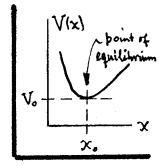
Schrödinger's Problem for a 1D Simple Harmonic Oscillator

Solos 10

C. Simple Harmonic Oscillator [Davydov, Sec. 26].

1. For any attractive potential V(x) which shows a minimum (or equilibrium pt) at some pt. X., do a Taylor expansion:

$$\rightarrow V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \dots$$
 (1)



near xo. Now at xo, have V'(xo) = O [i.e. the force is zero there], and have V"(x0)>0 [V(x) is concave upward]. Shift the zero of coordinates so that $x_0 = 0$ and $V(x_0) = V_0 = 0$. Then the leading term of V(x) is ...

$$V(x) = \frac{1}{2}kx^2$$
, near $x = 0$, $k = V''(0) > 0$, spring onst. (2)

This form of V(x) corresponds to a Hooke's Law force: F=- ox = - kx;

that is why k is called a "spring cost". Classically, a particle of mass in will execute a simple harmonic oscillation (SHO) about x=0 at the characteristic frequency: $\underline{\omega} = \sqrt{k/m}$ (so long as the oscillation amplitude is not too large). Since $k = m\omega^2$, V in Eq. (2) is sometimes written: $V(x) = \frac{1}{2} m\omega^2 x^2$.

The approximate form V= = 2kx2, for small oscillations of m about an equilibrium pt. in an essentially arbitrary but smoothly varying) attractive potential, has a ~ universal application -- this is the way bound states begin in most potential wells. The classical efth-of-motion, viz.

 $\rightarrow m\ddot{x} = -kx$, $^{n}/(\ddot{x} + \omega^2 x = 0)$, also has many applications; it is applied whenever the system of interest can be thought of as being connected by springs. There are successful theories of the inbrations of diatomic molecules, crystal vibrations (phonons), etc. based on this simple idea. So now we want the QM -- i.e. a solution to:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2}m\omega^2x^2\right) \psi = 0$$

$$\int \frac{Schrödinger's}{for a 1D SHO@fry. \omega}.$$

(4)

Simple Harmonic Oscillator (contd)

2. It is convenient to write Schrödinger's Egtn, Eq. (4) in terms of dimen-Scanless variables ξ (position) and λ lenergy), as defined by ...

$$\underline{\xi} = (\sqrt{m\omega/\hbar}) \times , \quad \underline{\lambda} = 2E/\hbar\omega \implies \frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2) \psi = 0.$$

As 151 > 00, the egth behaves asymptotically as...

$$\rightarrow \frac{d^2 \psi}{d \xi^2} - \xi^2 \psi \approx 0 \implies \underline{\psi(\xi)} \simeq \exp\left(\pm \frac{1}{2} \xi^2\right), \text{ as } |\xi| \rightarrow \infty.$$

 $\Psi \sim e^{+\frac{1}{2}\xi^2}$ is ruled out because Ψ can never be infinite (2sp. at $|\xi| = \infty$). To pick off the $\Psi \sim e^{-\frac{1}{2}\xi^2}$, we look for a solution of the form...

$$\rightarrow \Psi(\xi) = u(\xi) \exp\left(-\frac{1}{2}\xi^2\right), \qquad (7)$$

where U(\$) is a <u>polynomial</u> in \$ to be found. Limiting U(\$) to a combination of powers of \$, say ξ^n at most, ensures $\Psi(\xi) \to 0$ as $|\xi| \to \infty$. Put (7) into (5) to get:

$$\frac{d^2u}{d\xi^2} - 2\xi \frac{du}{d\xi} + (\lambda - 1)u = 0$$
| Hermite's Differential Eqtn (8)
(a confluent hypergeometric ODE)

3. The easiest way to "solve" Eq. (8) is to recognize it as a confenent hypergeometric ODE, i.e. an ODE of the form...*

$$\rightarrow z \frac{d^2u}{dz^2} + (c-z) \frac{du}{dz} - au = 0 \int_{\frac{1}{2}}^{w_f} \frac{z = \frac{1}{2}\xi^2}{2}, \frac{2a = -(\lambda - 1)}{2a = -(\lambda - 1)}, \frac{c = \frac{1}{2}}{2}.$$

Such an equation has a power series solution of the form ...

$$\rightarrow \mathcal{U}(\xi) = F(a,c; z) = \frac{\Gamma(c)}{\Gamma(a)} \sum_{k=0}^{\infty} \left[\frac{\Gamma(a+k)}{\Gamma(c+k)\Gamma(k+1)} \right] z^{k}, \quad \mathcal{U}_{\chi} = \frac{1}{2} \xi^{2}; \quad (10)$$

is an independent solution for U(5) is $Z^{1-c}F(a-c+1, 2-c; Z)$; this solution is an independent solution to the ODE when $c \neq integer$ (as is time, here). The F^{1s} are called "confluent <u>hypergeometric series</u>", and they are "polynomials" of or degree unless the index a=-n is some (-) we integer, with

Davydorques a concise recount of this ODE in his Appendix D, p. 619.

n=0,1,2,3,.... Since, in $V(\xi)=u(\xi)\exp(-\frac{1}{2}\xi^2)$, we need $u(\xi)=$ polynomial of finite degree (to keep V from diverging as $|\xi|\to\infty$) we impose the condition that in fact $\underline{a=-n}$. This quantizes the SHO energies, as...

$$\Rightarrow \alpha = -\frac{1}{2}(\lambda - 1) = -n \Rightarrow \lambda = 2E/\hbar\omega = 2n + 1;$$
by $E_n = (n + \frac{1}{2})\hbar\omega$, $w_1 = 0, 1, 2, ...$ \leftarrow allowed SHO energies. (11)

For each n-value, there is an eigenfen solution for U(E). It is a polynomial of nth degree, called a Hermite polynomial "Hn(E), and defined by ...

The normalized wevefons for the stationary states of the SHO are then

$$\Psi_{n}(\xi) = \mathcal{N}_{n} H_{n}(x) \exp\left(-\frac{1}{2}\xi^{2}\right), \quad \mathcal{N}_{n} = 1/(2^{n}n!\sqrt{\pi})^{1/2}$$
 (13)

The treatment of the SHO problem via the large number of tabulated results available for the confluent hypergeometric ODE is very compact... and similar compact treatments can be done for many other QM problems (and Just ODE's in general). This is a persuasive argument for learning the intricacies of hypergeometric of confluent hypergeometric ODE's, if you do not know them already.

4. A less alignet way of solving Hermite's Egtn (8) is by Frobenius' Method,

Viz. // put power series: $u(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$, into: $u'' - 2\xi u' + (\lambda - 1)u = 0$; Solve for $\{a_n\}$.

If When a=-n, the series coefficient in Eq.(10): $\frac{\Gamma(a+k)}{\Gamma(a)}$ = a(a+1)... (a+k-1), will be wantsh for all k>n; the power series truncates at the term $2^k|_{k=n}$.

By carrying out the operation in Eq. (14), we find $u''-2\xi u'+(\lambda-1)u=0$ requirec: $\sum_{n=0}^{\infty} [fcn \circ f \ n \notin a_n] \xi^n=0$, and then by setting the $[\]=0$, we obtain

$$\rightarrow a_{n+2} = \left[\frac{2n+1-\lambda}{(n+1)(n+2)}\right] a_n, \text{ for } n=0,1,2,3,...$$

This is the "recursion relation" for the series coefficients that is specific to Hermite's ODE. Since we are solving a 2nd order ODE, there are two arbitrary consts in the solution; in (15), we can choose these to be a a 4 91. Then we generate two classes of solutions, of ± parity, as follows:

$$\underline{\underline{I}} : \underbrace{a_0 \neq 0, \ a_1 = 0}_{\text{a_1} = 0} \implies \begin{cases} a_z = \frac{1}{2}(1 - \lambda)a_0, \ a_4 = \frac{1}{12}(5 - \lambda)a_z, \text{ etc.}; \\ a_1 = a_3 = a_5 = \dots = 0; \\ \lambda \psi(-\xi) = (+) \psi(+\xi) \end{cases}$$

$$\underbrace{a_0 \neq 0, \ a_1 = 0}_{\text{a_1} = 0} \implies \begin{cases} a_1 = a_3 = a_5 = \dots = 0; \\ \psi(\xi) = \psi(\xi)e^{-\frac{1}{2}\xi^2}, \text{ have } \underbrace{(+) \text{ parity}}_{\text{a_1} = 0}.$$
(16A)

$$\underline{\underline{II}} \cdot \underline{0}_{0} = 0, \, \underline{0}_{1} \neq 0 \implies \begin{cases}
0_{1} = \underline{0}_{4} = \underline{0}_{6} = \dots = 0; \\
0_{3} = \frac{1}{6}(3-\lambda)\underline{0}_{1}, \, \underline{0}_{5} = \frac{1}{10}(7-\lambda)\underline{0}_{3}, \, \underline{\text{etc.}}, \, \underline{\psi}(-\xi) = \underline{\psi}(+\xi)
\end{cases}$$

$$\underline{\underline{II}} \cdot \underline{0}_{0} = 0, \, \underline{0}_{1} \neq 0 \implies \begin{cases}
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\end{cases}$$

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\end{cases}$$

$$\underline{\underline{II}} \cdot \underline{0}_{0} = 0, \, \underline{0}_{1} \neq 0 \implies \begin{cases}
0_{1} = \underline{0}_{1} = 0, \, \underline{0}_{1} \neq 0, \, \underline{0}_{2} = 0; \\
0_{1} = 0, \, \underline{0}_{1} \neq 0, \, \underline{0}_{2} = 0; \\
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0_{3} = 0, \, \underline{0}_{3} = 0; \\
0_{4} = 0, \, \underline{0}_{3} =$$

Class I & II solutions, of ±parity, are chosen to emulate the reflection symmetry of the SF10 potential V(x)= ½ kx², by V(-x) = V(x). We did this also for the rectangular potential well (see Notes, pp. 90125 1-2, Eq.(4)).

An essential requirement for the series solutions $u(\xi) = \sum_{k=0}^{\infty} a_k \xi^k$ as generated above are that they do not $\to \infty$ as fast as $\exp(+\frac{1}{2}\xi^2)$, when $|\xi| \to \infty$; otherwise $\Psi(\xi) = u(\xi) e^{-\frac{1}{2}\xi^2}$ will diverge. A way to ensure that this is true is to make the $u(\xi)'^s = \operatorname{polynomials}$ of finite degree. Look at (15):

$$\frac{\alpha_{n+2}/\alpha_n = [(2n+1)-\lambda]/(n+1)(n+2)}{m},$$

Evidently, if we impose that the parameter $\lambda = 2E/\hbar \omega$ [from Eq. (5)] is

Such that $\underline{\lambda=2n+1}$, then in (17) we have $a_{n+2}=0$, and also all the sub-Sequent an vanish for N>n+z. The series $u(\xi)=\sum_{k=0}^{\infty}a_k\xi^k \rightarrow \sum_{n=0}^{\infty}a_k\xi^k$ becomes a polynomial of finite degree n, and as $|\xi| \rightarrow \infty$, the wavefor $\Psi \sim \xi^n e^{-\frac{1}{2}\xi^2}$ properly vanishes. This condition quantizies the SHO energies, as...

$$\lambda = 2n+1 \implies \boxed{E_n = (n+\frac{1}{2}) \hbar \omega}, \quad w_j = 0, 1, 2, ...$$

This result confirms the energies quoted in Eq. (11), p. Sol= \$ 12 preceding.

REMARKS On the quantized SHO.

- 1. As for the rectangular potential well (pp. Sol=s 1-4), the system quantization results from boundary conditions imposed on 4; here 41x) > 0 as 1x1+00.
- 2. The condition $\lambda=2n+1$ in (18) is a way of ensuring $\Psi=ue^{-\frac{1}{2}\xi^2}$ vanishes at ∞ . One can show it is the only way. Any choice $\frac{4}{2}$ $\lambda \neq 2n+1$ will give an ∞ series for $u(\xi)=\sum_{k}a_k\xi^k$, and it can be shown that this series diverges faster than $e^{+\frac{1}{2}\xi^2}$ as $|\xi| \to \infty$. So $\lambda \neq 2n+1 \Rightarrow \Psi=ue^{-\frac{1}{2}\xi^2}$ diverges.
- 3. The choice λ = 2n+1 in the Series for $\mathcal{N}(x)$ allows us to write ...

$$\rightarrow u(\xi) = FI_n(\xi) = \sum_{k=0}^{\infty} a_k \xi^k$$
, $u_j = \frac{2(k-n)}{(k+1)(k+2)} a_k \{FIermite\}$

as particular solutions to Exermite's ODE, Eq. 18). More on these, later.

4: The energies in Eq. (18) bear on <u>Planck's Hypothesis</u> (p. Intro. 4, Eq. (10)). He could (and did) picture the atomic oscillators that emitted radiation from the walls of his BB cavity as obeying a SHO egtn: $\dot{\phi} + \omega^2 \dot{\phi} = 0$, $^{9}\phi = 0$ ribration amplitude, and $\omega = 0$ oscillation freq. Then, by solving this egtn for ϕ , and insisting ϕ be finite, he would get: $E_n = (n + \frac{1}{2}) t_i \omega$, as above. Planck used just the ntw part of E_n , discarding the "gero-point" energy $\frac{1}{2}t_i\omega$. But the $\frac{1}{2}t_i\omega$ is needed for consistency "uncertainty relations.

Study of SHO eigenfons. The Hulz) as explicit polynomials.

5. We shall now study the SHO eigenfons $V_n(\xi) = N_n H_n(\xi) e^{-\frac{1}{2}\xi^2}$ in detail. We do this not only because the SHO is an important QM system, but also because the analysis that follows is typical of what can be done for other "interesting" QM wavefons, and we should look at the details for at least one example. What we shall do here is:

(A) Find explicit forms for the Hermite polynomials.

(B) Show that H'n = 2n Hn-1. Then find the "generating for" for the Hn (E).

(C) Establish Rodrigues' Formula: Hnlx)=(-1 ex2 (d/dz) e-32.

(D) Show orthogonality & find normalization for the SHO Yn (E)'s.

When we are done, we will be able to show (among other things) how the QM SHO emulates a <u>classical</u> oscillator when n > 00 (Correspondence Principle works!).

(A) Find Hermite polynomials explicitly.

→ By Eq. (19) where:
$$H_n(\xi) = \sum_{k=0}^{n} a_k \xi^k$$
, $a_k = \frac{2(k-n)}{(k+1)(k+2)} a_k$. (20)

By repeating the recursion from an down to as or a1, one finds ...

$$\alpha_{N} = \left[\frac{2^{N}}{N!} \left(-\right)^{\frac{N}{2}} \left(\frac{N}{2}\right)!\right] \alpha_{0} \int_{-\infty}^{\infty} for N \qquad (21)$$

$$\alpha_{N} = \left[\frac{2^{N-1}}{N!} \left(-\right)^{\frac{N-1}{2}} \left(\frac{N-1}{2}\right)!\right] \alpha_{1} \int_{-\infty}^{\infty} for N \qquad (21)$$

The costs as & an are still free. It is constromery to choose them so that the highest order term in the series for Hn has a coefficient an = 2n. Thus:

$$\frac{n \text{ even} : \text{ Choose} : a_0 = (-)^{\frac{n}{2}} n! / (\frac{n}{2})! \implies a_n = 2^n;}{n \text{ odd} : \text{ Choose} : a_1 = 2 \cdot (-)^{\frac{n-1}{2}} n! / (\frac{n-1}{2})! \implies a_n = 2^n.}$$

The resulting Hermite polynomials are then of the form (for n=both evan 4 odd):

$$\longrightarrow F_{1n}(\xi) = (2\xi)^{n} - \frac{n(n-1)}{1!} (2\xi)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!} (2\xi)^{n-4} - \dots$$
 (23)

It is easy to see that for n=odd : Hnlo)=0; the last term in the series oc 3.

In the other hand, when $n=even: H_n(0)=a_0=(-)^{\frac{n}{2}}n!/(\frac{n}{2})!$. The first few polynomials that follow from (23) are...

$$\rightarrow$$
 H₀(ξ) = 1, H₁(ξ) = 2 ξ , H₂(ξ) = 4 ξ ²-2, H₃(ξ) = 8 ξ ³-12 ξ , ...

(B) Show H'n = 2n Hn-1. Find generating for for the Hn (5).

First show the identity. The Hn(3) satisfy the ODE: $\frac{d^2}{d\xi}H_n-2\xi\frac{d}{d\xi}H_n+2nH_n$ =0. If we operate through this egts by d/dx, we can write...

But Eq. (25) is also satisfied by Hny. Then: Hn = CHny, where C = cust. To fix C, look at Hn & Hny as 3 > large. The leading terms are...

$$\frac{49}{H_n'} = C H_{n-1}$$
, with $C = 2n$. (26)

This relation is useful in finding the "generating fen" g(s, \(\xi\)) for the Hermite polynomials. By definition, g(s, \(\xi\)) is that fen which—expanded in a Taylor Series in S— has the Hn(\(\xi\)) as expansion coefficients, i.e.

$$\rightarrow \xi(s,\xi) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi). \tag{27}$$

To find an explicit form for g (whose uses will be come apparent), differentiate (27) by 3/3%, and use (26)...

But \$15,0) can be evaluated from the defining extra (27), as ...

$$\rightarrow g(s,0) = \sum_{k=0}^{\infty} \frac{S^{2k}}{(2k)!} H_{2k}(0) = \sum_{k=0}^{\infty} (-)^k \frac{S^{2k}}{k!} = e^{-S^2}.$$
 (29)

Rodrigues' Formula for Hy. Orthogonality & Normalization of Vn. Solas U.

At this print, we have an expression for the generating for &, i.e...

$$+g(s,\xi)=\sum_{n=0}^{\infty}\frac{s^n}{n!}H_n(\xi)=e^{-s^2+2s\xi}=e^{\xi^2-(s-\xi)^2}.$$
 (30)

This shows glo, = Holz = 1, so the norm is correct, per Eq. (24).

(C) Establish Rodrigues' Formula: Hn(3)=1-1" e32 (d/d2)" e-32.

The Taylor Series for the generating form in Eq. (30) can also be written: $g(s,\xi) = \sum_{n=0}^{\infty} \frac{s^n}{n!} \left[\left(\frac{\partial}{\partial s} \right)^n g(s,\xi) \right]_{s=0}^s, \quad so: H_n(\xi) = \left[\left(\frac{\partial}{\partial s} \right)^n g(s,\xi) \right]_{s=0}^s$ i.e., $H_n(\xi) = e^{\xi^2} (\partial |\partial s|^n e^{-(s-\xi)^2}|_{s=0}^s$ (31)

It is clear why g is called a "generating fon"... the Hn (3) are generated by g and its derivatives. To simplify (31), note that we are differentiating a fon of (5-8) only, so that the operation 3/35 is equivalent to -3/35, and $(3/35)^n = (-)^n (3/35)^n$. Then we have...

This is Rodrigues' formula, as desired.

(D) Orthogonality & normalization for the SHO eigenstates $V_n(x)$. Write the SHO eigenfens as

$$\frac{\Psi_n(x) = N_n e^{-\frac{1}{2}\xi^2} H_n(\xi)}{\xi = \sqrt{m\omega/\hbar} x}.$$
 (33)

We want to demonstrate <u>orthogonality</u>, i.e. $\int_{0}^{\infty} \Psi_{n}^{*}(x) \Psi_{m}(x) dx = 0$, when $m \neq n$. And we want to <u>normalize</u> the Ψ_{n} , i.e. find the enst Nn such that $\int_{0}^{\infty} |\Psi_{n}(x)|^{2} dx = 1$. Both tasks are accomplished by considering the following integral over generating fens:

→
$$J(s,t) = \int_{-\infty}^{\infty} g(s,\xi) g(t,\xi) e^{-\xi^2} d\xi$$
. (34)

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In detail, (34) neads... p form in Eq. (30) def of g in Eq. (27)

T(s,t) = \int_{\infty} e^{-5^2+25\xi} e^{-t^2+2t\xi} e^{-\xi^2} d\xi = \int_{m,n=0}^{\infty} \frac{s^n}{n!} \frac{t^m}{m!} \int_{\infty} e^{-\xi^2} H_m(\xi) H_n(\xi) d\xi

The LHS integral is tabulated...

Expand this result in a power series and rewrite (35) as...

$$\left[\sum_{n=0}^{\infty} \frac{S^{n}}{n!} (\sqrt{\pi} 2^{n}) t^{n} = \sum_{n=0}^{\infty} \frac{S^{n}}{n!} \left\{ \sum_{m=0}^{\infty} \left(\frac{1}{m!} \int_{-\infty}^{\infty} e^{-\xi^{2}} H_{m}(\xi) H_{n}(\xi) d\xi \right) t^{m} \right\}, \quad (37)$$

For (37) to be an identity, must have...

A Imn = 0 for m = n, so: \$ e^-\xi^2 Hm(\xi) Hn(\xi) d\xi = 0, when m = n.

For: $\psi_{k}(x) = N_{k}e^{-\frac{1}{2}\xi^{2}}H_{k}(\xi)$, have: $\int_{-\infty}^{\infty} \psi_{m}^{*}(x)\psi_{n}(x)dx = 0$, $m \neq n$. [38]

B Inn = √π 2", for m=n → ∫ e-ξ² H²(ξ)dξ = √π 2"·n!;

... then $\iint_{-\infty}^{\infty} |\psi_n(x)|^2 dx = \frac{|N_n|^2}{\sqrt{m\omega/k}} \int_{-\infty}^{\infty} e^{-\xi^2} H_n^2(\xi) d\xi = 1$,

... requires / $N_n = (\sqrt{m\omega/\hbar}/\sqrt{\pi} \cdot 2^n n!)^{1/2}$, normin cost.

With these results, we can write down the orthonormal SHO eigenfons:

$$\psi_{n}(x) = \left(\frac{\alpha/\sqrt{\pi}}{2^{n}n!}\right)^{1/2} e^{-\frac{1}{2}\alpha^{2}x^{2}} H_{n}(\alpha x), \quad \alpha = \sqrt{m\omega/\hbar}$$

$$ta has dimensions$$
obeying:
$$\int_{-\infty}^{+\infty} \psi_{k}^{*}(x) \psi_{n}(x) dx = \delta_{kn} = \sigma_{kn} \text{ wave # (inverse)}$$

The ground state wavefor (state with n=0 & energy Eo= = thw) is

ground }
$$\frac{y_0(x)}{x} = (\alpha/\sqrt{\pi})^{1/2} e^{-\frac{1}{2}\alpha^2x^2}$$
.

This is a Gaussian distribution of spatial extent $\Delta x \sim \frac{1}{\alpha} = \sqrt{\hbar/m\omega}$.