10-09-19_AESCM_lesson-06

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1 AESCM lesson 06

- **Hour: 2**
- **Professor: Pere Alemany**

1.1 Independent particle approximation for the N-electron problem

There are two basic **delicious flavors** of independent electron approximations where electrons are not correlated (expect for they must obey Pauli's principle). - Non-interacting (Hartree-like) - Hartree-Fock

1.1.1 Non-interacting (Hartree-like) electron approximations

In non-interacting theories there isn't any explicit interaction term! (although the potential includes it to a certain extent).

All calculations based on the Kohn-Sham methods consider a non-interacting Hamiltonian.

In Hartree-like methods there's no need to construct an antisymmetric wave function literally!

The GS is found by occupying the levels following the exclusion principle.

Expectation values

N-electron states are specified by the set of occupation numbers $n_1^0 = 0, 1$ of independent particle states with energies ϵ_1^0

1.2 The periodic nature of $V_{ext}(R)$

In a macroscopic sample of a material, N is within the order of 10^{23} (which is a very big lot, the N-electron problem cannot be solved even with the indpendent particle approximation).

However, we can take advantage of the fact that many solids have periodic structures in the shape of **crystal lattices** to reduce the calculation of N independent electron equations to KN_{cell} independent electron equations within one single unit cell.

1.2.1 The lattice of translations

The set of all translations forms a lattice of points in space in which any translation can be written as integral multiples of a set of primitive vectors.

The choice of primitive vectors is not unique!! It's enough if they cover all lattice points.

1.2.2 The 14 Bravais lattices in 3D space

1.3 The basis of atoms

Lattice points are obtained by applying the translation vectors to a reference point.

Atomic positions in a basis of S atoms are given by a set of vectors $\{\tau_i\}_S$ defined relative to any point in the lattice

1.3.1 Bloch functions and bands of eigenvalues

1.3.2 Conservation of crystal momentum

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