We can think of $\vec{A}(\vec{r},t)$ as a generalized coordinate (of infinite dimensionality), with generalized velocity $\dot{\vec{A}}(\vec{r},t)$. The normal modes are again plane waves. In this case there is no restriction on $\vec{k}$ (continuously infinite # of degrees of freedom!), but due to the masslessness of photons (or Gauss' law) only transverse polarizations are allowed.

→ Chapter 18.

7.2 The Hamilton operator for the harmonic oscillator in coordinate basis representation

$$i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$$

with (for 1 particle in 1 dimension)

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2$$

The time evolution is trivial once we have solved the eigenvalue problem

$$\hat{H}|E_n\rangle = E_n|E_n\rangle$$

It is given by

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_n |E_n\rangle\langle E_n| e^{-iE_nt/\hbar}$$

Let's look at this eigenvalue problem.

First, for any $|\psi\rangle$,

$$\langle \hat{H} \rangle = \frac{1}{2m} \langle \psi | \hat{P}^2 | \psi \rangle + \frac{1}{2} m\omega^2 \langle \psi | \hat{X}^2 | \psi \rangle$$

$$= \frac{1}{2m} \langle \psi | \hat{P}^+ \hat{P} | \psi \rangle + \frac{1}{2} m\omega^2 \langle \psi | \hat{X}^+ \hat{X} | \psi \rangle$$

$$= \frac{1}{2m} \langle \hat{P}\psi | \hat{P}\psi \rangle + \frac{1}{2} m\omega^2 \langle \hat{X}\psi | \hat{X}\psi \rangle \geq 0$$

So, since $|\psi\rangle$ can also be any eigenstate, we see that $\hat{H}$ cannot have any negative eigenvalues.

In the $\hat{X}$-basis the eigenvalue equation reads

$$\langle x | \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2 | E \rangle = E \langle x | E \rangle$$

$$\uparrow$$

$$\int dx' |x'\rangle\langle x'| , \quad \langle x | \hat{P}^2 | x' \rangle = -\hbar^2 \delta(x-x') \frac{d^2}{dx'^2}$$

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

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

How to solve this differential equation? Watch closely!

1) Introduce dimensionless variables:

$$x \rightarrow \xi = \frac{x}{x_0} \qquad (x = x_0 \xi)$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2} + \frac{2mE x_0^2}{\hbar^2} \psi - \frac{m^2\omega^2 x_0^4}{\hbar^2} \xi^2 \psi = 0$$

Any x_0 with units of length will make the equation dimensionless, but each problem has its own natural length scale which, if you use it for scaling, makes the equations look particularly simple.

Here, we see that by choosing $\boxed{x_0 = \sqrt{\frac{\hbar}{m\omega}}}$ the last term gets a coefficient of unity.

Similarly we can measure the energy in "natural units",

$$\boxed{\varepsilon \equiv \frac{E}{\hbar\omega}} = \frac{E m x_0^2}{\hbar^2}$$

$$\Rightarrow \boxed{\frac{d^2\psi}{d\xi^2} + (2\varepsilon - \xi^2)\psi(\xi) = 0}.$$

2) Try to figure out the behavior of the solution in certain limits: $\xi \to 0$, $\xi \to \infty$

(i) $\xi \to \infty$ $(\xi \gg 2\varepsilon)$ $\Rightarrow \psi'' - \xi^2\psi = 0$

$$\Rightarrow \boxed{\psi \xrightarrow[\xi \gg 2\varepsilon]{} A' \xi^m e^{\pm \xi^2/2}}$$

(Check: $\psi' \to A'\left(m\xi^{m-1} e^{\pm\xi^2/2} \pm \xi^{m+1} e^{\pm\xi^2/2}\right)$

$$\psi'' \to A'\left(m(m-1)\xi^{m-2} \pm m\xi^m \pm (m+1)\xi^m + \xi^{m+2}\right)e^{\pm\xi^2/2}$$

$$= \xi^2 A' \xi^m e^{\pm\xi^2/2}\left(1 \pm \frac{2m+1}{\xi^2} + \frac{m(m-1)}{\xi^4}\right)$$

$$\xrightarrow[\xi\to\infty]{} \xi^2\psi \checkmark \quad)$$

Now, only the solution $\sim e^{-\xi^2/2}$ will be normalizable,

so we discard the solution $\sim e^{+\xi^2/2}$.

(ii) $\xi \to 0$ $(\xi \ll 2\varepsilon)$ $\Rightarrow$ $\psi'' + 2\varepsilon\psi = 0$

$$\Rightarrow \psi \xrightarrow[\xi\to 0]{} A\cos(\sqrt{2\varepsilon}\,\xi) + B\sin(\sqrt{2\varepsilon}\,\xi)$$

Consistency with dropping the term $\sim \xi^2\psi$ in the differential equation requires that we expand the sin and cos and also drop all terms $\sim \xi^2$ and higher:

$$\psi \xrightarrow[\xi\to 0]{} A + C\xi + O(\xi^2) \qquad (C = \sqrt{2\varepsilon}\,B)$$

From (i) ⊕ (ii) we infer

$$\boxed{\psi_m(\xi) = u_m(\xi)\, e^{-\xi^2/2}} \qquad (*)$$

where $u_m(\xi) \xrightarrow[\xi\to 0]{} A + C\xi +$ higher powers

and $u_m(\xi) \xrightarrow[\xi\to\infty]{} A'\xi^m +$ lower powers

We do not know yet which values of m are allowed.

(iii) Plug the ansatz $(*)$ back into the equation for ψ:

$$\Rightarrow \boxed{u'' - 2\xi u' + (2\varepsilon - 1)\, u = 0} \qquad (**)$$

If we make a power-law ansatz

$$u(\xi) = \xi^\alpha \sum_{n=0}^{\infty} C_n \xi^n$$

(ii) convinces us that $\alpha = 0$ should work:

$$u(\xi) = \sum_{n=0} C_n \xi^n$$

Feeding this into (**) gives

$$\sum_{n=0}^{\infty} C_n \left[n(n-1)\xi^{n-2} - 2n\xi^n + (2\varepsilon-1)\xi^n \right] = 0$$

or (setting $n = n'+2$, $n' \geq 0$ in the first term, since it really only starts at $n=2$)

$$\sum_{n=0}^{\infty} \left[C_{n+2}(n+2)(n+1) + C_n(2\varepsilon - 1 - 2n) \right] \xi^n = 0 \qquad \forall \xi \,!$$

$$\Rightarrow \boxed{C_{n+2} = C_n \frac{2n+1-2\varepsilon}{(n+2)(n+1)}}$$ recursion relation for the expansion coefficients!

So if we specify somehow C_0, C_1, the recursion relation generates all other C_n for us.

$$\Rightarrow u(\xi) = C_0 \left[1 + \frac{1-2\varepsilon}{(0+2)(0+1)}\xi^2 + \frac{1-2\varepsilon}{(0+2)(0+1)} \frac{4+1-2\varepsilon}{(2+2)(2+1)}\xi^4 + \dots \right]$$

$$+ C_1 \left[\xi + \frac{2+1-2\varepsilon}{(1+2)(1+1)}\xi^3 + \frac{2+1-2\varepsilon}{(1+2)(1+1)} \frac{6+1-2\varepsilon}{(3+2)(3+1)}\xi^5 + \dots \right] \qquad (\#)$$

For large ξ, $u(\xi) \to \xi^m$ with a finite power m. The above series does not do this unless we ensure that the series breaks off after a finite number of steps!

This forces discrete values for ε. For any other value of ε (such that the series in (#) does not break off) it can be shown that the series behaves for large ξ as $\xi^m e^{+\xi^2}$ such that $u(\xi)e^{-\xi^2/2} \sim \xi^m e^{+\xi^2/2}$,

i.e. the other, non-normalizable solution that we had to throw away.

(iv) So, which values of ε make the series break off?

Answer $\quad 2\varepsilon = 2m+1 \quad \Rightarrow \quad \boxed{\varepsilon_m = \frac{2m+1}{2}, \; m = 0,1,2,\ldots}$

For m even, we must also set $c_1 = 0$ (otherwise the odd-power series does not truncate), and for odd m we must set $c_0 = 0$.

So for $\begin{Bmatrix}\text{odd}\\ \text{even}\end{Bmatrix} m$, $u(\xi)$ has only $\begin{Bmatrix}\text{odd}\\ \text{even}\end{Bmatrix}$ powers of ξ.

The highest power is ξ^m, since for $2m+1-2\varepsilon = 0$ the next higher coefficient c_{m+2} vanishes.

So we have a discrete eigenvalue spectrum

$$\boxed{E_m = \left(m+\tfrac{1}{2}\right)\hbar\omega \qquad m = 0,1,2,\ldots}$$

with eigenfunctions

$$\psi_m(\xi) = \begin{Bmatrix} c_0 + c_2\xi^2 + c_4\xi^4 + \cdots + c_m\xi^m \\ c_1\xi + c_3\xi^3 + c_5\xi^5 + \cdots + c_m\xi^m \end{Bmatrix} \cdot e^{-\xi^2/2} \qquad \begin{Bmatrix} m \text{ even} \\ m \text{ odd} \end{Bmatrix}$$

The polynomials in curly brackets are called <u>Hermite polynomials, $H_n(\xi)$</u>:

$$H_0(\xi) = 1 \qquad\qquad H_3(\xi) = -12\left(\xi - \tfrac{2}{3}\xi^3\right)$$
$$H_1(\xi) = 2\xi \qquad\qquad H_4(\xi) = 12\left(1 - 4\xi^2 + \tfrac{4}{3}\xi^4\right)$$
$$H_2(\xi) = -2(1-2\xi^2)$$

The normalized solutions are

$$\boxed{\psi_n(x) = \underbrace{\left(\frac{m\omega}{\pi\hbar\, 2^{2n}(n!)^2}\right)^{1/4}}_{A_n} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega x^2}{2\hbar}}}$$

There is a short way to figure out the normalization constant that we will encounter a bit later.

A few notes about Hermite polynomials:

$$H_n'(\xi) = 2n\, H_{n-1}(\xi)$$

$$H_{n+1}(\xi) = 2\xi\, H_n(\xi) - 2n H_{n-1}(\xi)$$

$$\frac{1}{\sqrt{\pi}\, 2^n n!}\int_{-\infty}^{\infty} H_n(\xi)\, H_{n'}(\xi)\, e^{-\xi^2} = \delta_{nn'}$$ (orthonormality of normalized eigenfcts.)

(v) Propagator:

$$\boxed{\begin{aligned} \mathcal{U}(x,t;\, x',t') &= \langle x |\, \hat{\mathcal{U}}(t,t')\, | x' \rangle \\ &= \sum_{n=0}^{\infty} A_n H_n\left(\sqrt{\tfrac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega^2}{2\hbar} x^2} A_n H_n\left(\sqrt{\tfrac{m\omega}{\hbar}}\, x'\right) e^{-\frac{m\omega^2}{2\hbar} x'^2} \\ &\quad \cdot e^{-i(n+\frac{1}{2})\omega(t-t')} \end{aligned}}$$

In chapter 8 we will find an elegant way to do the sum over n analytically, with result

$$\boxed{\mathcal{U}(x,t;x't') = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega(t-t'))}}\; e^{\frac{im\omega}{\hbar}\frac{(x^2+x'^2)\cos(\omega(t-t')) - 2xx'}{2\sin(\omega(t-t'))}}}$$

Hard to believe, but true!

(vi) Discussion

(a) The energy is quantised. But unlike the infinitely high square well, where $E_n \sim n^2$, here $E \sim n$, i.e. the energy eigenvalues are equally spaced. This is related to the potential becoming wider in x at higher energies.

The quantization arises again (as in the case of the square well) by the requirement that the solution be normalizable, i.e. part of Hilbert space.

Classical limit:

A particle with mass 2g oscillating at $\omega = \frac{1\,\text{rad}}{\text{sec}}$ with amplitude $x_0 = 1\,\text{cm}$ has $E = \frac{1}{2} m\omega^2 x_0^2 = 1\,\text{erg}$

The gap between energy eigenvalue is

$$\Delta E = \hbar\omega \cong 10^{-27}\,\text{erg}$$

So for a classical, macroscopic particle, energy quantization is almost impossible to observe.

The classical particle's energy corresponds to motion in an excited state with quantum number

$$n = \frac{E}{\hbar\omega} - \frac{1}{2} \approx 10^{27}$$

"Correspondence principle": for quantum numbers approaching infinity, we regain the classical picture.

(b) We call the energy difference $\Delta E = \hbar\omega$ a quantum of energy. We can excite the particle in the harmonic oscillator potential by adding more and more energy quanta to its energy. In the case of the electromagnetic field in vacuum, one energy quantum corresponds to one <u>photon</u>. In the case of a crystal, one energy quantum of oscillatory energy corresponds to one <u>phonon</u>.

(c) The lowest energy eigenvalue is

$$E_0 = \frac{1}{2}\hbar\omega > 0$$

("zero-point energy"). It results from the uncertainty relation $\Delta X \cdot \Delta P \geq \frac{\hbar}{2}$ (resulting from $[\hat{X}, \hat{P}] = i\hbar$) which forbids to put the particle at rest at the potential minimum.

A crystal with $3N_0$ atomic degrees of freedom has ground state energy $\frac{1}{2}\hbar\omega(\vec{k},\lambda)$ in each mode, which has measurable consequences. The electromagnetic field in vacuum has ground state energy

$$E_0 = \int_0^\infty d\omega \, \frac{1}{2}\hbar\omega = \infty!$$

So if the state $\overline{|x=0, p=0\rangle}$ is forbidden by the uncertainty relation, what the lowest quantum mechanically allowed energy? Lets try to find a $|\psi\rangle$ that minimizes the total energy:

$$\langle\psi|\hat{H}|\psi\rangle = \langle\hat{H}\rangle = \frac{\langle\hat{P}^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle\hat{X}^2\rangle$$

$$= \frac{(\Delta P)^2 + \langle\hat{P}\rangle^2}{2m} + \frac{m\omega^2}{2}\left((\Delta X)^2 + \langle\hat{X}\rangle^2\right)$$

To minimize $\langle\hat{H}\rangle$ we should obviously consider only states with $\langle\hat{X}\rangle = \langle\hat{P}\rangle = 0$. In such states

$$\langle\hat{H}\rangle = \frac{(\Delta P)^2}{2m} + \frac{m\omega^2}{2}(\Delta X)^2 \underset{\Delta P\cdot\Delta X \geq \hbar/2}{\geq} \frac{\hbar^2}{8m(\Delta X)^2} + \frac{m\omega^2}{2}(\Delta X)^2$$

We can minimize $\langle\hat{H}\rangle$ by choosing a state which has a Gaussian wave function, because we showed earlier that Gaussians have $\Delta P\cdot\Delta X = \frac{\hbar}{2}$, i.e. the minimal possible uncertainty product:

$$\langle\hat{H}\rangle_{\text{Gaussian}} = \frac{\hbar^2}{8m(\Delta X)^2} + \frac{m\omega^2}{2}(\Delta X)^2$$

Let's minimize this with respect to the uncertainty $(\Delta X)^2$:

$$\frac{\partial\langle H\rangle_{\text{Gaussian}}}{\partial(\Delta X)^2} = 0 = -\frac{\hbar^2}{8m(\Delta X)^4} + \frac{1}{2}m\omega^2 \Rightarrow (\Delta X)^2 = \frac{\hbar}{2m\omega}$$

$$\langle H\rangle_{\min} = \frac{1}{2}\hbar\omega$$

$$\Rightarrow \psi_{\min}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega^2 x^2}{2\hbar}}$$

Since $\langle H\rangle_{\min} = \langle\psi_{\min}|\hat{H}|\psi_{\min}\rangle \leq \langle\psi|\hat{H}|\psi\rangle \;\; \forall|\psi\rangle$

this applies in particular to the ground state $|\psi_0\rangle$;

On the other hand, we showed in exercise 5.2.2. that the expectation value of $\hat{H}$ is lowest in the ground state:

$$E_0 = \langle \psi_0 | \hat{H} | \psi \rangle \leq \langle \psi | \hat{H} | \psi \rangle \quad \forall \, |\psi\rangle$$

$$\Rightarrow \langle \psi_0 | \hat{H} | \psi_0 \rangle = \langle \psi_{min} | \hat{H} | \psi_{min} \rangle = \frac{\hbar\omega}{2}$$

Since there was only one state with that energy, we have $|\psi_{min}\rangle = |\psi_0\rangle$.

This calculation is an example how you can try to find the ground state energy by a variational argument, without actually solving the Schrödinger equation. In most cases, this doesn't work exactly, however; we only get an upper bound for the ground state energy.

Here it works since the ground state wave function is a Gaussian that minimises the uncertainty product.

(d) The solutions for even (odd) n have even or odd parity:

$$\psi_n(-x) = \begin{cases} \psi_n(x) & n \text{ even} \\ -\psi_n(x) & n \text{ odd} \end{cases}$$

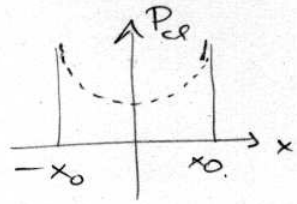
Like in the square well, even and odd solutions alternate.

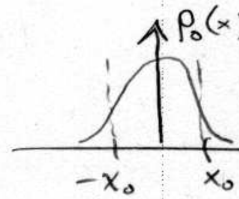
(e) The wave function does not vanish exactly at the classical turning points $\xi_n = \pm\sqrt{2n+1}$. However, for large n, the excursions into the classically forbidden region contribute very little to the total probality integral.

(f) The probability density looks very different from the classical case:

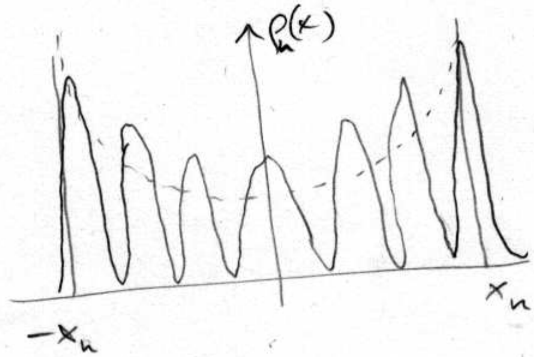
$$P_{cl} \sim \frac{1}{v(x)} = \frac{1}{\omega\sqrt{x_0^2 - x^2}} \qquad x_0 = \text{classical turning point}$$

This is peaked near the classical turning point, and minimal at $x=0$. In the quantum case, especially for the ground state $|\psi_0\rangle$, $|\psi(x)|^2$ goes the other way.





But for large n the classical limit is approached <u>on average</u>:



(see Fig. 7.2)

7.3. The harmonic oscillator in momentum eigenbasis

Same as in $\hat{X}$-basis, with $x \to p$, $m\omega \to \frac{1}{m\omega}$

7.4. The harmonic oscillator in the energy basis