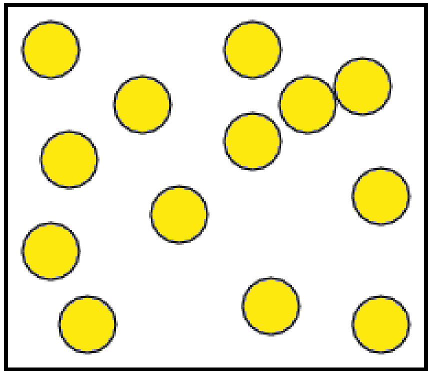
$$|\Psi(t)\rangle=e^{i(\sum_n\epsilon_n)(t-t_0)}|\Psi(t_0)\rangle$$

Perturbation Methods



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





The objective of all perturbative methods is to rewrite the fully interacting problem as an independent counter-part (h) corrected (somehow) by the interactions (H')

$$|\Psi\rangle \overset{?}{\approx} \sum_{m=0}^{\infty}\lambda^m\left|n^{(m)}\right\rangle$$

Introduction to Perurbation Methods: The limiting case of one-particle potentials

$$H \approx \sum_i \left(h\left(x_i\right) + \delta h\left(x_i\right) \right)$$

The two-level problem (I)

$$h+H'=E_1^{(0)}\left|1^{(0)}\right\rangle\left\langle 1^{(0)}\right|+E_2^{(0)}\left|2^{(0)}\right\rangle\left\langle 2^{(0)}\right|+V\left(\left|1^{(0)}\right\rangle\left\langle 2^{(0)}\right|+\left|2^{(0)}\right\rangle\left\langle 1^{(0)}\right|\right)$$

We want to find the states $|n\rangle$ such that:

$$h+H'=E_1|1\rangle\langle 1|+E_2|2\rangle\langle 2|$$

The problem can be solved by direct diagonalization of the matrix

$$\begin{pmatrix} E_1^{(0)} & V \\ V & E_2^{(0)} \end{pmatrix}$$

⇓

$$E_{1/2}=\frac{E_1^{(0)}+E_2^{(0)}}{2}\pm\sqrt{\frac{E_1^{(0)}-E_2^{(0)}}{4}+V^2}$$

The two-level problem (I)

$$H(\lambda)=h+\lambda H'$$

$$E_{1/2}(\lambda)=\frac{E_1^{(0)}+E_2^{(0)}}{2}\pm\sqrt{\frac{E_1^{(0)}-E_2^{(0)}}{4}+V(\lambda)^2}$$

$$\lambda V^2 \ll |E_1^{(0)}-E_2^{(0)}|$$

$$E_{1/2}(\lambda)=E_{1/2}^{(0)}\pm\frac{(V\lambda)^2}{E_1^{(0)}-E_2^{(0)}}+O(\lambda^4)$$

The question is: is it possible to obtain this power expansion without solving the full problem?

Static Perturbation Theory(I)

$$h+\lambda H' = \sum_n E_n^{(0)} |n^{(0)}\rangle\langle n^{(0)}| + \sum_{n,m} \lambda H'_{n,m} |n^{(0)}\rangle\langle m^{(0)}|$$

Now the PT is easily introduced by the following set of definitions

$$|n\rangle_\lambda = \sum_{m=0}^{\infty} \lambda^m |n^{(m)}\rangle$$

$$(h+\lambda H')|n(\lambda)\rangle\langle n(\lambda)| = E_n(\lambda)|n(\lambda)\rangle\langle n(\lambda)|$$

$$E_n(\lambda) - E^{(0)} = \sum_{m=0}^{\infty} \lambda^m \Delta E_n^{(m)}$$

$$|n(\lambda)\rangle \approx |n^{(0)}\rangle + \sum_{k\neq n} \frac{H'_{kn}}{E_n^{(0)}-E_k^{(0)}} + \dots$$

$$E_n(\lambda) \approx E_n^{(0)} + \lambda H'_{nn} + \sum_{k\neq m} \lambda^2 \frac{|H'_{nk}|^2}{E_n^{(0)}-E_k^{(0)}} + \dots$$

Static Perturbation Theory(II)

$$h+H'=E_1^{(0)}|1^{(0)}\rangle\langle 1^{(0)}|+E_2^{(0)}|2^{(0)}\rangle\langle 2^{(0)}|+V\left(|1^{(0)}\rangle\langle 2^{(0)}|+|2^{(0)}\rangle\langle 1^{(0)}|\right)$$

$$E_n(\lambda)\approx E_n^{(0)}+\lambda H'_{nn}+\sum_{k\neq m}\lambda^2\frac{|H'_{nk}|^2}{E_n^{(0)}-E_k^{(0)}}+\dots$$

V^2

0

$$E_{1/2}(\lambda)=E_{1/2}^{(0)}\pm\frac{(V\lambda)^2}{E_1^{(0)}-E_2^{(0)}}+O(\lambda^4)$$

By using PT I can find again the first order in the perturbative expansion of the exact solution

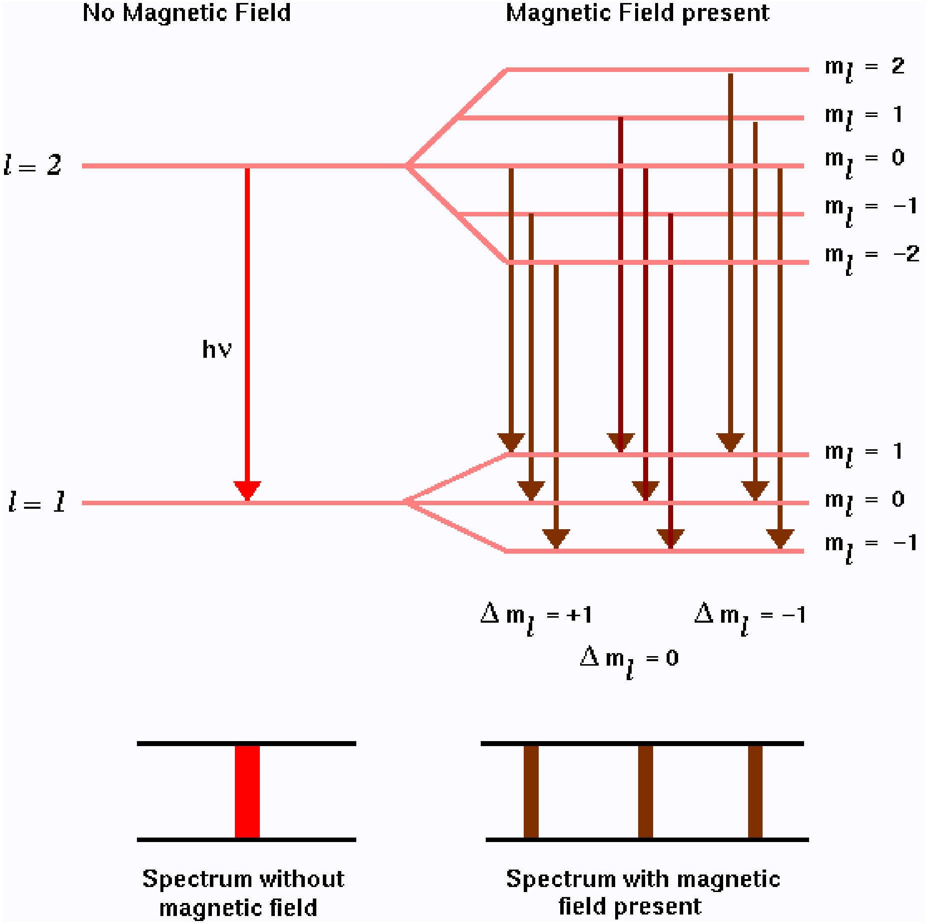
Static Perturbation Theory (III): The Zeeman Effect

$$H' \begin{cases} \text{Static Electric Field} \\ \text{Static Magnetic Field} \\ \text{Stress} \\ \dots \end{cases}$$

$$H'=-\vec{\mu}\cdot\vec{B}$$

$$\vec{\mu}=-\mu_B g\vec{J}$$

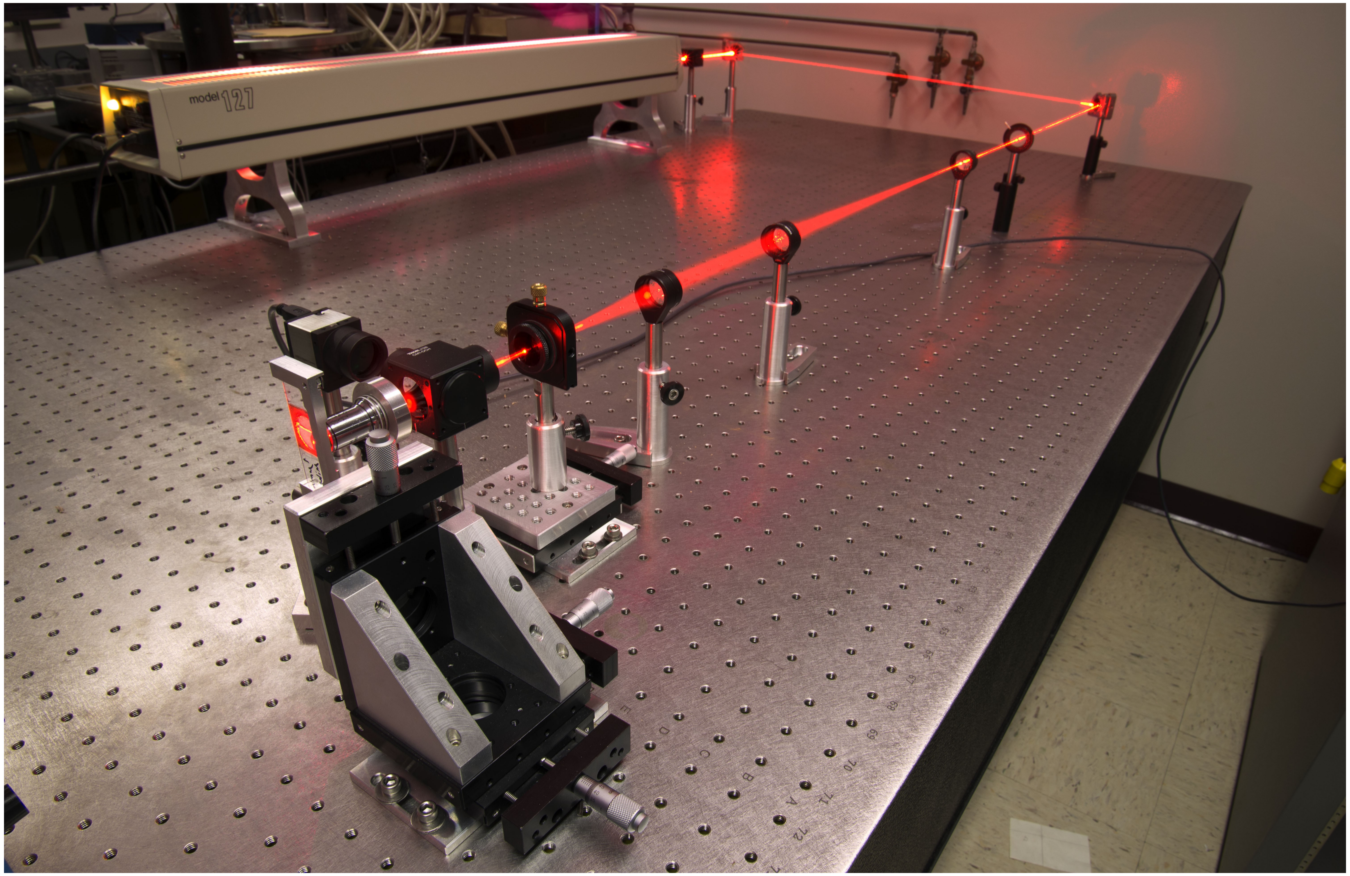
$$E_n(\lambda)\approx E_n^{(0)}+\lambda H'_{nn}$$



Time-Dependent Perturbation Theory

Time-Dependent Perturbation Theory (I)

$$H'(t) \propto \vec{r} \cdot \vec{E}(t)$$



Time-Dependent Perturbation Theory (II)

$$h+\lambda H'(t)=\sum_n E_n^{(0)}\left|n^{(0)}\right\rangle\left\langle n^{(0)}\right|+\sum_{n,m} H'_{n,m}(t)\left|n^{(0)}\right\rangle\left\langle m^{(0)}\right|$$

Interaction Representation

$$\left|n_I(t)\right\rangle=e^{iht}\left|n\right\rangle \qquad O_I(t)=e^{iht}\,O\,e^{-iht}$$

$$i\partial_t\left|n_I(t)\right\rangle=H'_I(t)\left|n_I(t)\right\rangle$$

$$\left|n_I(t)\right\rangle=\left|n_I(t_0)\right\rangle-i\int_{t_0}^{t}d\tau\,H_I'(\tau)\left|n_I(\tau)\right\rangle$$

$$\left|n_I(t)\right\rangle=\left|n_I\right\rangle-i\left|n_I\right\rangle\left(\int_{-\infty}^{t}d\tau\,H_I'(\tau)\right)$$

Time-Dependent Perturbation Theory (III)

$$|n_I(t)\rangle = |n_I\rangle - i|n_I\rangle\left(\int_{-\infty}^{t} d\tau\, H_I'(\tau)\right) \qquad |n_I(t)\rangle = \sum_m C_{nm}(t)|m\rangle$$

And now we expand again in powers of H'

$$C_{nm}(t)=\delta_{nm} - i\sum_\eta \int_{-\infty}^{t} \langle m|H'(t)|\eta\rangle C_{n\eta}(t)$$

$$\langle m|H_I'(t)|\eta\rangle = e^{i(E_\eta^{(0)}-E_m^{(0)})t}\langle m|H'|\eta\rangle$$

$$C_{nm}(t)=\delta_{nm} - i\sum_\eta \int_{-\infty}^{t} e^{i(E_\eta^{(0)}-E_m^{(0)})t}\langle m|H'|\eta\rangle C_{n\eta}(t)$$

Time-Dependent two level problem (I)

$$h+H'=E_1^{(0)}|1^{(0)}\rangle\langle 1^{(0)}|+E_2^{(0)}|2^{(0)}\rangle\langle 2^{(0)}|+\gamma\left(e^{i\omega t}|1^{(0)}\rangle\langle 2^{(0)}|+e^{-i\omega t}|2^{(0)}\rangle\langle 1^{(0)}|\right)$$

$$|1(t)\rangle=C_1(t)|1\rangle+C_2(t)|2\rangle$$

$$C_1(0)=1$$

$$C_2(0)=0$$

$$E_2>E_1$$

Boundary Conditions

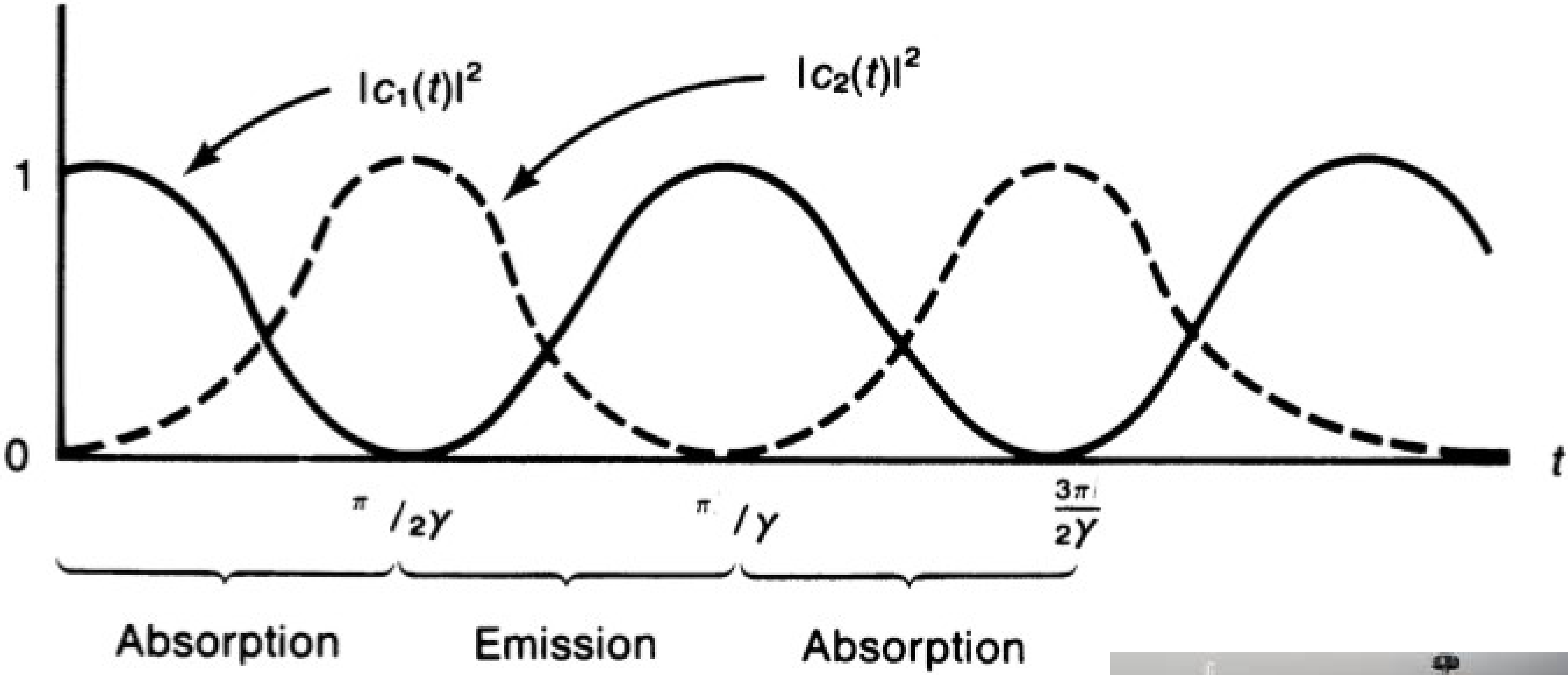
$$|c_2(t)|^2=\frac{\gamma^2}{\gamma^2+(\omega-\omega_{21})^2/4}\sin^2\left\{\left[\gamma^2+\frac{(\omega-\omega_{21})^2}{4}\right]^{1/2}t\right\}$$

$$\omega_{21}\equiv(E_2-E_1)$$

Time-Dependent two level problem (II)

Resonant Condition

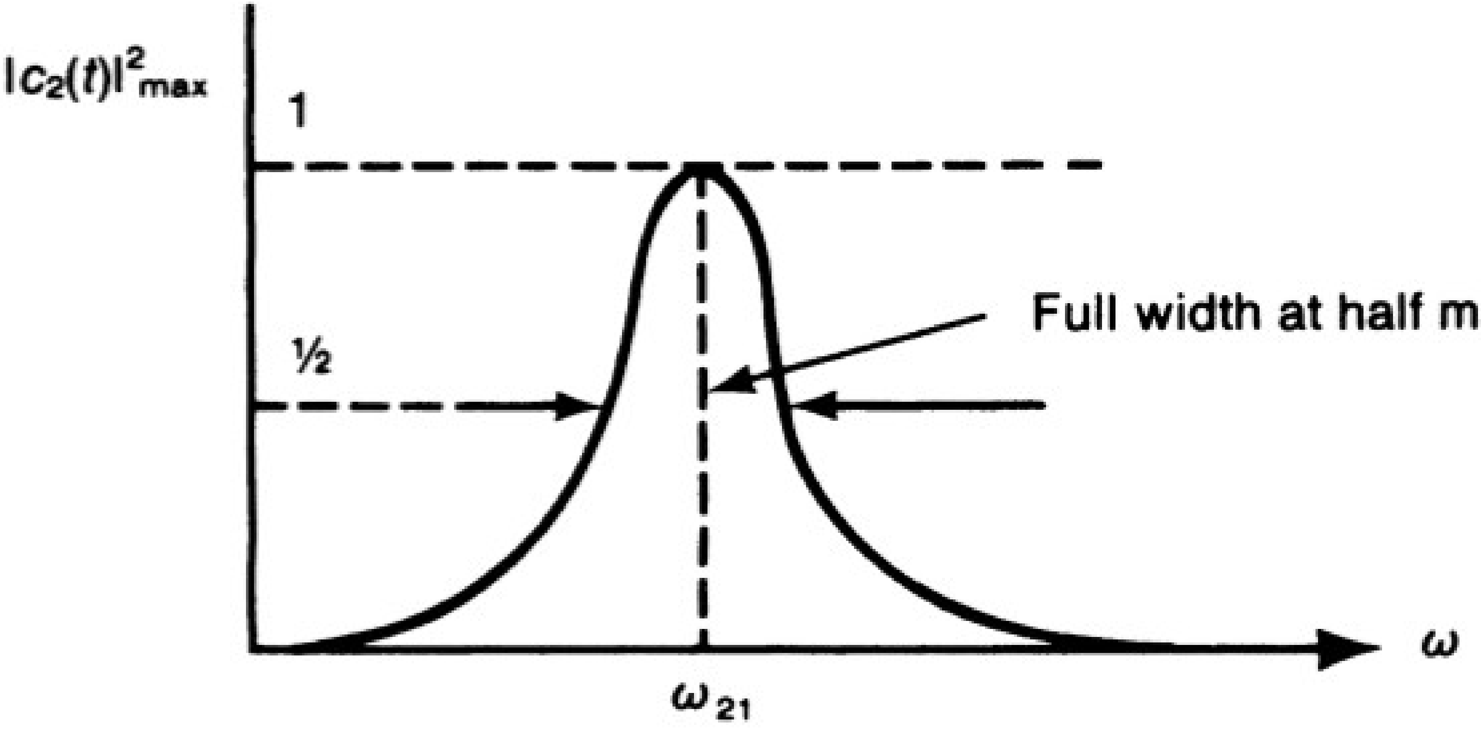
$$\omega \simeq \omega_{21} = (E_2 - E_1)$$



A maser (/ˈmeɪzər/) is a device that produces coherent electromagnetic waves through amplification by stimulated emission. The word "maser" is derived from the acronym MASER: "microwave amplification by stimulated emission of radiation".

Time-Dependent two level problem (III)

Resonant Condition ➡ $\omega \simeq \omega_{21} = (E_2 - E_1)$

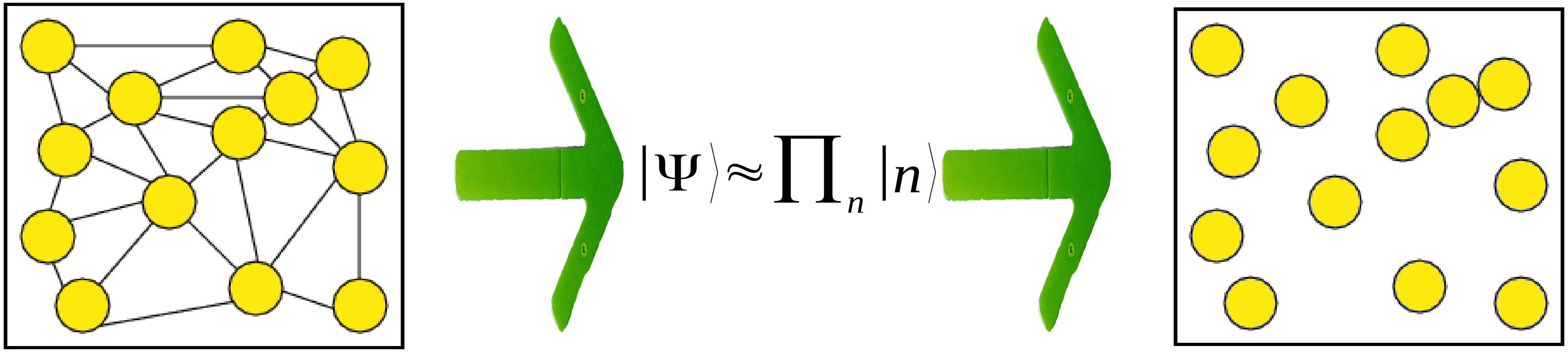


REAL many body interactions and
FICTITIOUS quasi-particles

Perturbation Theory for Many-Body Systems

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

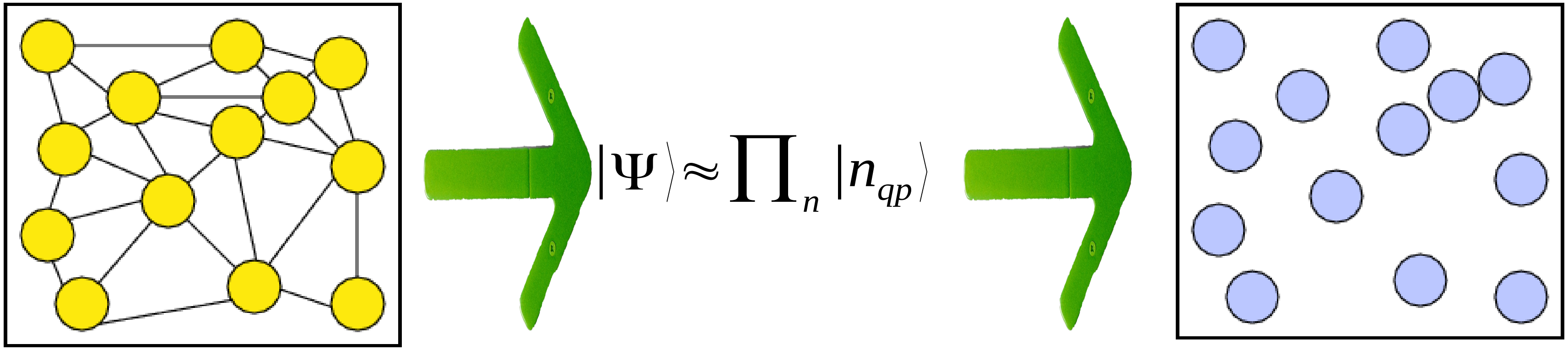
$$H=\sum_i h(x_i)$$



$$|\Psi\rangle\approx\prod_n |n\rangle$$

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

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



$$|\Psi\rangle\approx\prod_n |n_{qp}\rangle$$

Hartree-Fock

Hartree-Fock (I)

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

H'

$$|\Psi\rangle\approx\prod_n|n\rangle=|\Phi_0\rangle$$

$$\langle x_1\ldots x_N|\Phi_0\rangle\approx\sum_{Permutations}(-1)^P\prod_n\langle x_i|n\rangle$$

$\chi_n(x_i)$

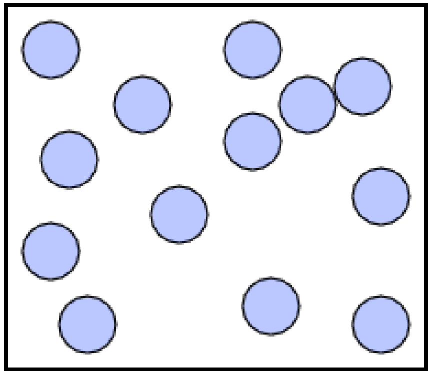
$$E_n(\lambda)\approx E_n^{(0)}+\lambda H'_{nn}+\sum_{k\neq m}\lambda^2\frac{|H'_{nk}|^2}{E_n^{(0)}-E_k^{(0)}}+\ldots$$

$$E_\Psi=\langle\Psi|H|\Psi\rangle\approx E_\Phi+\langle\Phi|H'|\Phi\rangle$$

Hartree-Fock (II)

$$E_\Psi = \langle \Psi | H | \Psi \rangle \approx E_\Phi + \langle \Phi | H' | \Phi \rangle$$

$$E_\Psi \approx \sum_n \left(\epsilon_n + \delta \epsilon_N^{HF} \right)$$



$$\delta \epsilon_i^{HF} \equiv \sum_{j \neq i} \left(\langle \chi_i | J_j(x) | \chi_i \rangle - \langle \chi_i | K_j(x) | \chi_i \rangle \right)$$

$$\mathcal{K}_j(\mathbf{x}_1)\chi_i(\mathbf{x}_1) = \left[\int d\mathbf{x}_2 \chi_j^*(\mathbf{x}_2) r_{12}^{-1} \chi_i(\mathbf{x}_2) \right] \chi_j(\mathbf{x}_1)$$

$$\mathcal{J}_j(\mathbf{x}_1) = \int d\mathbf{x}_2 |\chi_j(\mathbf{x}_2)|^2 r_{12}^{-1}$$

Hartree-Fock via Variational Methods (I)

If we concentrate on the fully interacting ground-state an approach alternative to perturbation theory is via variational minimization of the total Energy

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

The idea is to define a set of single-particle states such that the expectation value of H is minimal

$$\langle x_1 \dots x_N | \Phi_0 \rangle \approx \sum_{Permutations} (-1)^P \langle x_i | n \rangle$$

$$\Downarrow$$

$$\mathcal{L}[\{\chi_i\}] = E_{HF}[\{\chi_i\}] - \sum_{ij} \epsilon_{ij}(< i|j > - \delta_{ij})$$

$$E_{HF} \equiv \langle \Phi_0 | H | \Phi_0 \rangle$$

Hartree-Fock via Variational Methods (I)

$$\mathcal{L}[\{\chi_i\}] = E_{HF}[\{\chi_i\}] - \sum_{ij} \epsilon_{ij}(< i|j > -\delta_{ij})$$

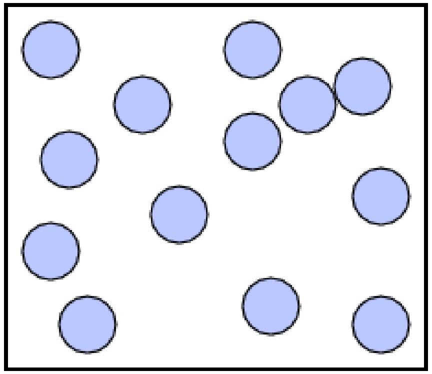
$$h(\mathbf{x}_1)\chi_i(\mathbf{x}_1) + \sum_{j\neq i}\left[\int d\mathbf{x}_2 |\chi_j(\mathbf{x}_2)|^2 r_{12}^{-1}\right]\chi_i(\mathbf{x}_1) - \sum_{j\neq i}\left[\int d\mathbf{x}_2 \chi_j^*(\mathbf{x}_2)\chi_i(\mathbf{x}_2) r_{12}^{-1}\right]\chi_j(\mathbf{x}_1) = \epsilon_i\chi_i(\mathbf{x}_1)$$

$$\left[h(\mathbf{x}_1) + \sum_{j\neq i}\mathcal{J}_j(\mathbf{x}_1) - \sum_{j\neq i}\mathcal{K}_j(\mathbf{x}_1)\right]\chi_i(\mathbf{x}_1) = \epsilon_i\chi_i(\mathbf{x}_1)$$

$$H = \sum_i \left(h(x_i) + \delta h_{HF}(x_i)\right)$$

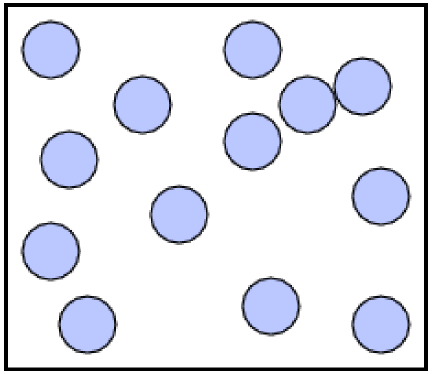
$$\mathcal{K}_j(\mathbf{x}_1)\chi_i(\mathbf{x}_1) = \left[\int d\mathbf{x}_2 \chi_j^*(\mathbf{x}_2) r_{12}^{-1}\chi_i(\mathbf{x}_2)\right]\chi_j(\mathbf{x}_1)$$

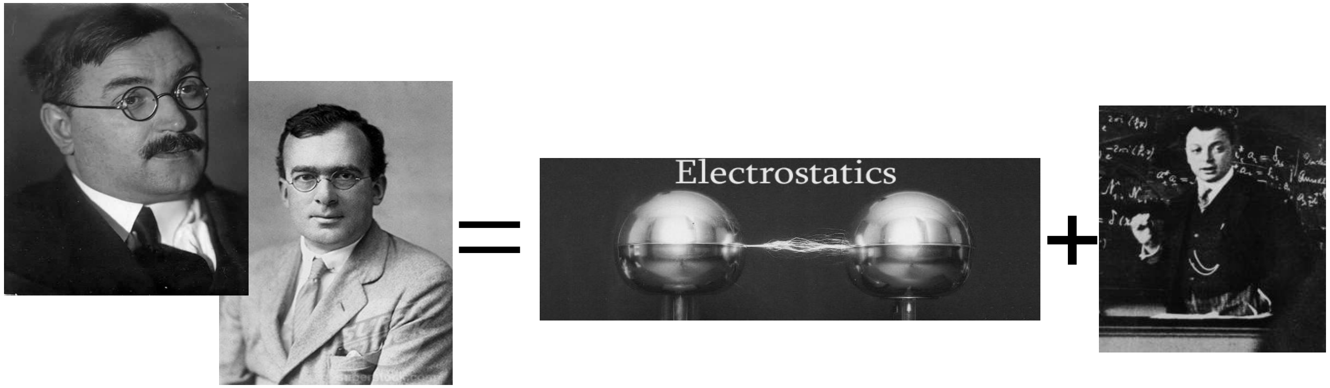
$$\mathcal{J}_j(\mathbf{x}_1) = \int d\mathbf{x}_2 |\chi_j(\mathbf{x}_2)|^2 r_{12}^{-1}$$



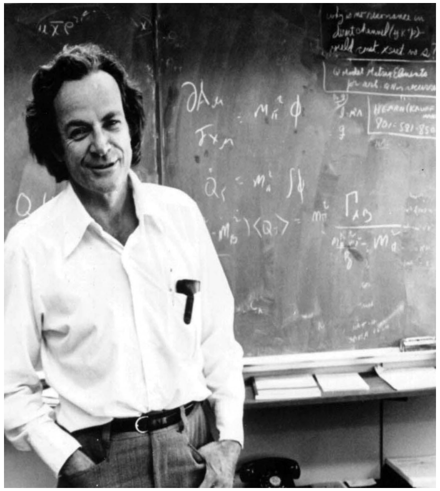
Hartree Fock…

$$H = \sum_i \left(h(x_i) + \delta h_{HF}(x_i) \right)$$

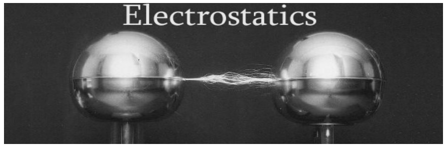




Hartree Fock lacks of CORRELATION



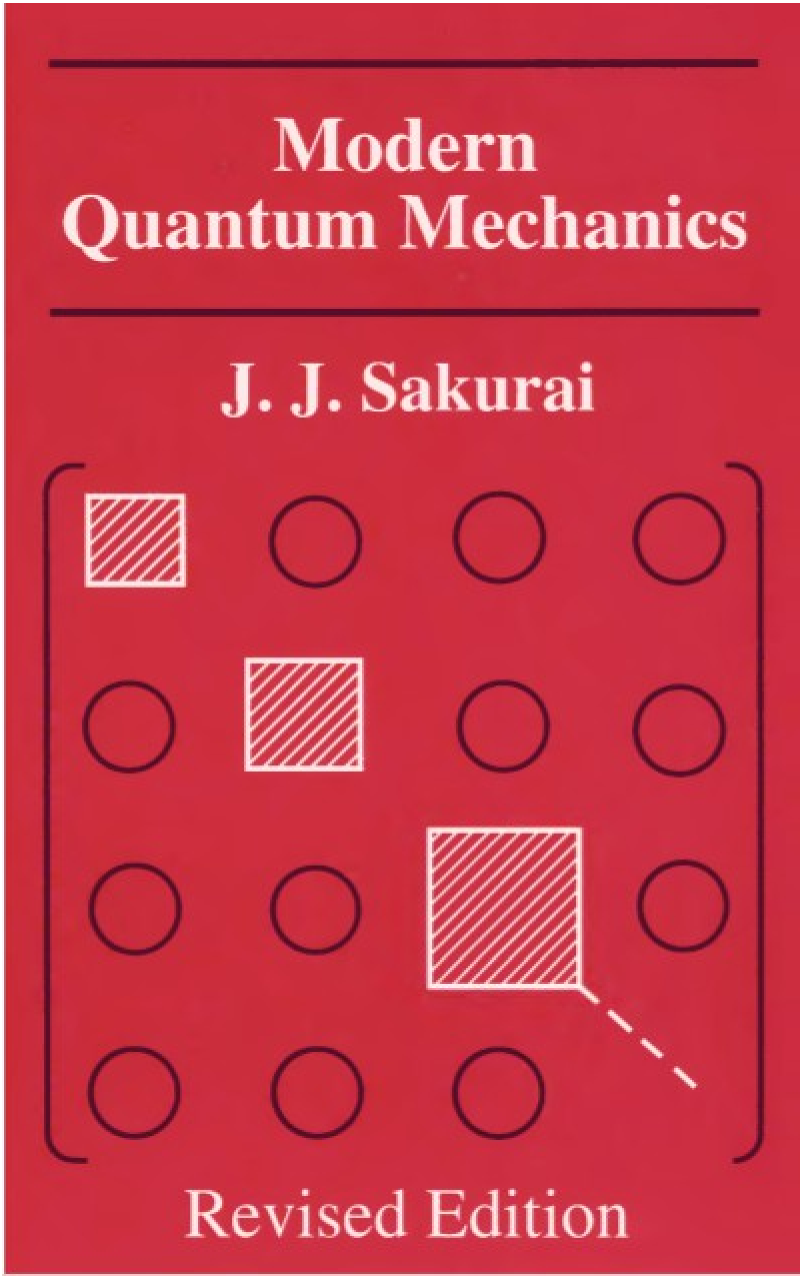
=



+

+

References



Modern
Quantum Mechanics

J. J. Sakurai

Revised Edition