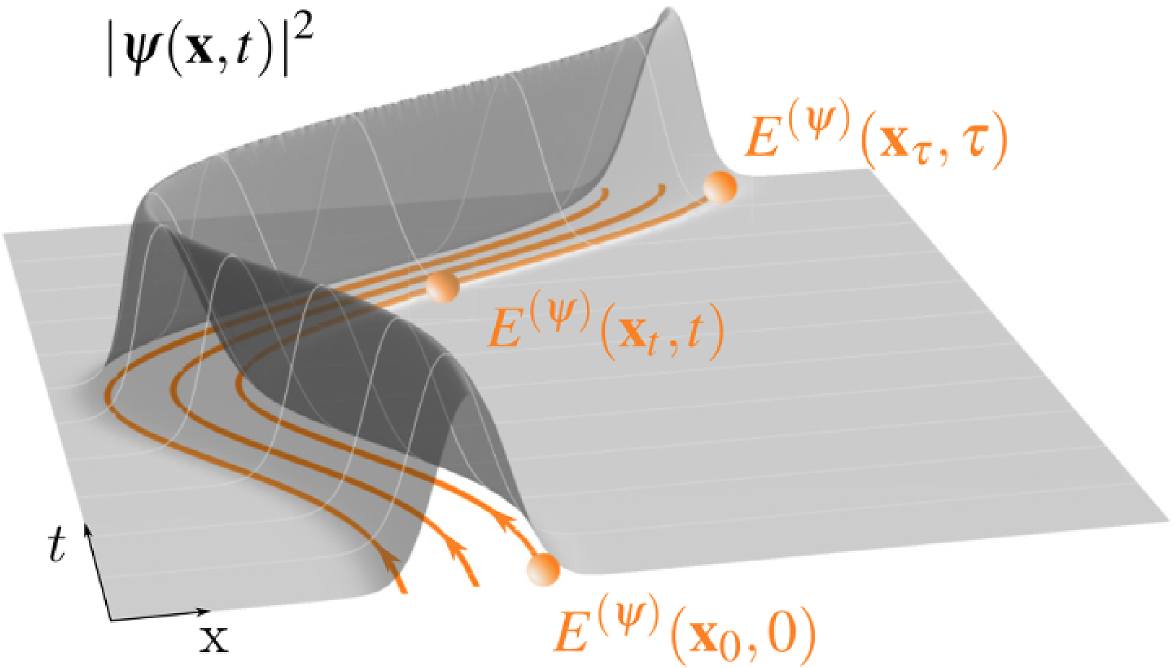
PHYS-C0252 - Quantum Mechanics Part 2
16.11.2020-04.12.2020

Tapio.Ala-Nissila@aalto.fi



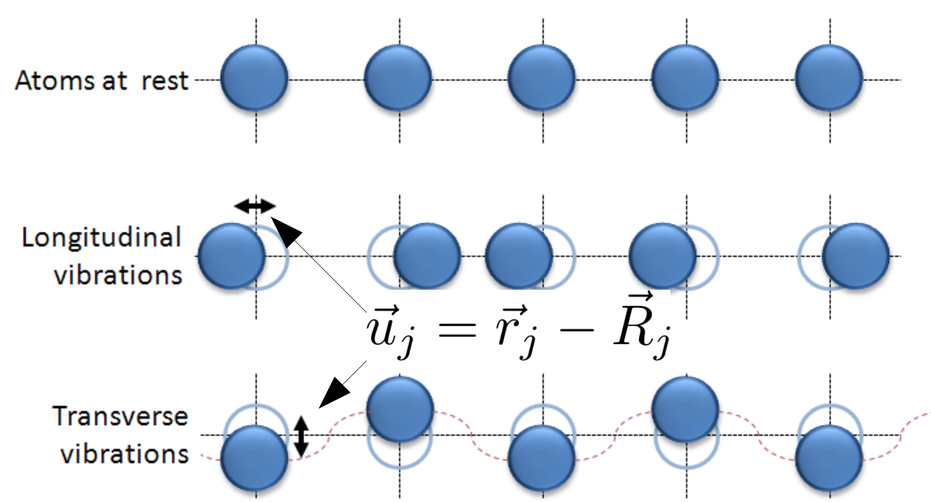
1. Harmonic Oscillators

1.1 Classical Harmonic Oscillators

- Harmonic oscillators appear in *many applications* in physics (lattice vibrations i.e. phonons, photons etc.)
- For interacting atoms in a classical solid lattice we can write in general

$$H = \sum_{i=1}^{N} \frac{\vec{p_i}^{\,2}}{2m} + V(\vec{r_1}, \vec{r_2}, \ldots, \vec{r_N})$$

Ideal lattice positions $\vec{R}_j$



For *small displacements* $\vec{u}_j = \vec{r}_j - \vec{R}_j$ around the equilibrium positions $\vec{R}_j$ the interaction potential can be expanded in Taylor series as

$$V \approx V_0 \sum_{i,j} \underbrace{\frac{\partial V^j}{\partial x_i}}_{=0} u_{x_{ij}} + \frac{1}{2} \sum_{i,j;k,l} \frac{\partial^2 V^{kl}}{\partial x_i \partial x_j} u_{x_i k} u_{x_j l}$$

which is called the Harmonic Approximation

- By diagonalizing (in normal coordinates) the classical harmonic Hamiltonian can be written as

$$H(q_1,\ldots,q_N,p_1,\ldots,p_N)=\sum_{i=1}^{3N}\left(\frac{p_i^2}{2m}+\frac{1}{2}m\omega^2 q_i^2\right)$$

for identical *but distinguishable* particles in 3D space.

- The equations of motion can be obtained from the standard Hamilton equations as

$$\dot{p}_i=-\frac{\partial H}{\partial q_i}$$

$$\dot{q}_i=\frac{\partial H}{\partial p_i}$$

- The equations of motion are linear and can be easily solved (1D homework problem)...

1.2 Quantum Harmonic Oscillators

- Consider a single 1D QHO whose Hamiltonian is given by

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{Q}^2$$

which we have obtained by simple quantization from the classical Hamiltonian as $x \to \hat{Q}, p \to \hat{P}$ where

$$[\hat{Q}, \hat{P}] = \imath\hbar$$

Next it is useful to define adimensional operators as

$$\hat{q} \equiv \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} \hat{Q}; \;\; \hat{p} \equiv \left(\frac{1}{m\hbar\omega}\right)^{\frac{1}{2}} \hat{P}$$

which now satisfy

$$[\hat{q}, \hat{p}] = \imath$$

This gives us the Hamiltonian

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{p}^2 + \hat{q}^2)$$

The next trick is to introduce two new operators that are Hermitian conjugates as

$$\hat{a} \equiv \frac{q + \imath p}{\sqrt{2}}; \;\; \hat{a}^\dagger \equiv \frac{\hat{q} - \imath p}{\sqrt{2}};$$

that now satisfy

$$[\hat{a}, \hat{a}^\dagger] = 1$$

The 1D Q.H.O. Hamiltonian can now be written as

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) = \hbar\omega(\hat{a}\hat{a}^\dagger - \frac{1}{2}) = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$$

Note that no matter how you write this, it has to be Hermitian (why?)

- The importance of this form is that it allows us to obtain a fully algebraic solution for the QHO without having to explicitly solve for the Schrödinger equation. The formal solution is given by

$$\hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})|\nu\rangle = N|\nu\rangle$$

where *N* is the eigenvalue of the operator $\hat{a}^\dagger \hat{a}$ which is called the *number operator*

$$\hat{N} \equiv \hat{a}^\dagger \hat{a}$$

It obeys (homework)

$$[\hat{N}, \hat{a}] = -\hat{a};\; [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$$

- Let us assume that $\hat{N}$ has a complete set of orthogonal eigenvectors s.t. $\hat{N}|n\rangle = n|n\rangle$. Then it follows that

$$\hat{N}\hat{a}|n\rangle = \hat{a}(\hat{N} - 1)|n\rangle = (n-1)\hat{a}|n\rangle$$

Similarly

$$\hat{N}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(\hat{N}+1)|n\rangle = (n+1)\hat{a}^\dagger|n\rangle$$

It was shown in Lecture 6 that the eigenvalues must be non-negative and the spectrum is bounded from below by the ground state for which *n* = 0.

- The squared norm of $\hat{a}^\dagger|n\rangle$ can be calculated as

$$(\langle n|\hat{a})(\hat{a}^\dagger|n\rangle) = \langle n|(\hat{N}+1)|n\rangle = (n+1)\langle n|n\rangle$$

and thus $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$

Thus any eigenstate | n > can be written as

$$|n\rangle = (n!)^{-1/2}(\hat{a}^\dagger)^n|0\rangle$$

Another important result is that the all the matrix elements can be simply calculated as

$$\langle n'|\hat{a}^\dagger|n\rangle = (n+1)^{1/2}\delta_{n',n+1}$$
$$\langle n'|\hat{a}|n\rangle = n^{1/2}\delta_{n',n-1}$$

- Finally, we can read off the eigenvalues of the Hamiltonian as

$$\hat{H}|n\rangle \equiv E_n|n\rangle = \hbar\omega(n+\frac{1}{2})|n\rangle$$