Normal coördinates and quantum mechanics

CMC 2013 October 24

Consider a quantum system with Hamiltonian H. The stationary states are the eigenstates of H: $H|E\rangle = E|E\rangle$. The state vector $|\psi(t)\rangle$ can be written in terms of an arbitrary basis, $\{|j\rangle\}$, as

$$|\psi(t)\rangle = \sum_{j} |j\rangle\langle j|\psi(t)\rangle = \sum_{j} \eta_{j}(t)|j\rangle,$$

where the "original coördinates" are the amplitudes $\eta_j(t) = \langle j | \psi(t) \rangle$. The state vector can also be written in terms of the energy eigenbasis as

$$|\psi(t)\rangle = \sum_{E} |E\rangle \langle E|\psi(t)\rangle = \sum_{E} \zeta_{E}(0)e^{-iEt/\hbar}|E\rangle,$$

where the amplitudes

$$\zeta_E(t) = \langle E|\psi(t)\rangle = \langle E|e^{-iHt/\hbar}|\psi(0)\rangle = e^{-iEt/\hbar}\langle E|\psi(0)\rangle = e^{-iEt/\hbar}\zeta_E(0)$$

are the normal coördinates because they oscillate sinusoidally in time.

The original coördinates are related to the normal coördinates by

$$\eta_j(t) = \langle j | \psi(t) \rangle = \sum_E \underbrace{\langle j | E \rangle}_{= a_{jE}} \langle E | \psi(t) \rangle = \sum_E a_{jE} \zeta_E(0) e^{-iEt/\hbar} \,.$$

The energy eigenstates are the normal modes; they are related to the basis $|j\rangle$ by

$$|E\rangle = \sum_{j} |j\rangle\langle j|E\rangle = a_{jE}|j\rangle.$$

The matrix elements a_{jE} give the "shape" of normal mode E in the original basis.

The only difference with what we are doing in linear mechanical systems is that the variables are real instead of complex and thus obey second-order, linear differential equations in time, instead of the first-order, linear Schrödinger equation. Once one is past that difference, the whole thing is identical. If we were to master the bra-ket notation for the real vector spaces in mechanics, the question of which order to write the indices in and whether to use a transformation matrix or its transpose would disappear as questions, since the bra-ket notation takes care of all that without any need for thinking.