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Many body Problem.

Bohr: Independent-particle-model
"Planetary" model of the atom (different of the true planetary motion)

Atoms: Hartree-Fock scheme.
Molecules: ″ ″ ″ ASP-MO-LCAO-SCF
Solid State Band Theory. (more general than H.F. scheme)
Nuclei Shell model - magic numbers.

Biological systems (aperiodic systems)

Schrödinger equations. (non-relativistic)

1) $\mathcal{H}_{op} \Psi = -\frac{h}{2\pi i} \frac{\partial \Psi}{\partial t}$

2) $\mathcal{H} \Psi = E \Psi$ Requirements. 1) $\int |\Psi|^2 (dx) = \text{finite}$.
2) Ψ finite everywhere.

the hamiltonian:

$$\mathcal{H}_{op} = \sum_i \mathcal{H}_i + \frac{1}{2!} \sum_{ij}{}' \mathcal{H}_{ij} + \frac{1}{3!} \sum_{ijk}{}' \mathcal{H}_{ijk} + \cdots\cdots$$

∞-order perturbation theory. diagram technique.
Feynman, Schwinger, Dyson, Hubbard, van Hove, ...
$\Psi(t)$ Evolution operator.
$\Psi(t) = U(t) \, \Psi(0)$
$\Psi(0)$ comes from the experimental situation.

Pauli suggests the knowledge of the prob. distribution in x and p.
1) and 2) are connected by Fourier transform. There are another important connection with Stat. Mech by the temperature trick.

Let's consider

$$\mathcal{H}\Psi = E\Psi$$

Partition technique

Ritz: Complete basis $\{f_\ell\}$

$$\Psi = \sum_\ell f_\ell c_\ell \qquad \text{assuming} \qquad \langle f_k | f_\ell \rangle = \delta_{k\ell}$$

Introducing $\mathcal{H}_{k\ell} = \langle f_k | \mathcal{H} | f_\ell \rangle$

we get $\mathbb{H}\mathbb{C} = E\mathbb{C}$ where $\mathbb{C} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$

$f_1, f_2, \ldots, f_n, \ldots$ spans the whole Hilbert space of the n particles,

We want to divide the space into the subspaces a and b by the operators O and P such that $O + P = 1$

$$\mathbb{H} = \begin{pmatrix} \mathbb{H}_{aa} & \mathbb{H}_{ab} \\ \mathbb{H}_{ba} & \mathbb{H}_{bb} \end{pmatrix} \qquad \mathbb{C} = \begin{pmatrix} \mathbb{C}_a \\ \mathbb{C}_b \end{pmatrix}$$

so we can get,

$$\mathbb{H}_{aa}\mathbb{C}_a + \mathbb{H}_{bb}\mathbb{C}_b = E\mathbb{C}_a$$
$$\mathbb{H}_{ba}\mathbb{C}_a + \mathbb{H}_{bb}\mathbb{C}_b = E\mathbb{C}_b$$

Solving:

$$\mathbb{C}_b = (E\cdot\mathbb{1}_{bb} - \mathbb{H}_{bb})^{-1}\mathbb{H}_{ba}\mathbb{C}_a$$

$$[\mathbb{H}_{aa} + \mathbb{H}_{ab}(E\mathbb{1}_{bb} - \mathbb{H}_{bb})^{-1}\mathbb{H}_{ba}]\mathbb{C}_a = E\mathbb{C}_a$$

we started from the S eq. for the entire Hilbert space.

$$\mathbb{H}\mathbb{C} = E\mathbb{C}$$

and we get

$$\mathcal{H}_{aa}\mathbb{C}_a = E\mathbb{C}_a$$

another S eq for finite dimensions.

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$$\mathcal{H}_{aa} = \mathbb{H}_{aa} + \mathbb{H}_{ab}(E\mathbb{1}_{bb} - \mathbb{H}_{bb})^{-1}\mathbb{H}_{ba}$$

Applications: ionic crystals, lattice vibrations.

Simple cases.

1) order of subspace $(a) = 1$

$$\mathcal{H}_{11}c_1 = Ec_1 \qquad \text{if} \quad c_1 \neq 0.$$

$$E = \mathcal{H}_{11} = H_{11} + \mathbb{H}_{1b}(E\cdot\mathbb{1}_{bb} - \mathbb{H}_{bb})^{-1}\mathbb{H}_{b1} \equiv f(E)$$

This is a condensed form of ∞-order perturbation theory.

Solution by recursion:

$$E^{(0)}, E^{(1)}, E^{(2)}, \ldots, E^{(k)}, E^{(k+1)}, \ldots \qquad E^{(k+1)} = f\{E^{(k)}\}$$

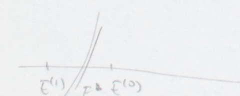
(iteration procedure)

This has bracketing behaviour. $E^{(k)}$ and $E^{(k+1)}$ brackets a true eigenvalue.

Write now:

$$E - f(E) = 0$$

To solve it we can use the Newton-Raphson formula which connects with the variation principle.



2) order of subspace $(a) = 2$

application: chemical bond. (we can get the Pauling concept of electronegativity)

This very useful for models in which the system is truncated or separated by our physical ideas.

Let's go back to relations betw. IPM and the many body system.
We separate out only one element:

$$\underbrace{f_1}_{a}, \underbrace{f_2, f_2, f_3, \ldots}_{b}$$

$$O + P = 1$$

Properties: $O^2 = O \qquad O^+ = O \qquad Tr(O) = 1$

$$P = 1 - O \quad \text{orthogonal complement.}$$

Φ = any trial function.

$O\Phi = \varphi \qquad$ (φ is our previous f_1)

$\langle\varphi|\varphi\rangle = 1 \quad$ equivalent to ~~then~~ $\quad \langle\Phi|O|\Phi\rangle = 1$

then

$$E = \langle\varphi|\mathcal{H} + \mathcal{H}\frac{P}{E-\mathcal{H}}\mathcal{H}|\varphi\rangle = \langle\Phi|O\mathcal{H}O + O\mathcal{H}\frac{P}{E-\mathcal{H}}\mathcal{H}O|\Phi\rangle$$

and $\quad \Phi = \varphi + \frac{P}{E-\mathcal{H}}\mathcal{H}\varphi = \left(O + \frac{P}{E-\mathcal{H}}\mathcal{H}O\right)\Phi$

This formalism does not distinguish betw. degenerate levels and non-degenerate.

Perturbation theory

$$\mathcal{H} = \mathcal{H}_0 + V$$

V not necessarily small.

From $\mathcal{H}_0\varphi_0 = E_0\varphi_0$

we can construct our project. $O\Phi = \varphi_0$

then: $\mathcal{H}_0 O = E_0 O$

$\qquad O\mathcal{H}_0 = E_0 O$

Applications. Schrödinger treatment of the Stark effect

London & Eisenschitz theory of van der Walls forces. etc

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Note: $P = 1 - O$ then $OP = PO = 0$

Using this property:

$$E = \langle\varphi_0|E_0 + V + V\frac{P}{E-\mathcal{H}}V|\varphi_0\rangle$$

$$\Phi = \left(1 + \frac{P}{E-\mathcal{H}}V\right)\varphi_0$$

This the essential of the modern many body problem approach.

Reaction operator. $\quad V + V\frac{P}{E-\mathcal{H}}V = t$

$$1 + \frac{P}{E-\mathcal{H}}V = W = \text{wave operator.}$$

$$E = E_0 + \langle\varphi_0|t|\varphi_0\rangle$$

$$\Phi = W\varphi_0$$

this looks like 1st order perturbation theory since

$$\langle\mathcal{H}\rangle = \langle\varphi_0|\mathcal{H}_0 + V|\varphi_0\rangle = E_0 + \langle\varphi_0|V|\varphi_0\rangle$$

Defining $\quad T = \frac{P}{E-\mathcal{H}}$

Reaction operator:

$$t = V + V\frac{P}{(E_0 - \mathcal{H}_0) - (V - \langle t\rangle_0)}V$$

or: $\quad t = VW$

Notice: in fact $\frac{P}{E-\mathcal{H}}$ is a short hand for the operator.

$\cancel{P\left(\alpha O + P\frac{1}{E-\mathcal{H}}\right)P} \qquad P\left(\alpha O + P(E-\mathcal{H})P\right)^{-1}P$

Brueckner theory:

$$\mathcal{H}_{op} = \sum_i \mathcal{H}_i + \sum_{i<j} \mathcal{H}_{ij} + \sum_{i<j<k} \mathcal{H}_{ijk} + \dots$$

$$= \overbrace{\sum_i (\mathcal{H}_i + u_i)}^{\mathcal{H}_0} - \overbrace{\sum_i u_i + \sum_{i<j} \mathcal{H}_{ij} + \sum_{i<j<k} \mathcal{H}_{ijk} + \dots}^{V}$$

at our disposal.

$$\mathcal{H}_{op} = \mathcal{H}_0 + V$$

V is the perturbation.

Hartree: $\delta \langle \mathcal{H} \rangle = 0$. (variation principle)

the best value for energy.

$$\sum_i (\mathcal{H}_i + u_i)\varphi_0 = E_0 \varphi_0 \qquad \varphi_0 = \psi_1 \psi_2 \dots \psi_N.$$

$$(\mathcal{H}_i + u_i)\psi_i = \epsilon_i \psi_i \qquad E_0 = \epsilon_1 + \epsilon_2 + \dots + \epsilon_N$$

~~Exact SCF~~

$$\cancel{E = E_0 + \langle \varphi_0 | t | \varphi_0 \rangle}$$

~~Hartree ...~~

$$u_i = \underbrace{u_i^{(2)}}_{\text{two body}} + u_i^{(3)} + \dots$$

$$u_i^{(2)} = \sum_{j \neq i} (\Psi_j | \mathcal{H}_{ij} | \Psi_j)$$

$$u_i^{(3)} = \frac{1}{2} \sum_{jk \neq i}{}' \langle \Psi_j \Psi_k | \mathcal{H}_{ijk} | \Psi_j \Psi_k)$$

Exact SCF

$$E = E_0 + \langle \varphi_0 | t | \varphi_0 \rangle$$

$$t = -\sum_i u_i + \tau = -\sum_i u_i + \sum_{i<j} \tau_{ij} + \sum_{i<j<k} \tau_{ijk} + \dots$$

$$u_i^{(2)} = \sum_{j \neq i} (\psi_j | \tau_{ij} | \psi_j)$$

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$$u_i^{(3)} = \frac{1}{2!} \sum_{j,k \neq i}{}' (\psi_j \psi_k | \tau_{ijk} | \psi_j \psi_k)$$

Then: Hartree $\tau = \sum_{i<j} \mathcal{H}_{ij} + \sum_{i<j<k} \mathcal{H}_{ijk} + \dots$

Brueckner $\tau = \sum_{i<j} \tau_{ij}$

$$E = E_0 + \langle \varphi_0 | t | \varphi_0 \rangle = \langle \varphi_0 | \sum_i (\mathcal{H}_i + u_i) + t | \varphi_0 \rangle =$$

$$= \langle \varphi_0 | \sum_i \mathcal{H}_i + \tau | \varphi_0 \rangle = \langle \varphi_0 | \sum_i \Big(\mathcal{H}_i + \tfrac{1}{2} u_i^{(2)} + \tfrac{1}{3} u_i^{(3)} +$$

$$+ \tfrac{1}{4} u_i^{(4)} + \dots + \tfrac{1}{N} u_i^{(N)} \Big) | \varphi_0)$$

This is not an upper bound of the energy but the energy itself.

$$(\mathcal{H}_i + u_i)\psi_i = \epsilon_i \psi_i$$

without the coefficients we counted wrongly the many particle interactions for example: ~~...~~ $\frac{1}{2}$ without the $\frac{1}{2}$ the two body interactions would be counted twice.

$$\varphi_0 = \psi_1 \psi_2 \psi_3 \dots \psi_k \dots \psi_N$$

$$\varphi_{se} = \psi_1 \psi_2 \psi_3 \dots \psi'_k \dots \psi_N \qquad \psi'_k \perp \psi_k \text{ (single excited state)}$$

then: Hartree $\langle \varphi_{se} | V | \varphi_0 \rangle = 0$, $\langle \varphi_{se} | \mathcal{H} | \varphi_0 \rangle = 0$

Brueckner $\langle \varphi_{se} | t | \varphi_0 \rangle = 0$ ~~...~~

$\Psi = \varphi_0 +$ doubly excited terms and higher

Calculations

$$\begin{tikzcd}
 & V \arrow[r] & t \arrow[r] & \tau \arrow[dr] & \\
u_i \arrow[ur] \arrow[rr] & & (\mathcal{H}_i + u_i) \arrow[rr] & & \psi_i \arrow[llll, bend left]
\end{tikzcd}$$

Some recent developments in the many-body problem.

D. Ter Haar.

Summary.

1.- Introduction

2.- The general state of theoretical Physics.

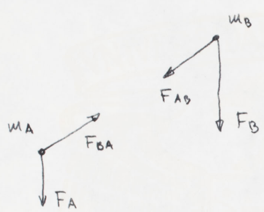

Fig. 1. Motion of two interacting particles in a common uniform gravitational field.

$$\underline{F}_{AB} + \underline{F}_{BA} = 0 \qquad (1)$$

$$\underline{F}_{AB} = - \underline{F}_{BA} = -\nabla_B U_{AB} = \nabla_A U_{AB} \qquad (2)$$

$$\underline{F}_A = m_A \underline{g} \qquad \underline{F}_B = m_B \underline{g} \qquad (3)$$

$$m_A \ddot{\underline{x}}_A = -\nabla_A U_{AB} - \nabla_A U \qquad m_B \ddot{\underline{x}}_B = -\nabla_B U_{AB} - \nabla_B U \qquad (4)$$

$$(m_A + m_B)\, \underline{X} = m_A \underline{x}_A + m_B \underline{x}_B \qquad \underline{x} = \underline{x}_A - \underline{x}_B \qquad (5)$$

$$M \ddot{\underline{X}} = M \underline{g} \qquad (6a)$$

$$\mu \ddot{\underline{x}} = -\nabla U_{AB} \qquad (6b)$$

$$M = m_A + m_B \qquad \mu = \frac{m_A m_B}{M} \qquad (7a)$$

3. Collective behaviour and quasi-particles.

$$H = H(\underline{x}_1, \ldots, \underline{x}_N, \underline{p}_1, \ldots, \underline{p}_N) \qquad (7b)$$

$$H(\xi_1, \ldots, \xi_{3N}; \pi_1, \ldots, \pi_{3N}) = \sum H_j(\xi_j, \pi_j) \qquad (8)$$

$$H(\xi_1, \ldots, \xi_{3N}; \pi_1, \ldots, \pi_{3N}) = \sum H_j(\xi_j, \pi_j) + H'(\xi_1, \ldots, \xi_{3N}; \pi_1, \ldots, \pi_{3N}) \qquad (9)$$

$$H_{com} = \frac{\underline{P}^2}{2M} + \underline{g} \cdot \underline{X} \qquad (10)$$

$$H_{rel} = \frac{\underline{p}^2}{2\mu} + U_{AB}(\underline{x}) \qquad (11)$$

$$H = \sum_j \frac{p_j^2}{2m_j} + \sum_j U(\underline{x}_j) + \frac{1}{2} \sum_{j \neq n} U_{jn}(\underline{x}_j, \underline{x}_n) \qquad (12)$$

$$H' = \sum_j H_j \quad , \quad H_j = \frac{p_j^2}{2m_j} + U(\underline{x}_j) + V_j(\underline{x}_j) \qquad (13)$$

$$H' = \sum_j \frac{p_j^2}{2\mu'} + \frac{1}{2} \sum_j U_{jn}(\underline{x}_j, \underline{x}_n) \qquad (14)$$

$$H'' = \sum_j \frac{p_j^2}{2\mu} \qquad (15)$$

$$H = H_{coll} + H_{part} + H_{int} \qquad (16)$$

$$H_{coll} = H_{coll}(\xi, \pi) \qquad (17)$$

$$H_{part} = H_{part}(x, p) \qquad (18)$$

$$H_{coll} = \sum_j \tfrac{1}{2} A_j \pi_j^2 + \sum_j f_j(\xi_j) \qquad (19)$$

$$f_j = \tfrac{1}{2} B_j \xi_j^2 \qquad (20)$$

(energy packets $h\nu_j$, where $(2\pi\nu_j)^2 = B_j A_j$)

4. Applications.

5. Conclusion:

List of quasi-particles:

Quasi-particle.	Brief description.
Total mass of system	Particle considered in calculating center of mass motion.
Reduced mass	✓ ✓ ✓ ✓ relative motion.
Conduction electron.	Electron surrounded by "cloud of interaction" with lattice
Hole	Conduction electron with a negative effective mass.
Electron	Electron surrounded by "cloud of int" with electr. mag. field
Phonon	Lattice vibration, sound wave.
Exciton	Electron-hole pair which is bound together.
Polaron	Conduction electron surrounded by a "polarization" cloud.
Spin-wave.	State in a ferromagnetic in which a "wrong" spin is distributed over the lattice.
Plasmon	Sound wave in a system of charged particles (i.e in a plasma)
Roton	Excitation in liquid helium.