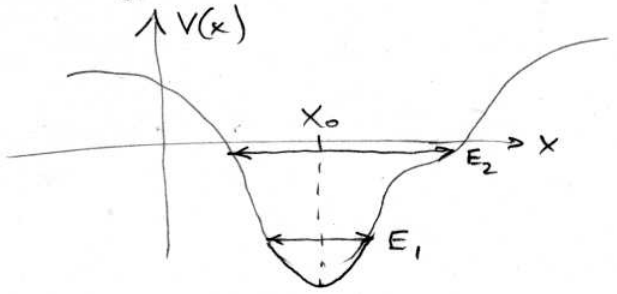
Chapter 7: The harmonic oscillator

7.1. The harmonic oscillator as a model for small excitations near the ground state.

Classical mechanics of a particle in an external force (possibly generated by the interaction with many other particles):

$$\mathcal{H}(x,p) = T + V = \frac{p^2}{2m} + V(x)$$

Classically, a particle with zero kinetic energy T placed at the minimum of $V(x)$, $V_0 = V(x_0)$, will remain there if left alone. Giving the particle some kinetic energy will allow the particle to explore some region around x_0:



The classically allowed range in x depends on the particle's total energy $E = T + V$.

For small T, the excursions around x_0 are limited, and the potential can be expanded with good accuracy around x_0, to second order, for all x-values accessible to the particle:

$$V(x) = V_0 + \underbrace{\left.\frac{dV}{dx}\right|_{x_0}}_{=0} (x - x_0) + \frac{1}{2!} \left.\frac{d^2V}{dx^2}\right|_{x_0} (x - x_0)^2 + \cdots$$

V_0 is an arbitrary normalization constant that drops out from physically relevant energy differences.
For small enough x (i.e. for small enough $E - V_0$) we can truncated the expansion at second order.

$$\Rightarrow \mathcal{H}(x,p) \approx \frac{p^2}{2m} + \frac{1}{2} \left.\frac{d^2V}{dx^2}\right|_{x_0} (x - x_0)^2$$

$\rightarrow$ harmonic oscillator!

Now consider 2 particles in external potentials of equal shape (at least around their equilibrium positions) and coupled to each other by an attractive potential that again can be modelled by a harmonic oscillator (for simplicity we assume the same restoring force for all three potentials):

$$\mathcal{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2} m\omega^2 \left(x_1^2 + x_2^2 + (x_1 - x_2)^2\right)$$

($x_{1/2}$ = displacement from equilibrium for particle 1/2; $x_1 - x_2$ = distance between particles)

$$= \mathcal{H}_1 + \mathcal{H}_2 + \frac{m\omega^2}{2} (x_1 - x_2)^2 \,.$$

This can be decoupled into 2 uncoupled harmonic oscillators:

$$X_I = \frac{x_1 + x_2}{\sqrt{2}} \,, \quad X_{II} = \frac{x_1 - x_2}{\sqrt{2}} \,, \quad p_1^2 + p_2^2 = p_I^2 + p_{II}^2 = m^2\left(v_I^2 + v_{II}^2\right)$$

$$\Rightarrow \boxed{\mathcal{H} = \frac{p_I^2}{2m} + \frac{1}{2} m\omega^2 X_I^2 + \frac{p_{II}^2}{2m} + \frac{3}{2} m\omega^2 X_{II}^2} \,.$$

We can think about this as follows:

Let's rewrite

$$\mathcal{H} = \frac{1}{2m}\sum_{i=1}^{2}\sum_{j=1}^{2} p_i \delta_{ij} p_j + \underbrace{\frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2} x_i V_{ij} x_j}_{\frac{1}{2}m\omega^2\left[x_1^2 + x_2^2 + (x_1 - x_2)^2\right]}$$

with $V_{11} = V_{22} = 2m\omega^2$

$V_{12} = V_{21} = -m\omega^2$

By switching to normal coordinates x_I, x_{II}, we go to a basis that diagonalizes V. The structure of the kinetic energy $\sim \delta_{ij}$ remains unaffected by this unitary basis-transformation.

Now look at the general case with N particles of mass m:

$$V(x_1, x_2, \ldots, x_N) = \frac{1}{2}\sum_{i,j=1}^{N} \left.\frac{\partial^2 V}{\partial x_i \partial x_j}\right|_{\vec{0}} x_i x_j + \ldots$$

(we shift the coordinate systems for x_i so that the minimum of V is at $x_1 = x_2 = \ldots = x_N = 0$, and normalize the minimum to $V_0 = 0$).

For small excitation energies the Hamiltonian is

$$\mathcal{H}(x_1, \ldots, x_N; p_1, \ldots, p_N) \cong \sum_{i,j=1}^{N} \frac{p_i \delta_{ij} p_j}{2m} + \frac{1}{2}\sum_{i,j=1}^{N} x_i V_{ij} x_j$$

where $V_{ij} \equiv \left.\frac{\partial^2 V}{\partial x_i \partial x_j}\right|_0 = \left.\frac{\partial^2 V}{\partial x_j \partial x_i}\right|_0 = V_{ji}$

$\Rightarrow$ V_{ij} is a real, symmetric, i.e. Hermitean matrix and thus diagonalizable.

The unitary coordinate transformation that diagonalises V decouples $\mathcal{H}$ into a sum of non-interacting harmonic oscillators.

Examples:

(A) A crystal in 3 dimensions, consisting of N_0 (point-like) atoms: $3N_0$ degrees of freedom (displacements from equilibrium positions)

For small displacements, V will be quadratic in the coordinates, and T is quadratic in the momenta

$\longrightarrow \exists$ $3N_0$ normal coordinates in which $\mathcal{H}$ is a sum over decoupled harmonic oscillators.

These normal modes are collective excitations travelling across the lattice (plane waves with wave number $\vec{k}$).
Possible oscillations are either parallel to $\vec{k}$ ("longitudinal polarization") or in one of the two transverse directions to $\vec{k}$ ("transverse polarization"), labelled by polarization index $\lambda = 1, 2, 3$. Modes are labelled by $(\vec{k}, \lambda)$; there are N_0 possible $\vec{k}$ vectors, times 3 polarizations.
These modes form a complete set for expanding any excitation state of the system. The expansion coefficients are $a(\vec{k}, \lambda)$, the normal frequencies are $\omega(\vec{k}, \lambda)$.

(B) The electromagnetic field in free space: described by vector potential $\vec{A}(\vec{r}, t)$.

We can think of $\vec{A}(\vec{r},t)$ as a generalized coordinate (of infinite dimensionality), with generalized velocity $\dot{\vec{A}}(\vec{r},t)$. The normal modes are again plane waves. In this case there is no restriction on $\vec{k}$ (continuously infinite # of degrees of freedom!), but due to the masslessness of photons (or Gauss' law) only transverse polarizations are allowed.

→ Chapter 18

7.2 The Hamilton operator for the harmonic oscillator in coordinate basis representation

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

with (for 1 particle in 1 dimension)

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

The time evolution is trivial once we have solved the eigenvalue problem

$$\hat{H}|E_n\rangle = E_n|E_n\rangle$$

It is given by

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_n |E_n\rangle\langle E_n| e^{-iE_n t/\hbar}$$