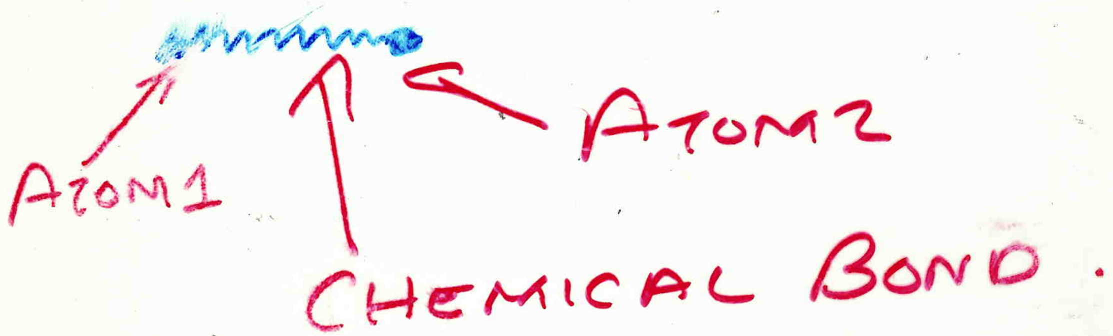
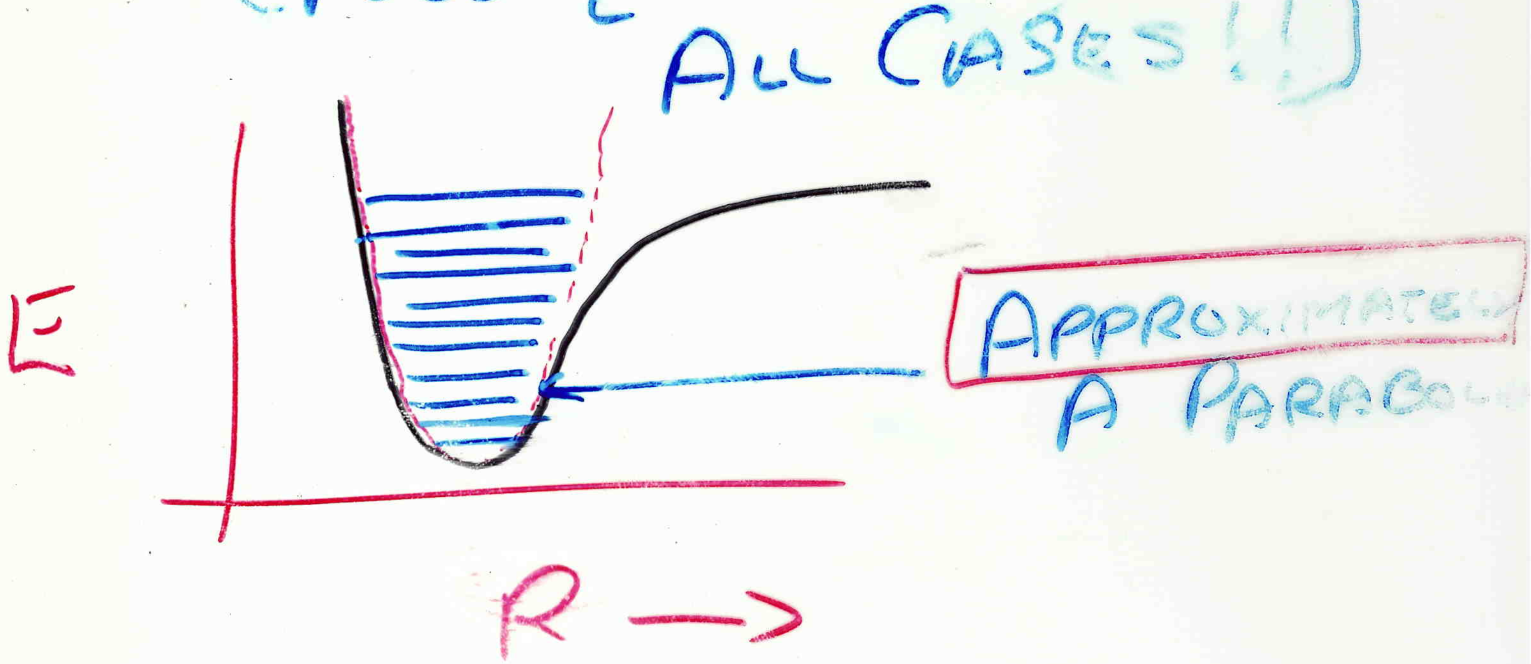
HARMONIC OSCILLATOR

WHY?



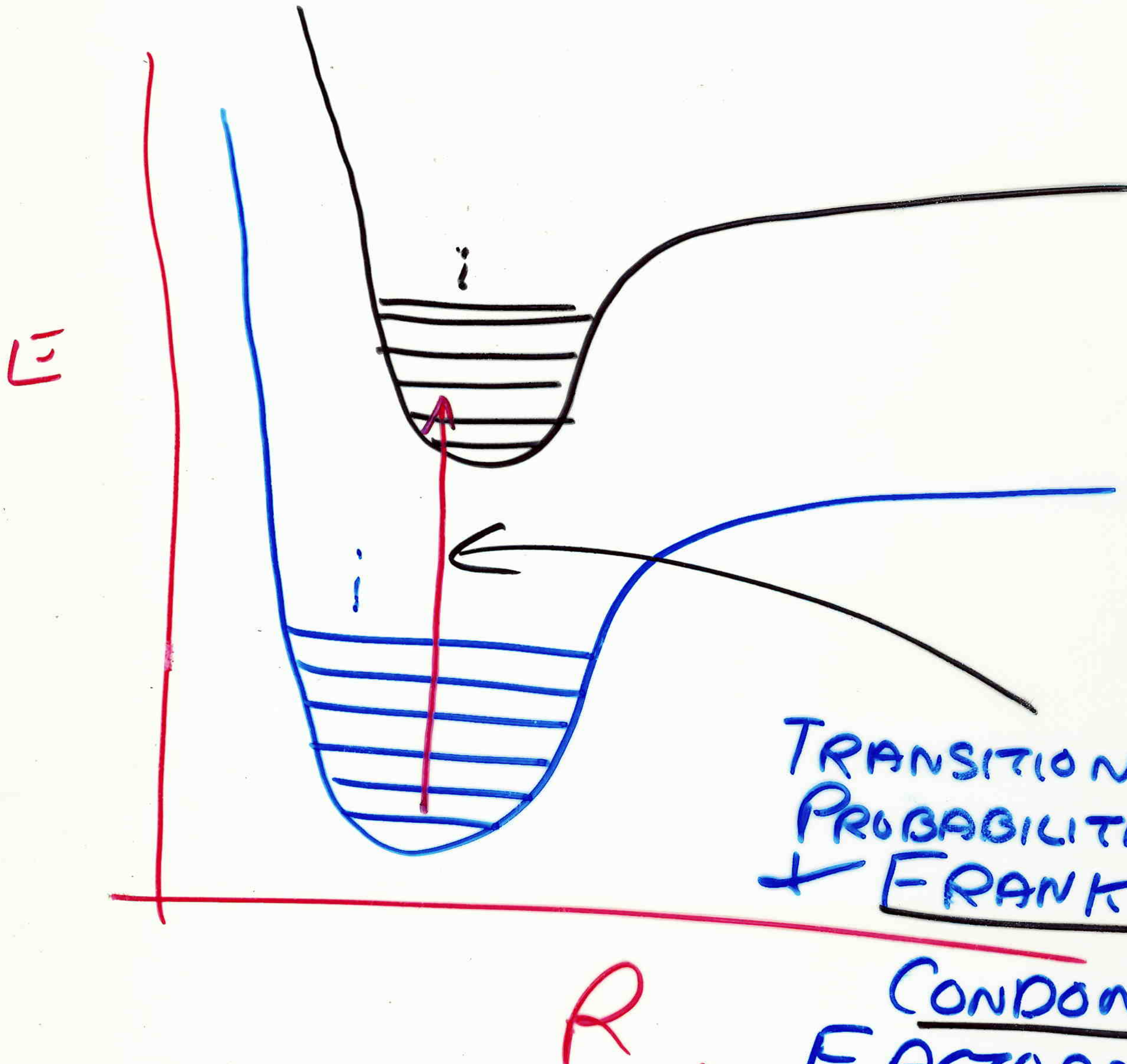
[ASSUME THIS IS A SPRING!!]

WORKS WELL IN MANY CASES [OF COURSE NOT ALL CASES!!]



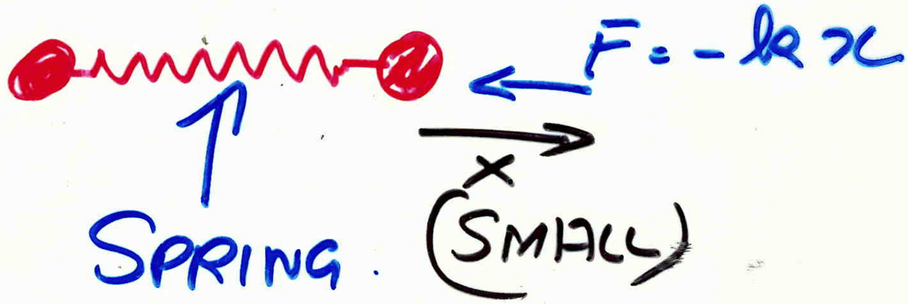
WE CAN DO A LOT. WITH JUST HO!!

Eg.



TRANSITION PROBABILITIES + FRANK-CONDON FACTORS FROM H.O.

The Story Of The Spring



$$F = -kx$$

[A Restoring Force]

Potential Energy While It Oscillates!

$$E = -\int F\,dx = \int +kx \cdot dx$$

$$= +\frac{1}{2}kx^2.$$

8. So (as usual :-)) we write the solution to the Harmonic oscillator as:
$$\psi(x) = \exp\left[-\frac{\alpha}{2}x^2\right] f(x) \tag{13.6}$$
and again we want to approximate $f(x)$ as a power series (as we did earlier for the hydrogen atom).

9. And when substitute this into the differential equation we can get an equation that involves the coefficients of the power series used to approximate the function $f(x)$. And we can equate like powers of x^i for all values i. We end up with another *special function* as a solution to this equation. And this function is known as the Hermite polynomials!! I am gonna solve this on the board so you guys have an idea how one would solve such an equation.

$$\psi''(x) = e^{-(\alpha/2)x^2}\left[f''(x) - 2\alpha x f'(x) + \alpha^2 x^2 f(x) - \alpha f(x)\right]$$

Eq. (13.2): $f''(x) - 2\alpha x f'(x) + \alpha^2 x^2 f(x) - \alpha f(x) + (\lambda - \alpha^2 x^2) f(x)$

$\therefore f''(x) - 2\alpha x f'(x) + (\lambda - \alpha) f(x) = 0$

$y = \sqrt{\alpha}\, x$; $\quad f(x) \equiv H(y)$

$\frac{df}{dx} = \sqrt{\alpha}\,\frac{dH}{dy}$

$\frac{d^2f}{dx^2} = \alpha\,\frac{d^2H}{dy^2}$.

$$\boxed{\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + \left(\frac{\lambda}{\alpha} - 1\right)H = 0}$$

$$f''(x) - 2\alpha x\, f'(x) + (1-\alpha) f(x) = 0 \rightarrow (A).$$

$$f(x) = \sum_{i=0}^{\infty} a_i\, x^i .$$

$$f'(x) = \sum_{i=1}^{\infty} a_i \cdot x^{i-1}$$

$$f''(x) = \sum_{i=2}^{\infty} a_i\, i\,(i-1)\, x^{i-2}$$

Using these in Eq. (A) :

$$\left[\sum_{i=2}^{\infty} a_i\, i(i-1) x^{i-2}\right] - 2\alpha\left[\sum_{i=1}^{\infty} a_i \cdot i\, x^{i}\right] + (1-\alpha)\left[\sum_{i=0}^{\infty} a_i x^{i}\right] = 0$$

$$\Rightarrow \left[\sum_{k=0}^{\infty} a_{k+2}(k+2)(k+1)\, x^{k}\right] - 2\alpha\left[\sum_{k=1}^{\infty} a_k \cdot k\, x^{k}\right] + (1-\alpha)\left[\sum_{k=0}^{\infty} a_k x^{k}\right] = 0$$

$$\Rightarrow x^0\left[a_2 \cdot 2 + (\lambda-\alpha)\,a_0\right] +$$

$$x^1\left[a_3(3)(2) - 2\alpha\,a_1 + (\lambda-\alpha)\,a_1\right] +$$

$$x^2\left[a_4(4)(3) - 2\alpha\,a_2(2) + (\lambda-\alpha)\,a_2\right] +$$

$$x^3\left[a_5(5)(4) - 2\alpha\,a_3(3) + (\lambda-\alpha)\,a_3\right] +$$

$$\ldots\ldots = 0 \longrightarrow (B)$$

This is basically:

$$c_0 x^0 + c_1 x^1 + c_2 x^2 + \ldots\ldots + \ldots = 0.$$

And for the left side to be equal to zero,

$$c_0 = c_1 = c_2 = \ldots = c_i = 0.$$

$$\Rightarrow a_2 = -\frac{a_0(\lambda-\alpha)}{2}.$$

or $a_{k+2} = -\,a_k\left[\left(\frac{\lambda-\alpha}{2}\right) - 2\cancel{\alpha}(k)\right]$

This is because Eq. B can also be written as:

$$x^0\left[2a_2 + (A-\alpha)a_0\right] + \sum_{k=1}^{\infty} x^k\left[a_{k+2}(k+2)(k+1) - a_k\left(2\alpha k - (A-\alpha)\right)\right] = 0.$$

Now as $k \to \infty$.

$$a_{k+2} \approx \frac{2k\alpha}{k^2}a_k = \frac{2\alpha}{k}a_k$$

$\Rightarrow$ Eq B as $k \to \infty$.

$$\sum_k \frac{\alpha^k}{(k/2)!}x^k \approx e^{+\alpha x^2}.$$

That diverges as $x \to \infty$

So the series:

$$f(x) = \sum_{i=0}^{I_{max}} a_i x^i$$

Has to be TRUNCATED.

Say; for $k = I_{max}$

$(\lambda - \alpha) - 2\alpha I_{max} = 0.$

all 'a_k' for $k > I_{max}$

$a_k = 0.$

THE SERIES TRUNCATES

$\downarrow$

$\lambda - \alpha - 2\alpha I_{max} = 0.$

$\Rightarrow \lambda - \alpha[2I_{max} + 1] = 0 \rightarrow$ ©

AFTER Eq. (13.27) WE SAID:

$$\lambda = \frac{2mE}{\hbar^2}$$

$$\& \ \alpha^2 = \frac{mk}{\hbar^2}$$

$$\Rightarrow \frac{\lambda}{\alpha} = \frac{2mE}{\hbar^2} \frac{\hbar}{\sqrt{mk}}.$$

$$k = m\omega^2$$

$$\Rightarrow \frac{\lambda}{\alpha} = \frac{2mE}{\hbar m\omega} = \frac{2E}{\hbar\omega}.$$

Using this in Eq. (C)

$$\left(\frac{\lambda}{\alpha}\right) - \left(2\,\mathrm{I}mmanc + 1\right) = 0$$

$$\Rightarrow \frac{2E}{\hbar\omega} = 2I_{max} + 1$$

$$\Rightarrow E = \frac{\hbar\omega}{2}\left[2I_{max} + 1\right].$$

OR

$$E_n = \frac{\hbar\omega}{2}\left[2n + 1\right] = \left(n + \frac{1}{2}\right)\hbar\omega$$

[SINCE 'I_{MAX}' IS AN INTEGER WE JUST CALLED IN 'n'].

QUANTIZED STATES:

AGAIN! ENFORCED BY.

B.C.S (BOUNDARY CONDNS).

$\left(n+\frac{1}{2}\right)\hbar\omega$

SO WE HAVE THE H.O. ENERGY. LEVELS.

$$\psi_m(x) = e^{-\alpha x^2/2} \cdot \sum_{n=0}^{m} a_n x^n .$$

$\{a_n\}$ are given by Eq.

$$a_{n+2} = -\frac{a_n\left[(\lambda - \alpha) - 2\alpha n\right]}{(n+2)(n+1)}$$

(RECURSION RELATION)

TRADITIONALLY WHATS DONE IS :

$$x \rightarrow \frac{r}{\sqrt{\alpha}} .$$

HERMITE POLYNOMIALS

$$\& \ \psi_m(x) = e^{-r^2/2} \cdot H_m(r) .$$

ANOTHER IMPORTANT. RELATION THAT APPEARS DUE TO THE RECURSION RELATION :

FOR ODD EIGENSTATES!

$m = 1, 3, 5 ..$ $\left[E_m = (m+\frac{1}{2})\hbar\omega \right]$

ONLY ODD POLYNOMIALS.

$$H_m(x) = - H_m(-x)$$

(ODD SYMMETRY UNDER INVERSION)

FOR EVEN 'm' : EVEN POLYNOMIALS

& $H_m(x) = + H_m(-x)$. [EVEN SYMMETRY