Summary of the Previous Lecture

- Diagonalization of Hermitian matrices
  - Matrix representation of a Hermitian operator with eigenbasis becomes diagonal
  - Simultaneous diagonalization is possible for two commuting operators
- Function of operator: $e^{\Omega} = \sum_{n=0}^{\infty} \frac{1}{n!} \Omega^n$
  - $f(\Omega) = \begin{bmatrix} f(\omega_1) & & & \\ & f(\omega_2) & & \\ & & \ddots & \\ & & & f(\omega_n) \end{bmatrix}$ when $f(\Omega)$ is represented in the eigenbasis of Ω
  - $\frac{\partial}{\partial t}|\psi\rangle = i\Omega|\psi\rangle$ ➔ $|\psi(t)\rangle = e^{i\Omega t}|\psi(0)\rangle = U(t)|\psi(0)\rangle$ ➔ When Ω is Hermitian, $U(t)$ is unitary.

From Chap. 1 of “Principles of Quantum Mechanics”, Ramamurti Shankar, 2nd ed. Plenum Press (1994)

Peep into Quantum Mechanics I

- Postulate 1: the state of the particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space
  - However, the law of quantum mechanics doesn't tell us what the state space of Hilbert space should be.
  - Therefore state space should be found by experiment
  - Example space: space composed of $|0\rangle$ & $|1\rangle$

Peep into Quantum Mechanics II

- Postulate 2: the evolution of a "closed" quantum system is described by a unitary transformation
  - $|\psi\rangle\ at\ t_1 \xrightarrow{\text{unitary transformation}} |\psi'\rangle\ at\ t_2$
  - Example: $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

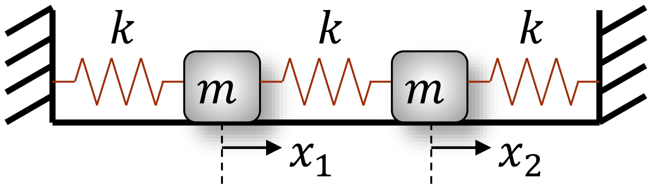
  $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $X|0\rangle = |1\rangle$, $X|1\rangle = |0\rangle$

- Postulate 2' (continuous time version): the time evolution of the state of a "closed" quantum system is described by Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = \mathcal{H}|\psi\rangle$$

  - $\hbar$ is Planck's constant, 1.054 $1.054 \times 10^{-34}\ (J \cdot s)$
  - $\mathcal{H}$ is called *Hamiltonian*. Hamiltonian describes how the system should evolve.

Analogy with Solution of Coupled Masses



Negative direction　　Positive direction

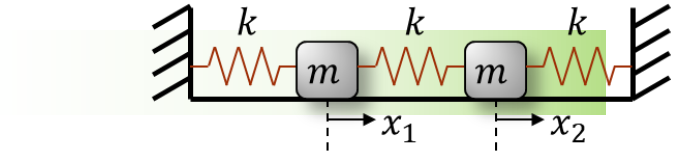
- Solve for x_1 and x_2.
  - $m\ddot{x}_1 = k(x_2 - x_1) - kx_1 = -2kx_1 + kx_2$
  - $m\ddot{x}_2 = -k(x_2 - x_1) - kx_2 = kx_1 - 2kx_2$
  - Initial condition: non-zero displacement $x_1(0)$, $x_2(0)$ and zero velocity $\dot{x}_1(t=0) = \dot{x}_2(t=0) = 0$
  - $m\begin{bmatrix}\ddot{x}_1\\ \ddot{x}_2\end{bmatrix} = \begin{bmatrix}-2k & k\\ k & -2k\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix} \Rightarrow m\begin{bmatrix}\ddot{x}_1\\ \ddot{x}_2\end{bmatrix} = \begin{bmatrix}-2k & k\\ k & -2k\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix}$

$\Rightarrow m\dfrac{d^2}{dt^2}\begin{bmatrix}x_1\\ x_2\end{bmatrix} = \begin{bmatrix}-2k & k\\ k & -2k\end{bmatrix}\begin{bmatrix}x_1\\ x_2\end{bmatrix}$

$\Rightarrow m\dfrac{d^2}{dt^2}|x\rangle = K|x\rangle \overset{Similarity?}{\Longleftrightarrow} i\hbar\dfrac{\partial}{\partial t}|\psi\rangle = \mathcal{H}|\psi\rangle$ Schrödinger equation

$|x(t)\rangle = U(t)|x(0)\rangle$　　　　$|\psi_{final}\rangle = U|\psi_{initial}\rangle$

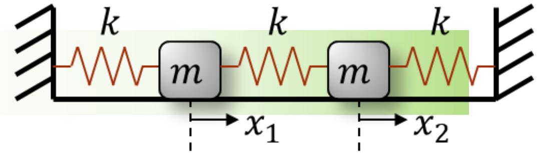
Solution of Coupled Masses



- $\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} = \begin{bmatrix} -2k/m & k/m \\ k/m & -2k/m \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \Omega \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ ➔ Matrix Ω is Hermitian
- We can view x_1, x_2 as the components of an abstract vector $|x\rangle$.
- Abstract form: $|\ddot{x(t)}\rangle = \Omega|x(t)\rangle$
- We can view the top equation as a projection of the abstract equation on the basis vectors $|1\rangle$, $|2\rangle$ which have the following physical significance:
  - $|1\rangle \Leftrightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \Leftrightarrow \begin{bmatrix} \text{first mass dispaced by unity} \\ \text{second mass undisplaced} \end{bmatrix}$
  - $|2\rangle \Leftrightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} \Leftrightarrow \begin{bmatrix} \text{first mass undisplaced} \\ \text{second mass dispaced by unity} \end{bmatrix}$
  - An arbitrary state, in which the masses are displaced by x_1 and x_2, is given in this basis by
    - $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \Leftrightarrow |x\rangle = x_1|1\rangle + x_2|2\rangle$
  - Representation of vector $|x\rangle$ in $|1\rangle$, $|2\rangle$ basis has simple physical interpretation, but not an ideal choice of basis to solve due to **coupling between x_1 and x_2.**

From Chap. 1 of “Principles of Quantum Mechanics”, Ramamurti Shankar, 2nd ed. Plenum Press (1994)

Solution of Coupled Masses



- Switch to a basis in which Ω is diagonal
  - Recall Ω is Hermitian ➔ normalized eigenvector basis $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$
  - The equations will become simplified into the following form:
    - $\Omega|\mathrm{I}\rangle = -\omega_{\mathrm{I}}^2|\mathrm{I}\rangle$
    - $\Omega|\mathrm{II}\rangle = -\omega_{\mathrm{II}}^2|\mathrm{II}\rangle$
- Find out eigenvectors
  - $\det(\Omega - \lambda I) = 0$
  - $$\det\begin{bmatrix} -\frac{2k}{m} - \lambda & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} - \lambda \end{bmatrix} = \left(\lambda + 2\frac{k}{m}\right)^2 - \left(\frac{k}{m}\right)^2 = \lambda^2 + 4\lambda\left(\frac{k}{m}\right) + 3\left(\frac{k}{m}\right)^2$$
    $$= \left(\lambda + \frac{k}{m}\right)\left(\lambda + 3\frac{k}{m}\right) = 0 \Rightarrow \lambda = -\frac{k}{m} \text{ and } \lambda = -3\frac{k}{m}$$
  - For $\lambda = -\frac{k}{m} = -\omega_{\mathrm{I}}^2$, $\omega_{\mathrm{I}} = \sqrt{k/m}$
    $$\begin{bmatrix} -\frac{2k}{m} + \frac{k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} + \frac{k}{m} \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 0 \Rightarrow a - b = 0 \Rightarrow |\mathrm{I}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
  - For $\lambda = -\frac{3k}{m} = -\omega_{\mathrm{II}}^2$, $\omega_{\mathrm{II}} = \sqrt{3k/m}$
    $$\begin{bmatrix} -\frac{2k}{m} + \frac{3k}{m} & \frac{k}{m} \\ \frac{k}{m} & -\frac{2k}{m} + \frac{3k}{m} \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 0 \Rightarrow a + b = 0 \Rightarrow |\mathrm{II}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

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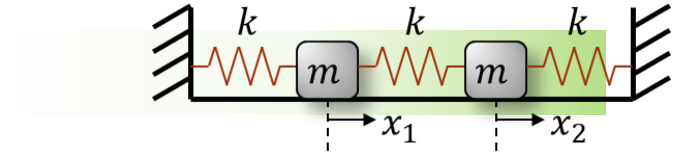
Solution of Coupled Masses



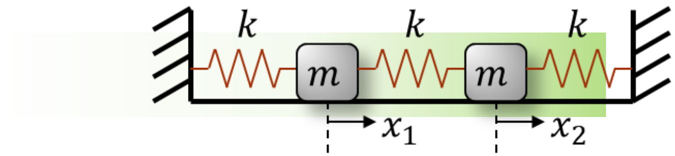
- Now the vector $|x(t)\rangle$ can be expanded in the basis of $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$ as $|x(t)\rangle = x_{\mathrm{I}}(t)|\mathrm{I}\rangle + x_{\mathrm{II}}(t)|\mathrm{II}\rangle$
- The representation of the equation $|\ddot{x}(t)\rangle = \Omega|x(t)\rangle$ in $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$ is $\begin{bmatrix}\ddot{x}_{\mathrm{I}}\\ \ddot{x}_{\mathrm{II}}\end{bmatrix} = \begin{bmatrix}-\omega_{\mathrm{I}}^2 x_{\mathrm{I}}\\ -\omega_{\mathrm{II}}^2 x_{\mathrm{II}}\end{bmatrix} = \begin{bmatrix}-\omega_{\mathrm{I}}^2 & 0\\ 0 & -\omega_{\mathrm{II}}^2\end{bmatrix}\begin{bmatrix}x_{\mathrm{I}}\\ x_{\mathrm{II}}\end{bmatrix}$
- $\begin{cases}\ddot{x}_{\mathrm{I}} = -\omega_{\mathrm{I}}^2 x_{\mathrm{I}}\\ \ddot{x}_{\mathrm{II}} = -\omega_{\mathrm{II}}^2 x_{\mathrm{II}}\end{cases}$
  - General solution of diff. eq. : $x_{\mathrm{I}}(t) = A\cos\omega_{\mathrm{I}}t + B\sin\omega_{\mathrm{I}}t$
  - If initial condition of $x_{\mathrm{I}}(t)$ is $x_{\mathrm{I}}(0)$, $A = x_{\mathrm{I}}(0)$
  - Use zero velocity initial condition: $\dot{x}_{\mathrm{I}}(t) = -A\omega_{\mathrm{I}}\sin\omega_{\mathrm{I}}t + B\omega_{\mathrm{I}}\cos\omega_{\mathrm{I}}t$ ➔ $B = 0$
  - $x_{\mathrm{I}}(t) = x_{\mathrm{I}}(0)\cos\omega_{\mathrm{I}}t$
  - Similarly for $x_{\mathrm{II}}(t)$, $x_{\mathrm{II}}(t) = x_{\mathrm{II}}(0)\cos\omega_{\mathrm{II}}t$
- $|x(t)\rangle = x_{\mathrm{I}}(0)\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle + x_{\mathrm{II}}(0)\cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle$
- If we define initial state vector as $|x(t=0)\rangle = x_{\mathrm{I}}(0)|\mathrm{I}\rangle + x_{\mathrm{II}}(0)|\mathrm{II}\rangle$, $x_{\mathrm{I}}(0) = \langle\mathrm{I}|x(t=0)\rangle$ and $x_{\mathrm{II}}(0) = \langle\mathrm{II}|x(t=0)\rangle$
- Then $|x(t)\rangle = \langle\mathrm{I}|x(t=0)\rangle\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle + \langle\mathrm{II}|x(t=0)\rangle\cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle$

$$= [\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle\langle\mathrm{I}| + \cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle\langle\mathrm{II}|]\ |x(t=0)\rangle$$

$$= U(t)\ |x(t=0)\rangle$$

➔ For this specific mechanical example, it is not unitary, but it is generally called as a propagator.

Solution of Coupled Masses



- Procedure

  Step (1). Solve the eigenvalue problem of Ω

  Step (2). Find the coefficients , $x_{\mathrm{I}}(0) = \langle \mathrm{I} | x(t=0) \rangle$ and $x_{\mathrm{II}}(0) = \langle \mathrm{II} | x(t=0) \rangle$ for the expansion $|x(t=0)\rangle = x_{\mathrm{I}}(0)|\mathrm{I}\rangle + x_{\mathrm{II}}(0)|\mathrm{II}\rangle$

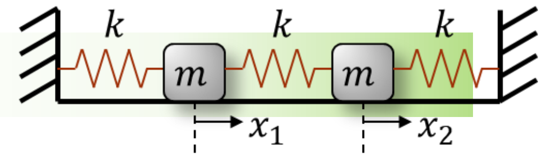
  Step (3). Append to each coefficient $x_i(0)$ $(i = \mathrm{I}, \mathrm{II})$ a time dependence $\cos \omega_i t$ to get the coefficients in the expansion of $|x(t)\rangle$.

- Step (2): to find out $x_{\mathrm{I}}(0)$ and $x_{\mathrm{II}}(0)$ in terms of $x_1(0)$ and $x_2(0)$:
  - $x_{\mathrm{I}}(0) = \langle \mathrm{I} | x(t=0) \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} = \frac{x_1(0) + x_2(0)}{\sqrt{2}}$
  - $x_{\mathrm{II}}(0) = \langle \mathrm{II} | x(t=0) \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} = \frac{x_1(0) - x_2(0)}{\sqrt{2}}$

- Step (3): $|x(t)\rangle = \frac{x_1(0)+x_2(0)}{\sqrt{2}} \cos \omega_{\mathrm{I}} t \, |\mathrm{I}\rangle + \frac{x_1(0)-x_2(0)}{\sqrt{2}} \cos \omega_{\mathrm{II}} t \, |\mathrm{II}\rangle$ where $\omega_{\mathrm{I}} = \sqrt{k/m}$ and $\omega_{\mathrm{II}} = \sqrt{3k/m}$

- Find out the location of mass: $x_1(t) = \langle 1 | x(t) \rangle$
  - By using $\langle 1 | \mathrm{I} \rangle = \frac{1}{\sqrt{2}}$ and $\langle 1 | \mathrm{II} \rangle = \frac{1}{\sqrt{2}}$, $x_1(t) = \frac{x_1(0)+x_2(0)}{2} \cos \omega_{\mathrm{I}} t + \frac{x_1(0)-x_2(0)}{2} \cos \omega_{\mathrm{II}} t$
  - Similarly, $x_2(t) = \langle 2 | x(t) \rangle = \frac{x_1(0)+x_2(0)}{2} \cos \omega_{\mathrm{I}} t - \frac{x_1(0)-x_2(0)}{2} \cos \omega_{\mathrm{II}} t$

Propagator



- Displacement:

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \frac{\cos\omega_{\mathrm{I}}t + \cos\omega_{\mathrm{II}}t}{2} & \frac{\cos\omega_{\mathrm{I}}t - \cos\omega_{\mathrm{II}}t}{2} \\ \frac{\cos\omega_{\mathrm{I}}t - \cos\omega_{\mathrm{II}}t}{2} & \frac{\cos\omega_{\mathrm{I}}t + \cos\omega_{\mathrm{II}}t}{2} \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$$

- Eigenbasis: $|x(t)\rangle = [\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle\langle\mathrm{I}| + \cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle\langle\mathrm{II}|]\ |x(t=0)\rangle$
- The final-vector is obtained from the initial-state vector upon multiplication by a matrix.
- This matrix is independent of the initial state. ➔ Propagator
- Procedure to solve $|\ddot{x(t)}\rangle = \Omega|x(t)\rangle$ using propagator

  Step (1). Solve the eigenvalue problem of Ω

  Step (2). Construct the propagator U in terms of the eigenvalues and eigenvectors.

  Step (3).$|x(t)\rangle = U(t)|x(t=0)\rangle$

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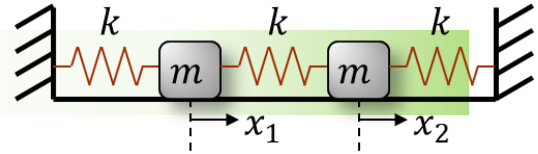
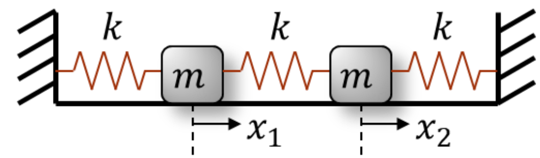
Normal Modes



- Two initial states for which the time evolution is particularly simple ➔ Eigenkets $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$
- $|\mathrm{I}(t)\rangle = U(t)|\mathrm{I}\rangle = [\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle\langle\mathrm{I}| + \cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle\langle\mathrm{II}|]|\mathrm{I}\rangle = \cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle$
- These two modes of vibration are called normal modes
  - $|\mathrm{I}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$ ➔ $|\mathrm{I}(t)\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}\cos\left(\sqrt{\frac{k}{m}}\,t\right)\\ \cos\left(\sqrt{\frac{k}{m}}\,t\right)\end{bmatrix}$ ➔ Center of mass mode
  - $|\mathrm{II}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$ ➔ $|\mathrm{II}(t)\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}\cos\left(\sqrt{\frac{3k}{m}}\,t\right)\\ -\cos\left(\sqrt{\frac{3k}{m}}\,t\right)\end{bmatrix}$ ➔ Breathing mode
- If the system starts off in a linear combination of $|\mathrm{I}\rangle$ and $|\mathrm{II}\rangle$, it evolves into the corresponding linear combination of the normal modes $|\mathrm{I}(t)\rangle$ and $|\mathrm{II}(t)\rangle$. Propagator $U(t) = [\cos\omega_{\mathrm{I}}t\,|\mathrm{I}\rangle\langle\mathrm{I}| + \cos\omega_{\mathrm{II}}t\,|\mathrm{II}\rangle\langle\mathrm{II}|]$ projects on each of them.

Summary of previous lecture

- $m\frac{\partial^2}{\partial t^2}|x\rangle = \Omega|x\rangle$ can be solved by finding $U(t)$ evolution operator satisfying $|x(t)\rangle = U(t)|x(0)\rangle$
  - The same solution $|x(t)\rangle$ can be represented in either $|1\rangle$, $|2\rangle$ basis or $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$ basis
  - $|x\rangle = x_1|1\rangle + x_2|2\rangle = x_1\begin{bmatrix}1\\0\end{bmatrix} + x_2\begin{bmatrix}0\\1\end{bmatrix}$
  - $|x\rangle = x_{\mathrm{I}}|\mathrm{I}\rangle + x_{\mathrm{II}}|\mathrm{II}\rangle = x_{\mathrm{I}}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} + x_{\mathrm{II}}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$
  - The normal modes have $\omega_{\mathrm{I}} = \sqrt{k/m}$ and $\omega_{\mathrm{II}} = \sqrt{3k/m}$ frequencies.



- Energy of the simple harmonic oscillator
  - $m\ddot{x} = kx$ with zero initial velocity $\left(\omega \equiv \sqrt{\frac{k}{m}}\right)$
  - $x = A\cos\sqrt{\frac{k}{m}}t \equiv A\cos\omega t$ ➔ $v = -A\omega\sin\omega t$
  - Total energy: $\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}m(-A\omega\sin\omega t)^2 + \frac{1}{2}k(A\cos\omega t)^2$
  - $= \frac{1}{2}m\omega^2A^2\sin^2\omega t + \frac{1}{2}kA^2\cos^2\omega t = \frac{1}{2}m\omega^2A^2$