

# Many-body situation.

If a body of mass " $m_1$ " moving in a force field, which is uncoupled.

(Their motion will not be changed by the presence of other balls)

By knowing the force on the ball at every point in space.

using Newton's Law.  $\leftarrow$  Problem. moving in an external field at time.

Now take the other body " $m_2$ " not attached is with " $m_1$ " by a spring. There is no force b/w the balls, naturally, But if some one stretched or compressed the spring, so mass " $m_1$ " will exert a force on " $m_2$ " and vice versa. So now one can not solve the trajectories of the ball A and B respectively - But the motion of the balls is still described perfectly well by Newtonian mechanics.

at every point in space  
It does not matter that the field is varying as long as long as  
the position or velocity of the ball

But the motion of A and B is linked with  $m_2$

Their equation of motions are coupled and must be solved simultaneously.

It is true that the balls still holds the Newton's Law, but the solution of the equation will not be easily calculate, because of the coupled motion. This thing leads to many-body problem.

However, it can be that if the <sup>masses</sup> balls are not connected by springs, then what will be happen?

The answer is, ~~bodies~~ <sup>bodies</sup> are like the electrons moving, as a single particles until they collide with each other. Now the problem is easy, first we will solve the equation of motion for a single particles individually, Thus we don't need to solve any <sup>until</sup> equation simultaneously, <sup>such times as they instantaneously scatter off each other.</sup>

But, this is not correct 100% did  
to describe these particles simply as  
single particles ~~that~~ because, in this case  
we are ignoring the effect of interaction  
b/w them when they collide to each  
other - so these are the quasi-particles. <sup>and scattering</sup>

• The appropriate Hamiltonian.

A solid can be described as  
a collection of heavy, positively-charged  
particles (nuclei) and lighter, negatively-charged  
particles (electrons). Each nucleus has a charge  
of  $Ze$ , where  $Z$  is the atomic number  
and  $e$  is the electronic charge. A system  
with  $N$  nuclei thus leads to a problem of

$N + ZeN$  interacting particles. This is a many-body  
problem, and demands a quantum mechanical  
approach because of the small mass of

the particles - called quantum many-body problem.

The exact many particle Hamiltonian for this many body system can be written as.

$$\hat{H}_{\text{Tot}} = \hat{T}_e(\vec{r}_i) + \hat{T}_N(\vec{R}_\alpha) + \hat{V}_{ee}(\vec{r}_i, \vec{r}_j) + \hat{V}_{NN}(\vec{R}_\alpha, \vec{R}_\sigma) + \hat{V}_{eN}(\vec{r}_i, \vec{R}_\alpha) \quad \text{--- (1)}$$

where.

$$\hat{T}_e(\vec{r}_i) = -\frac{\hbar^2}{2} \sum_i \frac{\nabla_{\vec{r}_i}^2}{m_e} \quad \text{is the kinetic energy operator for the electron; } m_e$$

is the mass of the electron at position  $\vec{r}_i$

$$\hat{T}_N(\vec{R}_\alpha) = -\frac{\hbar^2}{2} \sum_{\alpha} \frac{\nabla_{\vec{R}_\alpha}^2}{M_N} \quad \text{--- kinetic energy operator for the nucleus. } M_N \text{ --- mass of } \vec{R}_\alpha$$

$$\hat{V}_{ee}(\vec{r}_i, \vec{r}_j) = \frac{1}{4\pi\epsilon_0} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \quad \text{, Coulomb interaction b/w electrons and electrons.}$$

interaction b/w electrons and electrons.

$$\hat{V}_{NN} = \frac{1}{4\pi\epsilon_0} \sum_{\alpha \neq \sigma} \frac{e^2 z_\alpha z_\sigma}{|\vec{R}_\alpha - \vec{R}_\sigma|} \quad \text{b/w nuclei and nuclei}$$

where.

$z_\alpha$  is the charge on nucleus at position  $\vec{R}_\alpha$   
 and  $z_\sigma$  " " " " " "  $\vec{R}_\sigma$

$V_{eN} = -\frac{1}{4\pi\epsilon_0} \sum_{ij} \frac{e^2 Z_i Z_j}{|R_i - R_j|}$  - b/w.  $\bar{e}$  and Nuclei (7)  
 It is important to note that the kinetic and electron-electron terms in our

we can not solve this Hamiltonian exactly for the interaction particles system. In order to calculate the physically acceptable solutions which are the approximate eigenstates, we will use some approximations.

### Born-Oppenheimer Approximation

In the light of the Born-Oppenheimer approximation, we assume that the nuclei are much heavier, and therefore much slower than electrons. Hence nuclei can stay effectively frozen at fixed positions with only electrons being considered as mobile. The nuclei are deprived from this status, and reduced to a given source of positive charge, they become external to the electron cloud.

After applying this approximation, now we are dealing with a collection  $NZ$  interacting negative particles moving in the (given or external) potential of the nuclei.

Thus as the consequence of Born-Oppenheimer approximation on equ (0), the kinetic energy of the nuclei is zero and the ~~first~~<sup>2nd</sup> term disappears. The potential  $\hat{V}_{NN}(\bar{R}_X)$  term also reduced to a constant. We are then left with the kinetic energy of the electron gas, the potential energy due to electron-electron interaction and the potential energy of the electrons in the external potential of the nuclei. Therefore, the Hamiltonian operator  $\hat{H}$ , equ (1) now has only three terms: The kinetic energy of the electrons ( $\hat{T}_e$ ), the electron-electron interaction ( $\hat{V}_{ee}$ ) and the electron-nuclear ( $\hat{V}_{eN}$ ) interaction.