Tema 9: The harmonic oscillator

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$$V(x) \;=\; \frac{1}{2}kx^2 \quad ; \quad k \;=\; m\omega^2$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} \;+\; \frac{1}{2}m\omega^2 x^2\phi(x) \;=\; E\phi(x) \qquad \text{T.I.S.E.}$$

- change of variables

$$y \;=\; \sqrt{\frac{m\omega}{\hbar}}x \;=\; \alpha x$$

$$\frac{d}{dx} \;=\; \alpha\frac{d}{dy} \quad ; \quad \frac{d^2}{dx^2} \;=\; \alpha^2\frac{d^2}{dy^2} \quad ; \quad \alpha \;=\; \sqrt{\frac{m\omega}{\hbar}}$$

$$\left[\frac{d^2}{dy^2} \;+\; (\beta - y^2)\right]\Phi(y) \quad = \quad 0 \tag{1}$$

$\beta \;=\; \frac{2E}{\hbar\omega}$; $\Phi(y) \;=\; \phi(x)$ where y and β are dimensionless

- asymptotically for $y \to \infty$

$$\left[\frac{d^2}{dy^2} - y^2\right]\Phi^{as}(y) = 0 \tag{2}$$

We try $\Phi^{as}(y) = y^n e^{-\frac{y^2}{2}}$; n integer $\to$ satisfies the differential equation (2)

- we propose as a general solution $(\forall y)$

$$\Phi(y) = H(y)e^{-\frac{y^2}{2}}$$

so that (1) is fulfilled

$$H''(y) - 2yH'(y) + (\beta - 1)H(y) = 0 \tag{3}$$

we propose

$$H(y) = \sum_{k=0}^{\infty} a_k\, y^k \quad \text{power series}$$

since $V(x) = V(-x)$ in the sum only appear odd or even k 's

$$H'(y) = \sum_{k=1}^{\infty} k\, a_k\, y^{k-1}$$

$$\begin{aligned} H''(y) &= \sum_{k=2}^{\infty} k(k-1)\, a_k\, y^{k-2} \\ &= \sum_{p=0}^{\infty} (p+2)(p+1)\, a_{p+2}\, y^p \end{aligned}$$

Bring H' and H'' to (3)

$$\sum_{p=0}^{\infty}(p+2)(p+1)\ a_{p+2}\ y^p - 2y\left(\sum_{k=0}^{\infty} k\ a_k\ y^{k-1}\right) + (\beta-1)\sum_{k=0}^{\infty} a_k\ y^k = 0$$

$$\sum_{k=0}^{\infty}\left[(k+2)(k+1)\ a_{k+2}\ -\ (2k-\beta+1)\ a_k\right] y^k\ =\ 0 \qquad \forall y$$

$$\frac{a_{k+2}}{a_k}\ =\ \frac{2k+1-\beta}{(k+2)(k+1)} \qquad \text{recurrence relation}$$

$$\frac{a_{k+2}}{a_k}\ \to\ \frac{2}{k} \quad \text{when} \quad k \to\ \infty$$

$$e^{y^2}\ =\ \sum_{n=0}^{\infty}\frac{y^{2n}}{n!}\ =\ \sum_{k=0(\text{even})}^{\infty}\frac{y^k}{(\frac{k}{2})!}\ =\ \sum_{k=0(\text{even})}^{\infty} b_k\ y^k$$

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$$\frac{b_{k+2}}{b_k}\ =\ \left(\frac{\left[\frac{k+2}{2}\right]!}{\left[\frac{k}{2}\right]!}\right)^{-1}\ =\ \left(\frac{k}{2}+1\right)^{-1}\ \to\ \frac{2}{k}\ \text{when} \quad k \to\ \infty$$

$$e^{y^2} = \sum_{t=1(\text{odd})}^{\infty}\frac{y^{t-1}}{\left(\frac{t-1}{2}\right)!}$$

$$\to y e^{y^2}\ =\ \sum_{t=1(\text{odd})}^{\infty}\frac{y^t}{\left(\frac{t-1}{2}\right)!}\ =\ \sum_{t=1(\text{odd})}^{\infty} c_t\ y^t$$

$$\frac{c_{t+2}}{c_t}\ =\ \left(\frac{\left[\frac{t+1}{2}\right]!}{\left[\frac{t-1}{2}\right]!}\right)^{-1}\ =\ \left(\frac{t+1}{2}\right)^{-1}\ \to\ \frac{2}{t}\ \text{when} \quad t\ \to\ \infty$$

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If $H(y)$ is an infinite series, asymptotically

even series $y \rightarrow \infty$; $\Phi(y) = e^{y^2} e^{-\frac{y^2}{2}} = e^{\frac{y^2}{2}} \rightarrow \infty$ when $y \rightarrow \infty$

$$a_n \neq 0 \;;\; a_{n+2} = 0 \rightarrow \text{H(y) polynomial}$$

$$2n + 1 - \beta = 0 \rightarrow \quad \beta = 2n + 1 \quad (n = 0, 1, 2, \cdots)$$

We need

- a_0 for even eigenfunctions (generates $a_2,\ a_4, \cdots$)

  $(n = 0, 2, 4, \cdots)$; $a_1 = 0$

- a_1 for odd eigenfunctions (generates $a_3,\ a_5, \cdots$)

  $(n = 1, 3, 5, \cdots)$; $a_0 = 0$

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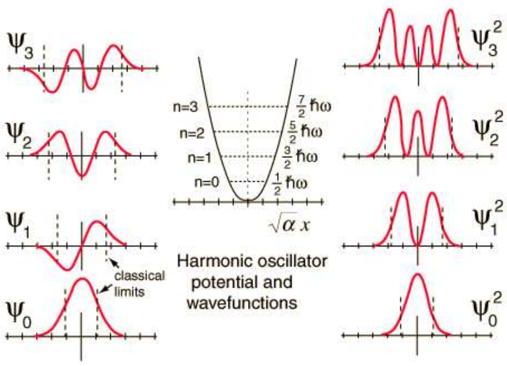
$$\beta = \frac{2E}{\hbar\omega} = 2n + 1 \rightarrow$$

$$E_n = \frac{1}{2}(2n + 1)\hbar\omega = \left(n + \frac{1}{2}\right)\hbar\omega \quad ; \quad n = 0, 1, 2, \cdots$$



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$$E_0 \;=\; \frac{1}{2}\hbar\omega \quad \text{zero point energy}$$

equidistant levels $E_{n+1} \;-\; E_n \;=\; \hbar\omega$
$H(y)$ **are the Hermite polynomials**

$$H_n(y) \;=\; (-1)^n e^{y^2} \; \frac{d^n e^{-y^2}}{dy^n}$$

We define $\alpha \;=\; \sqrt{\frac{m\omega}{\hbar}} \;\rightarrow\; y \;=\; \alpha\, x$

$$n \;=\; 0 \quad ; \quad \phi_0(x) \;=\; \left(\frac{\alpha}{\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}} \quad ; \quad H_0(y) \;=\; 1$$

$$n \;=\; 1 \;\; ; \;\; \phi_1(x) \;=\; \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{\frac{1}{2}} 2\alpha x e^{-\frac{\alpha^2 x^2}{2}} \quad ; \quad H_1(y) \;=\; 2y$$

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$$n \;=\; 2 \; ; \; \phi_2(x) \;=\; \left(\frac{\alpha}{8\sqrt{\pi}}\right)^{\frac{1}{2}} (4\alpha^2 x^2 - 2) e^{-\frac{\alpha^2 x^2}{2}} \quad ; \quad H_2 \;=\; 4y^2 \; - 2$$

$$\phi_n(x) = \Phi_n(y) = \left(\frac{\alpha}{2^n n! \sqrt{\pi}}\right)^{\frac{1}{2}} H_n(\alpha x) e^{-\frac{\alpha^2 x^2}{2}} \;=\; \mathcal{N}_n H_n(y) e^{-\frac{y^2}{2}} \quad \forall x$$

Normalized wave functions

$$\int_{-\infty}^{\infty} H_n^2(y) e^{-y^2} \; dy \;=\; \sqrt{\pi}\; 2^n \; n!$$

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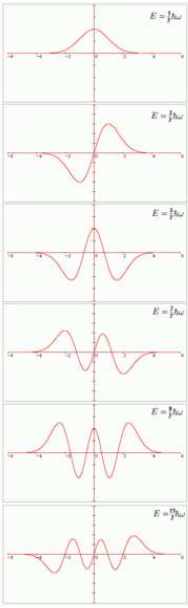

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Algebraic solution of the harmonic oscillator. Introduction to the second quantization 14 / 27

$$y = \alpha x \quad ; \quad \alpha = \sqrt{\frac{m\omega}{\hbar}} \quad ; \quad \eta = \frac{E}{\hbar\omega} = \frac{\beta}{2}$$

$$\hat{D} = \frac{d}{dy}$$

(1) $\left[\frac{d^2}{dy^2} + (\beta - y^2)\right]\Phi(y) = 0 \rightarrow$

$$\frac{1}{2}\left[-\hat{D}^2 + y^2\right]\Phi(y) = \eta\Phi(y)$$

$$\hat{D}^2 - y^2 = \left(\hat{D} - y\right)\left(\hat{D} + y\right) - 1$$

$$\hat{D}y \neq y\hat{D} \quad ; \quad \left[\hat{D}, y\right] = 1$$

$$\frac{1}{2}\left[1 - \left(\hat{D} - y\right)\left(\hat{D} + y\right)\right]\Phi = \eta\Phi$$

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$$-\frac{1}{\sqrt{2}}\left(\hat{D}\ -\ y\right)\frac{1}{\sqrt{2}}\left(\hat{D}\ +\ y\right)\Phi\ =\ \left(\eta-\frac{1}{2}\right)\Phi \tag{4}$$

$$b^{\dagger}\ =\ \frac{1}{\sqrt{2}}\left(y-\frac{d}{dy}\right)\quad ;\quad b\ =\ \frac{1}{\sqrt{2}}\left(y\ +\ \frac{d}{dy}\right)$$

$$b^{\dagger}b\ \Phi\quad =\quad \left(\eta-\frac{1}{2}\right)\Phi\qquad \textbf{Schrödinger eq.} \tag{5}$$

$\left[\mathbf{b},\mathbf{b}^{\dagger}\right]\ =\ \mathbf{1}$

$$\hat{\mathbf{x}}\ =\ \sqrt{\frac{\boldsymbol{\hbar}}{\mathbf{2m}\omega}}\left[\mathbf{b}\ +\ \mathbf{b}^{\dagger}\right]\ =\ \frac{\mathbf{1}}{\sqrt{\mathbf{2}}\alpha}\left[\mathbf{b}\ +\ \mathbf{b}^{\dagger}\right]$$

$$\hat{\mathbf{p}}\ =\ -\,\mathbf{i}\boldsymbol{\hbar}\frac{\mathbf{d}}{\mathbf{dx}}\ =\ -\,\mathbf{i}\boldsymbol{\hbar}\alpha\frac{\mathbf{d}}{\mathbf{dy}}\ =\ -\,\frac{\mathbf{i}\boldsymbol{\hbar}\alpha}{\sqrt{\mathbf{2}}}\left[\mathbf{b}\ -\ \mathbf{b}^{\dagger}\right]$$

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Number operator

$$\hat{N}\ =\ b^{\dagger}b \tag{6}$$

$$\hat{H}\ =\ \hbar\omega\left[\hat{N}\ +\ \frac{1}{2}\right]\ \rightarrow\ \text{eigenfunctions of } \hat{H}\ =\ \text{eigenfunctions of } \hat{N}$$

Eigenvalues of $\hat{H}\ \rightarrow\ E_n\ =\ \hbar\omega(n\ +\ \frac{1}{2})$ (n are eigenvalues of $\hat{N}$)

(5) and (6) $\hat{N}\Phi_n\ =\ \left(\eta-\frac{1}{2}\right)\Phi_n\ =\ n\ \Phi_n\ \rightarrow\ n\ =\ \eta-\frac{1}{2}$

($n\ =$ quanta of excitation, **phonons**)

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- (i) (5) multiplied by b on the left

$$bb^\dagger b\ \Phi_n \ = \ n\ b\ \Phi_n \qquad (bb^\dagger \ = \ 1 \ + \ b^\dagger b)$$

$$(1 \ + \ b^\dagger b) b\ \Phi_n \ = \ n\ b\ \Phi_n$$

$$b^\dagger b (b\ \Phi_n) \ = \ (n \ - \ 1)\ (b\ \Phi_n)$$

Φ_n eigenfunction of $\hat{N}$ associated to eigenvalue $n \ \rightarrow \ b\ \Phi_n$ eigenfunction of $\hat{N}$ associated to eigenvalue $n - 1$

$b \ =$ **annihilation operator** (annihilates one quantum of excitation = its number decreases by one unit)

Let's call the ground state $\Phi_{g.s.}$

$$b\ \Phi_{g.s.} \ = \ 0 \ \rightarrow \ (\hat{D} \ + \ y)\Phi_{g.s.} \ = \ 0 \tag{7}$$

$$\frac{d\ \Phi_{g.s.}}{dy} \ + \ y\ \Phi_{g.s.} \ = \ 0 \ \rightarrow \ \frac{d\ \Phi_{g.s.}}{dy} \ = \ -\,y\ \Phi_{g.s.} \ \rightarrow$$

$$\ln \Phi_{g.s.} \ = \ -\frac{y^2}{2} \ + \ A \ \rightarrow \ \Phi_{g.s.} \ = \ B\ e^{-\frac{y^2}{2}}$$

from (7) $\Phi_{g.s.}$ is eigenfunction of b associated to 0

$\rightarrow \ b^\dagger b\ \Phi_{g.s.} \ = \ 0 \ \rightarrow \ \Phi_{g.s.}$ is eigenfunction of $\hat{N}$ associated to $0 \quad \rightarrow \ \Phi_0$

$\rightarrow \ n_{g.s.} \ = \ 0 \ \rightarrow \ n \ = \ 0, 1, 2, \cdots$

■ (ii) (5) multiplied by $b^\dagger$ on the left

$$b^\dagger b^\dagger b \; \Phi_n \;=\; n \; b^\dagger \Phi_n$$

$$b^\dagger (b b^\dagger \;-\; 1) \Phi_n \;=\; n \; b^\dagger \Phi_n$$

$$b^\dagger b \left[b^\dagger \Phi_n \right] \;=\; (n \;+\; 1) \; \left[b^\dagger \Phi_n \right]$$

$b^\dagger \Phi_n$ is eigenfunction of $\hat{N}$ with eigenvalue $n \;+\; 1$

$b^\dagger$ **creation operator**

$$\Phi_1 \; \propto b^\dagger \Phi_0 \quad ; \quad \Phi_n \; \propto (b^\dagger)^n \Phi_0$$

($\propto$ because the normalization of $(b^\dagger)^n \Phi_0$ is not guaranteed)

$$n \;=\; 0 \;\; ; \quad \Phi_0 \; \propto e^{-\frac{y^2}{2}}$$

$$n \;=\; 1 \;\; ; \quad \Phi_1 \; \propto b^\dagger \; \Phi_0 \quad \propto \; y \; e^{-\frac{y^2}{2}}$$

$$n \;=\; 2 \;\; ; \quad \Phi_2 \; \propto b^\dagger \; \Phi_1 \quad \propto \; (2y^2 \;-\; 1) \; e^{-\frac{y^2}{2}} \cdots$$

we get the Hermite polynomials

- (iii) In Dirac's notation

  $|n>$ normalized eigenstate of $\hat{N}$ and $\hat{H}$

  $< n|n' > \; = \; \delta_{nn'}$

  - $(b^\dagger)^\dagger \; = \; b$ demonstration
    - $< n|b^\dagger|m > \; = \; < m|(b^\dagger)^\dagger|n >^* \qquad \forall m, n$

      but $b^\dagger|n > \; = \; \sqrt{n+1}|n+1 >$ and $b|n > \; = \; \sqrt{n}|n-1 >$

$$\sqrt{m+1}\;\delta_{m+1,n} \; = \; < m|(b^\dagger)^\dagger|n >^*$$

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$$< m|b|n >^* \; = \; \left[\sqrt{n}\;\delta_{m,n-1}\;\right]^*$$
$$= \; \sqrt{m+1}\;\delta_{m+1,n}$$
$$\forall m, n$$

$< m|(b^\dagger)^\dagger|n >^* \; = \; < m|b|n >^* \; \rightarrow$

$(b^\dagger)^\dagger \; = \; b \; \rightarrow \; b^\dagger \; = \; (b)^\dagger$

■

◆ $|n> \;=\; A\, b^\dagger|n-1>$

$$
\begin{aligned}
<n|n> \;&=\; |A|^2 <n-1|bb^\dagger|n-1> \\
&=\; |A|^2 <n-1|1 \;+\; b^\dagger b|n-1> \\
&=\; |A|^2(1 \;+\; n \;-\; 1) \;=\; n\;|A|^2
\end{aligned}
$$

$$\rightarrow \qquad |A| \;=\; \frac{1}{\sqrt{n}}$$

Take real A $\qquad b^\dagger|n> \;=\; \sqrt{n+1}|n+1>$

Analogously $\qquad b\;|n> \;=\; \sqrt{n}|n-1>$

■

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$$
\begin{aligned}
|n> \;&=\; \frac{(b^\dagger)^n|0>}{C} \\
&=\; \frac{(b^\dagger)^{n-1}b^\dagger|0>}{C} \\
&=\; \frac{(b^\dagger)^{n-1}|1>}{C} \;=\; \frac{(b^\dagger)^{n-2}\sqrt{2}\;|2>}{C} \\
&=\; \frac{\sqrt{n}\cdots\sqrt{2}\;\sqrt{1}\;|n>}{C} \;\rightarrow\; C \;=\; \sqrt{n!}
\end{aligned}
$$

$$|n> \;=\; \frac{(b^\dagger)^n}{\sqrt{n!}}|0>$$

Bibliography

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