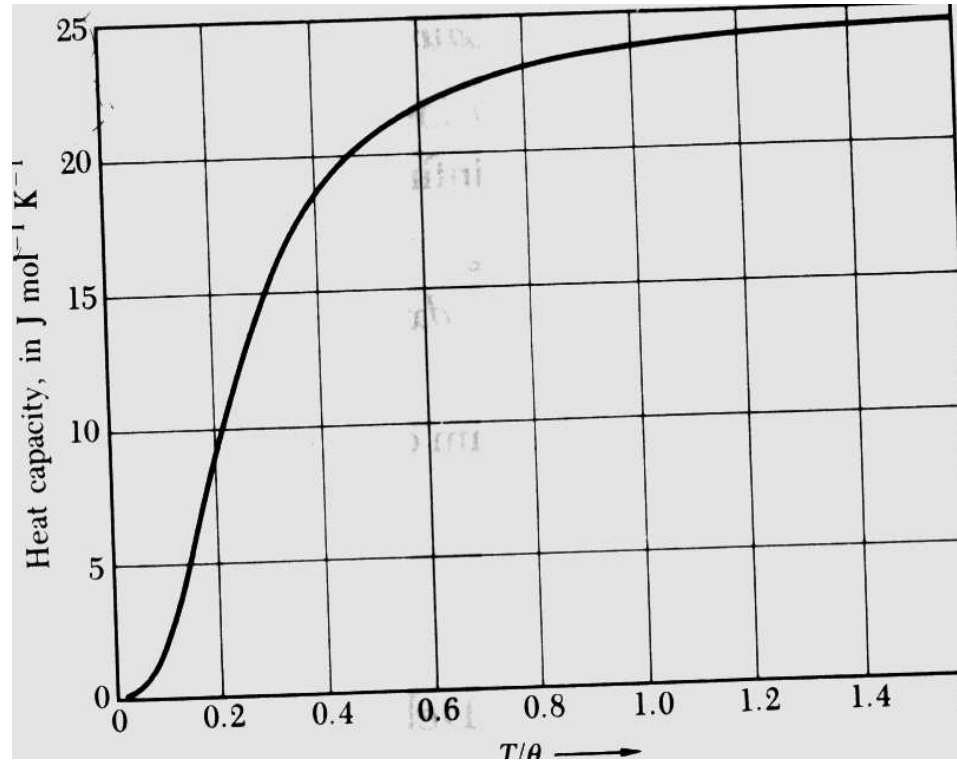




The Quantum Swing

Why Harmonic Oscillator?

- What is with specific heat of solids?



- Molecular vibrations?
- Light itself...really?



1D Harmonic Oscillator

- Hamiltonian (ω – “natural frequency”)

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

- What are the energy eigenvalues and eigenstates?
Need to solve

$$H\psi = E\psi$$

- Are there bound states? Extended states? Both?



1D Harmonic Oscillator

- What can we say without solving anything?
- Well, what do you expect classically? Any energy E is possible. Particle will be confined to $|x| \leq \sqrt{\frac{2E}{m\omega^2}}$
- Looks like we will have only bound states!
- Clearly, $\langle X \rangle = 0!$



1D Harmonic Oscillator

- Since, $\langle X \rangle = 0$, $\langle V(X) \rangle = \frac{1}{2}m\omega^2 \Delta x^2$
- Since bound state, $\langle P \rangle = 0$ and $\langle \frac{P^2}{2m} \rangle = \frac{\Delta p^2}{2m}$
- From uncertainty relation $\Delta p = \frac{\hbar}{\Delta x}$
- Total energy $E = \frac{\hbar^2}{2m\Delta x^2} + \frac{1}{2}m\omega^2 \Delta x^2$
- We can show this energy is minimum if $\Delta x = \sqrt{\frac{\hbar}{m\omega}}$,
for this value of Δx , $E \approx \hbar\omega$!
- Thus, uncertainty principle tells us that the minimum energy level of the harmonic oscillator must have energy of the order of $\hbar\omega$!
- Contrast this with classical result!



Solution of Quantum Swing

- **Solution of $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi$ is a bit technical**
- **Allowed energy levels $E_n = (n + \frac{1}{2}) \hbar \omega$, $n = 0, 1, 2, \dots$**
- **Lowest energy level $\frac{1}{2} \hbar \omega$! Very close to our estimate!**
- **Levels are equally spaced**
- **Energy eigenstates $\psi_n(x) = C_n H_n(\alpha x) e^{-\frac{1}{2} \alpha^2 x^2}$ with $\alpha = \sqrt{\frac{m\omega}{\hbar}}$, $C_n = \sqrt{\frac{\alpha}{\sqrt{\pi} 2^n n!}}$**
- **$H_n(\xi)$ are the Hermite polynomials which satisfy the differential equation $H_n''(\xi) - 2\xi H_n'(\xi) + 2n H_n = 0$**



Hermite Polynomials...What?

- $H_n(\xi)$ are the Hermite polynomials which satisfy the differential equation $H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n = 0$

$$H_0(\xi) = 1$$

$$H_1(\xi) = 2\xi$$

$$H_2(\xi) = 4\xi^2 - 2$$

$$H_3(\xi) = 8\xi^3 - 12\xi$$

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$$

$$H_6(\xi) = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120$$

$$H_7(\xi) = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi$$

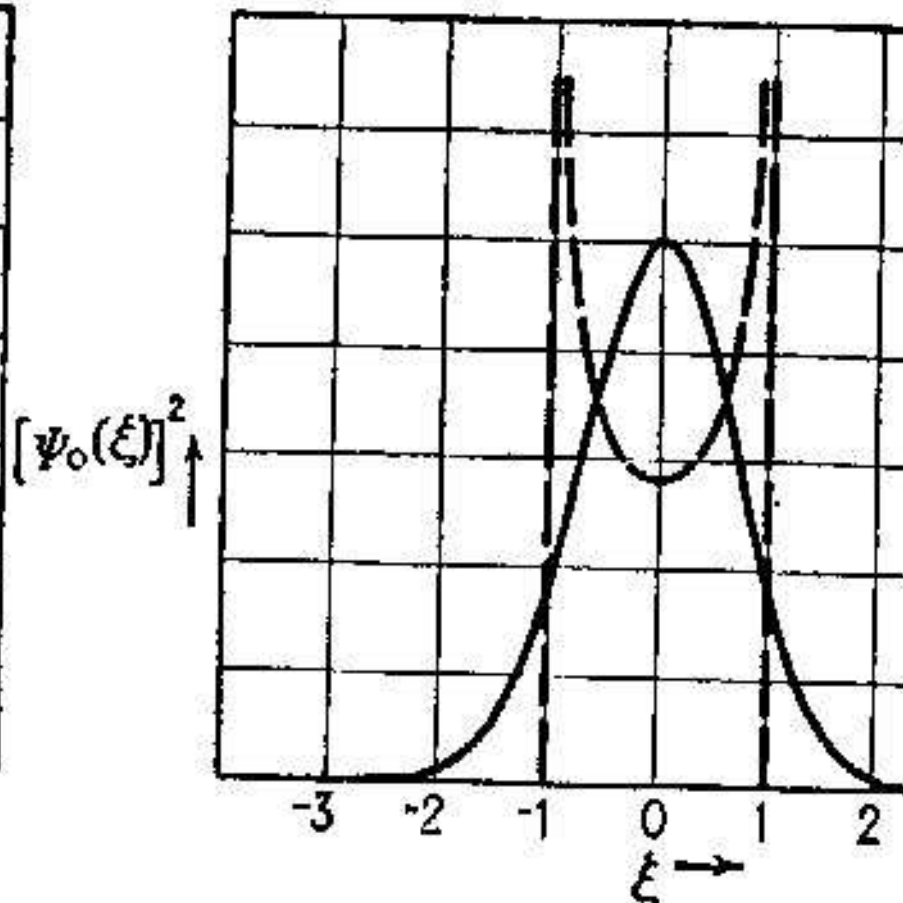
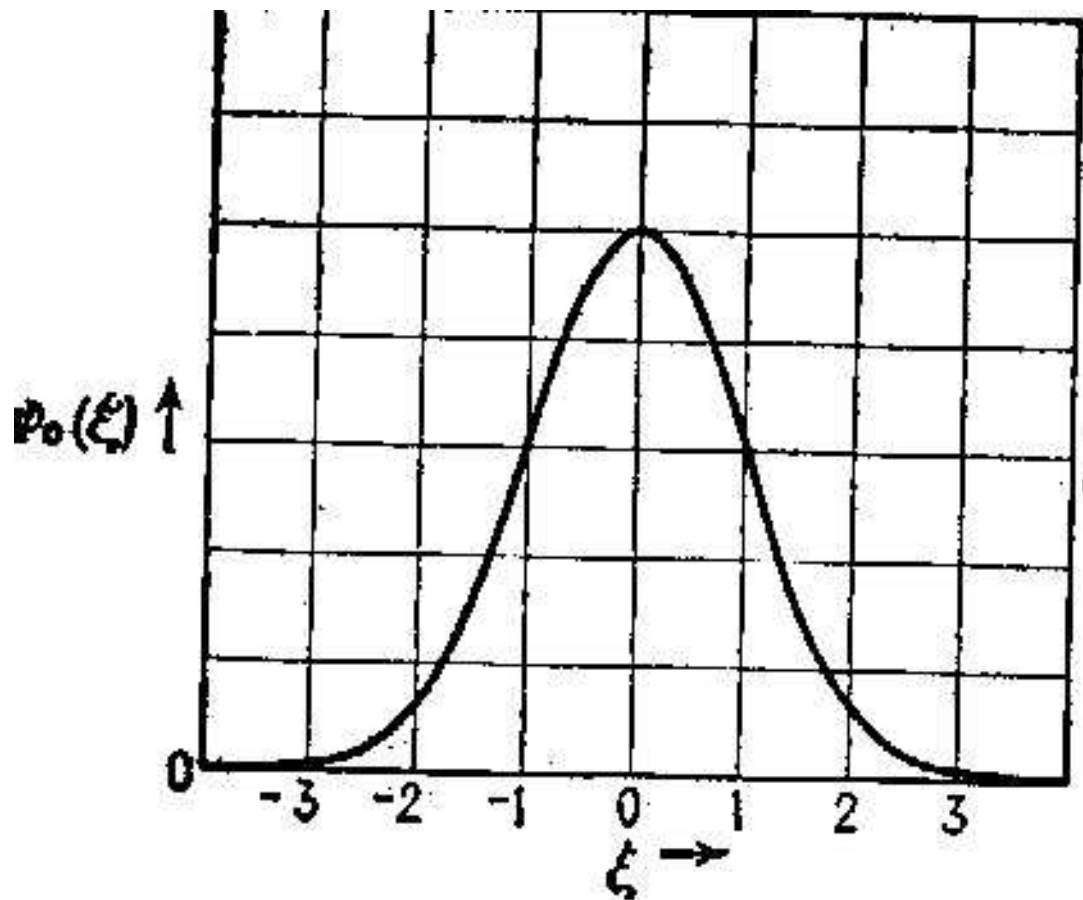
$$H_8(\xi) = 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680$$

$$H_9(\xi) = 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi$$

(Pauling and Wilson)

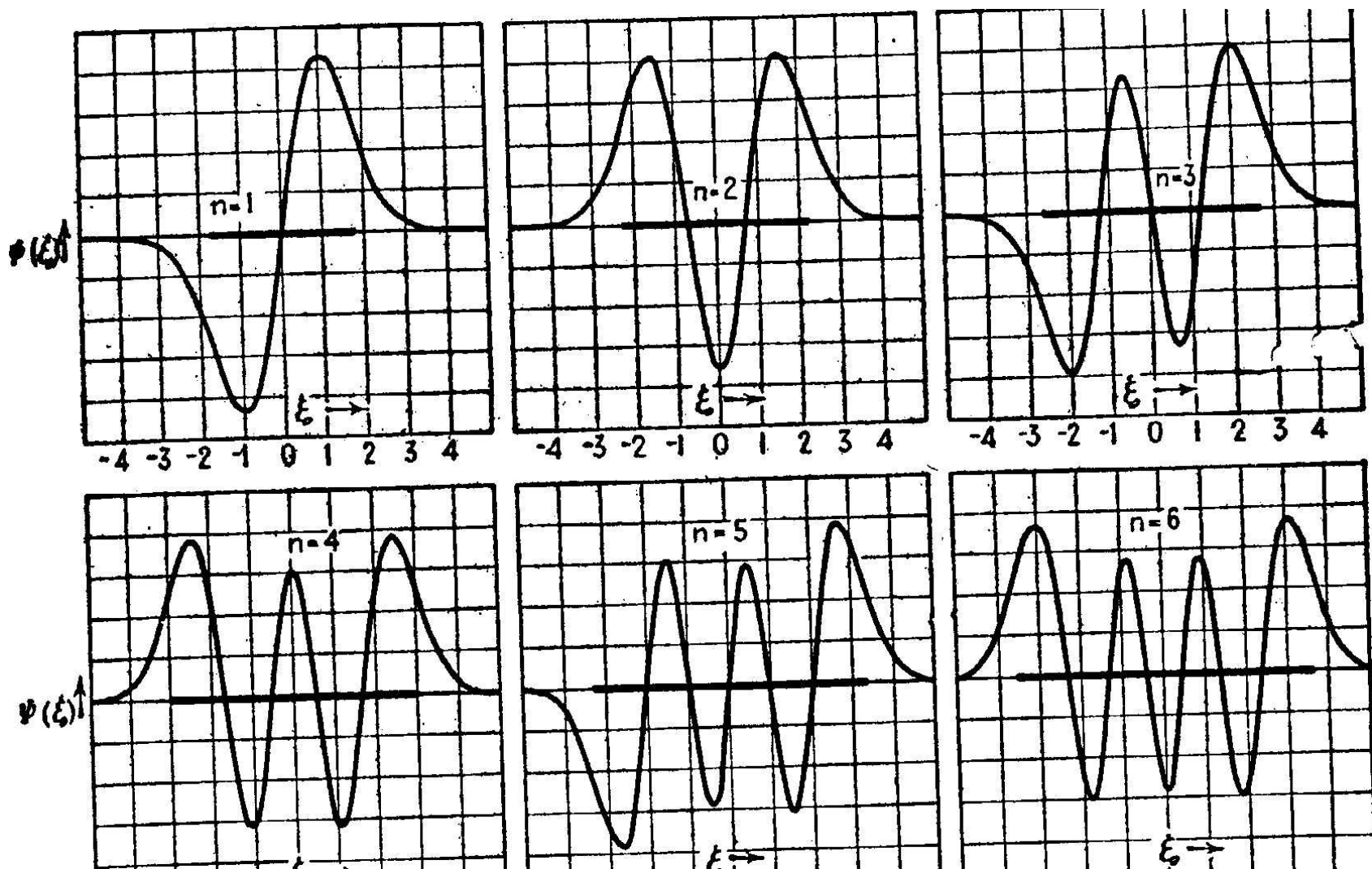
What does the ground state look like?

● $\psi_0(x) \sim e^{-\frac{1}{2}\alpha^2 x^2}$



(Pauling and Wilson)

What do other states look like?



(Pauling and Wilson)



Playing God with Quantum Swing!

- Much cleaner way to derive energy levels...play God with Dirac notation!
- Intrinsic length scale $x_o = \sqrt{\frac{\hbar}{m\omega}}$, momentum scale $p_o = \sqrt{\hbar m\omega}$
- Define *nondimensional operators* $\hat{X} = \frac{X}{x_o}$ and $\hat{P} = \frac{P}{p_o}$
- Hamiltonian $H = \hbar\omega \left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2 \right)$
- Commutation relation $[\hat{X}, \hat{P}] = i$



Playing God with Quantum Swing!

- **Define annihilation operator** $a = \frac{\hat{X} + i\hat{P}}{\sqrt{2}}$
- **Creation operator: Hermitian conjugate** $a^\dagger = \frac{\hat{X} - i\hat{P}}{\sqrt{2}}$
- **Clearly** $\hat{X} = \frac{a^\dagger + a}{\sqrt{2}}$ **and** $\hat{P} = \frac{a - a^\dagger}{\sqrt{2}i}$
- **Commutation relation** $[\hat{X}, \hat{P}] = i$ **implies** $[a, a^\dagger] = 1$
- **Hamiltonian** $H = \hbar\omega \left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2 \right) = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) !!$
- **Clearly, H and $a^\dagger a$ have the same eigenvectors!**
Thus, if $a^\dagger a |\alpha\rangle = \alpha |\alpha\rangle$, $H |\alpha\rangle = \hbar\omega \left(\alpha + \frac{1}{2} \right) |\alpha\rangle$
- **Anticipating, lets us call** $a^\dagger a = N$, **a Hermitian operator**



Playing God with Quantum Swing!

- **Suppose, $N|\alpha\rangle = \alpha|\alpha\rangle$, what is $a|\alpha\rangle$?**
- **$Na|\alpha\rangle = a^\dagger aa|\alpha\rangle = (aa^\dagger - 1)a|\alpha\rangle = (\alpha - 1)a|\alpha\rangle$! This implies $a|\alpha\rangle = C|\alpha - 1\rangle$, with $C = \sqrt{\alpha}$! Annihilation operator!**
- **Similarly, $a^\dagger|\alpha\rangle = \sqrt{\alpha + 1}|\alpha + 1\rangle$! Creation operator!**
- **“Clearly”:**
 $a^m|\alpha\rangle = \sqrt{\alpha(\alpha - 1)(\alpha - 2)\dots(\alpha - (m - 1))}|\alpha - m\rangle$...this necessarily implies that α has to be a nonnegative integer! Thus $\alpha = 0, 1, 2\dots$ etc. We have shown that the eigenvalues of N are nonnegative integers i. e., $N|n\rangle = n|n\rangle$!

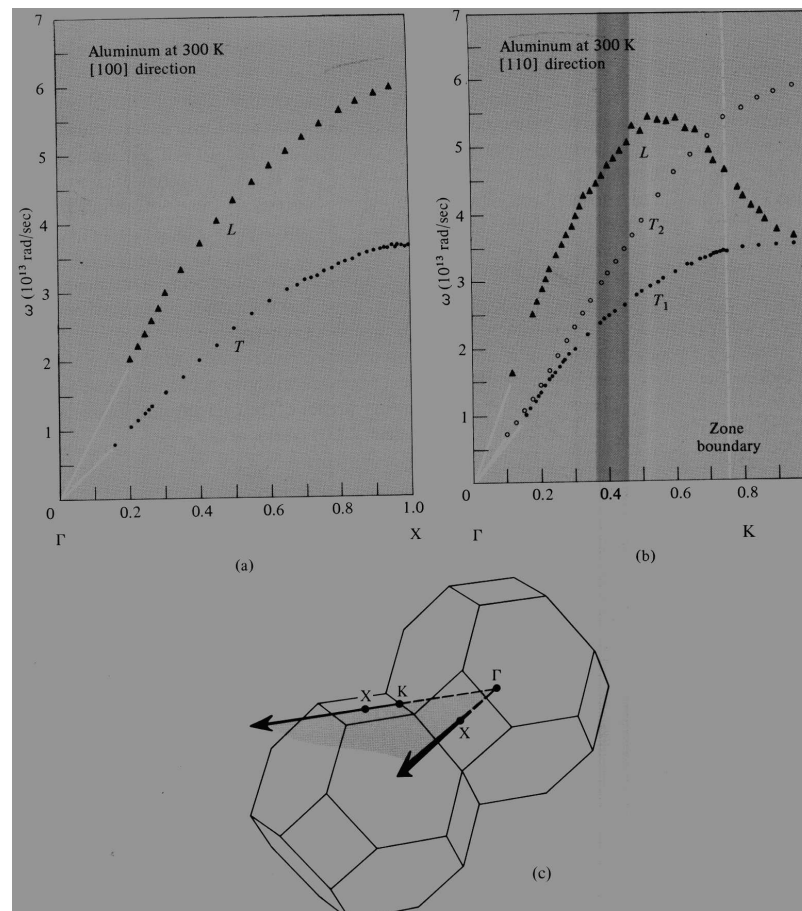


Playing God with Quantum Swing!

- $H = \hbar\omega \left(N + \frac{1}{2}\right), H|n\rangle = \underbrace{\hbar\omega \left(n + \frac{1}{2}\right)}_{E_n} |n\rangle$
- The ground state is $|0\rangle$...called “vacuum” state
- Any higher state can be generated from the ground state $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$
- Modern theory of solids is formulated using creation and annihilation operators, the number n being interpreted as the “number of particles”
- The above are called Bose operators (applicable to phonons); for electrons there are Fermi operators which satisfy *anti-commutation relations*!

Phonons in solids

- Quantized lattice vibrations! Phonon frequency depends on wavelength



Ashcroft and Mermin



Phonons, and other things

- Quantum mechanics explains specific heat anomaly (if $k_b T \ll \hbar \omega$, $C_v \sim e^{-\hbar \omega / k_b T}$, if $k_b T \gg \hbar \omega$, $C_v \sim k_b$ (Dulong-Petit)) Quantum alacrity!
- Can be used to understand molecular vibrations
- Quantum theory of light is developed in “exact analogy” with the theory of phonons...can show that light of frequency has energy levels $\hbar \omega (n + \frac{1}{2})$ where n is the number of photons...if you have large n you will have very intense light
- More interestingly this will tell you that “vacuum” in quantum mechanics is a VERY VERY VERY BUSY place!



Summary – Quantum Swing

- Energy levels go as $(n + \frac{1}{2}) \hbar\omega$
- There is a very nice way to do this using creation and annihilation operators
- Explains many things about materials – example specific heat anomaly
- Quantum swing is a very basic problem in physics, it will arise in one form or other in *many* problems