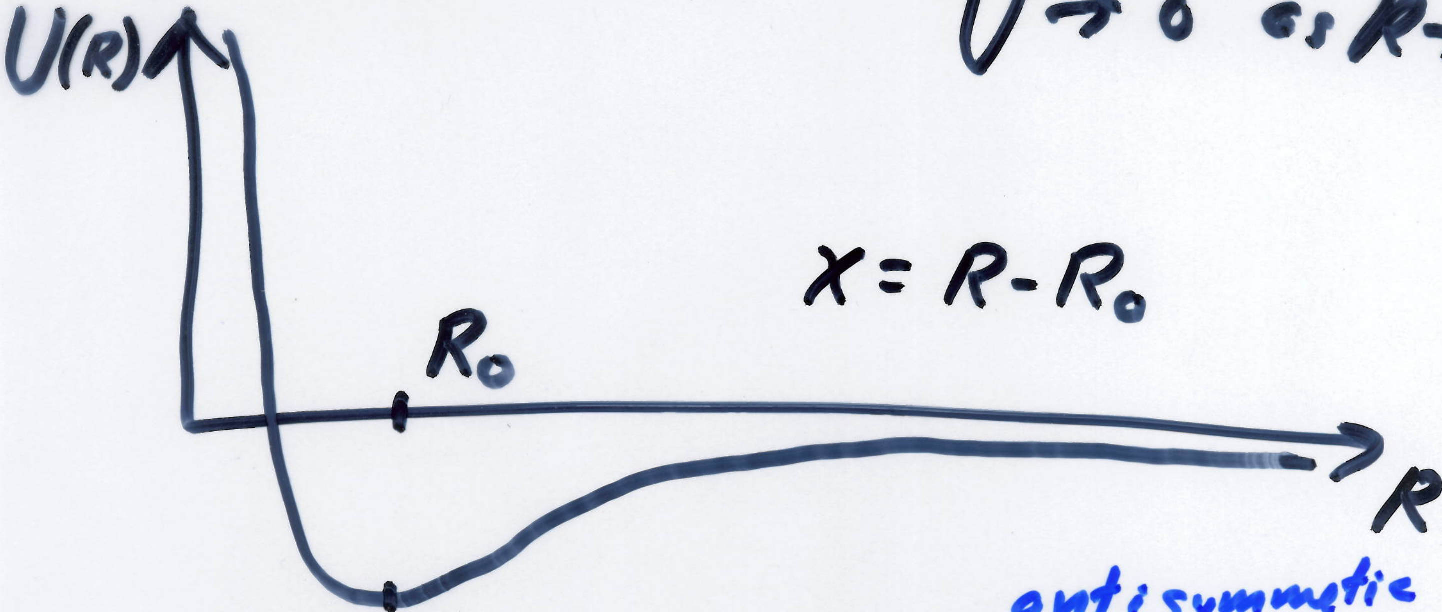
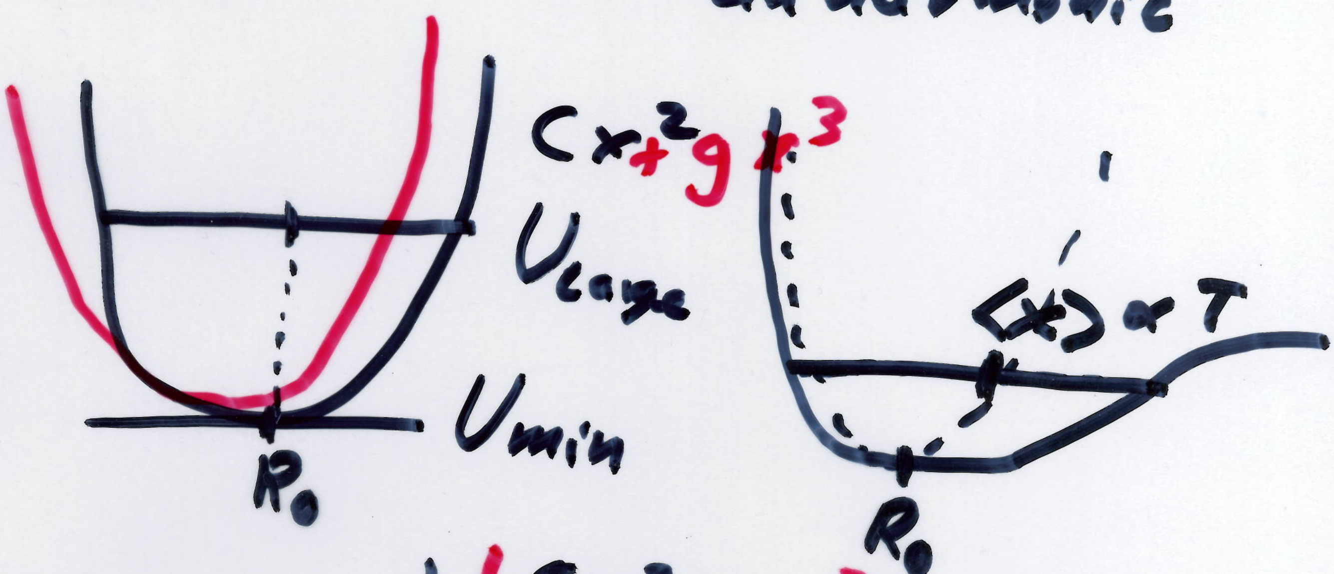
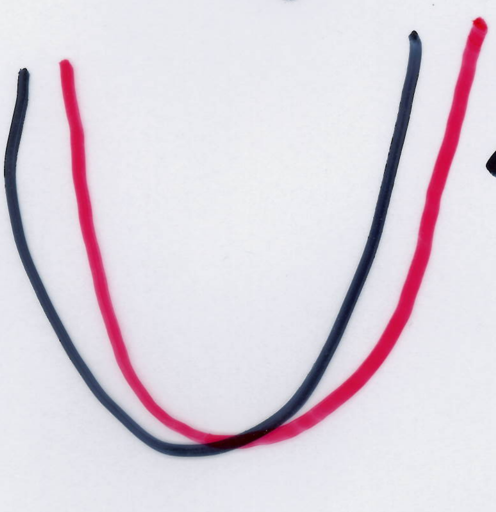
$U \to 0$ as $R \to \infty$



$x = R - R_0$

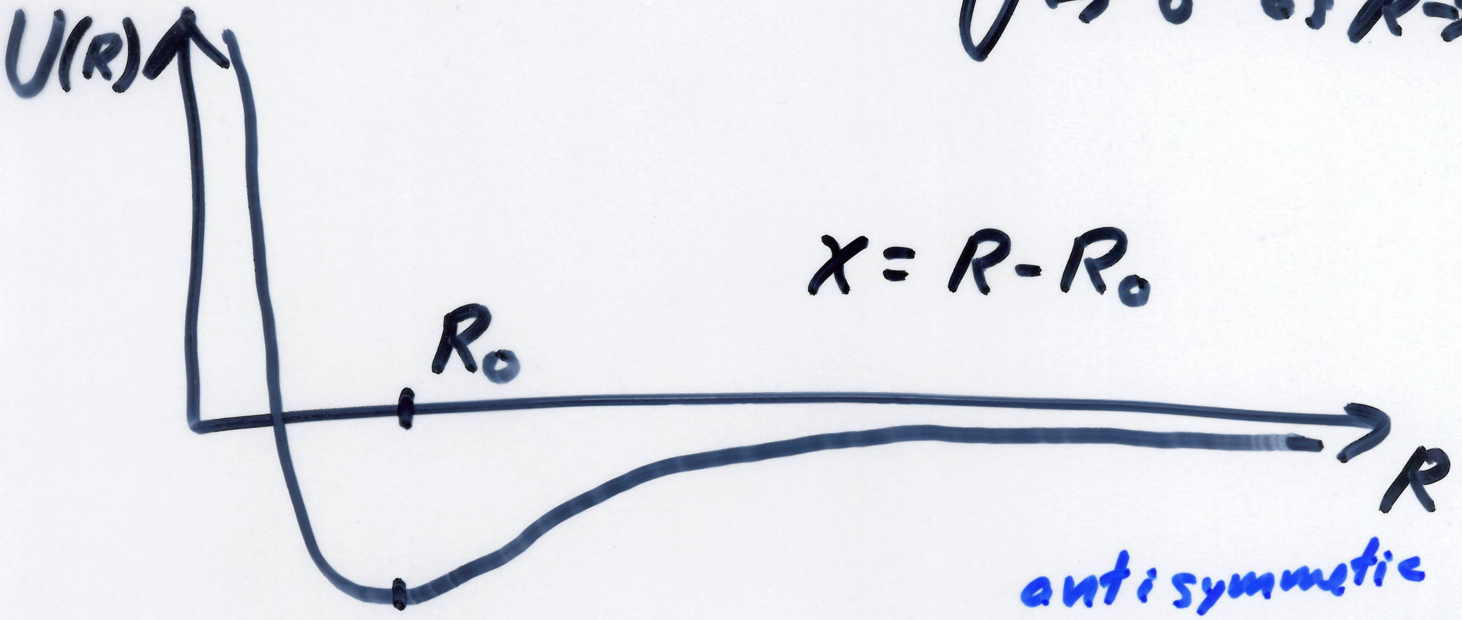
$$U(x) = U_0 + Cx^2 + \overbrace{-g x^3}^{\text{antisymmetic}} \underbrace{- \overbrace{f x^4}^{\text{symmetri}}}_{\text{anharmonic}} + \ldots$$





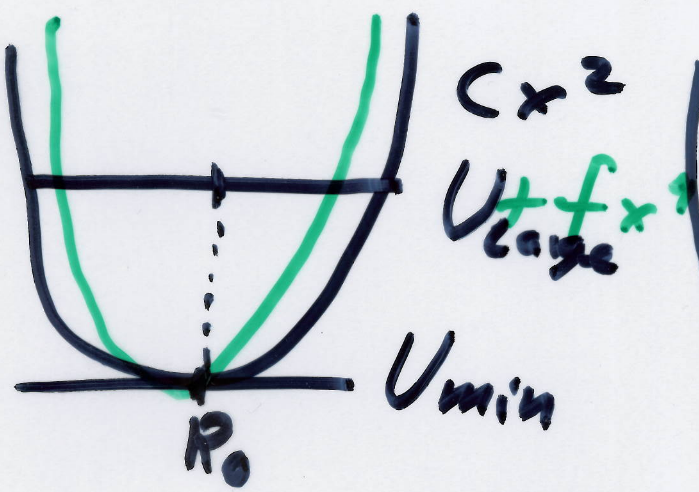
↑ no thermal expansion with only harmonic term

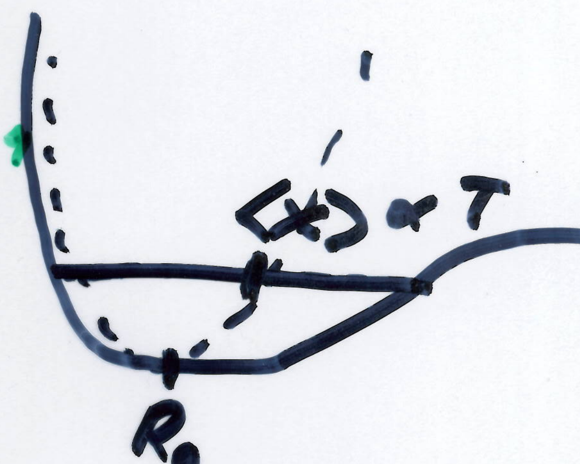
$U \to 0$ as $R \to \infty$



$x = R - R_0$

$$U(x) = U_0 + Cx^2 + \underbrace{\overbrace{-gx^3}^{\text{antisymmetric}} - \overbrace{fx^4}^{\text{symmetric}}}_{\text{anharmonic}} + \dots$$





$\leftarrow -fx^4$

no thermal expansion with only harmonic term

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x\, e^{-\frac{U(x)}{k_B T}}\, dx}{\int_{-\infty}^{\infty} e^{-\frac{U(x)}{k_B T}}\, dx}$$

$$U = Cx^2 - gx^3 - fx^4$$

Gaussian Integrals

$$I = \int_{x=-\infty}^{+\infty} e^{-x^2}\, dx \qquad I = \int_{y=-\infty}^{+\infty} e^{-y^2}\, dy$$

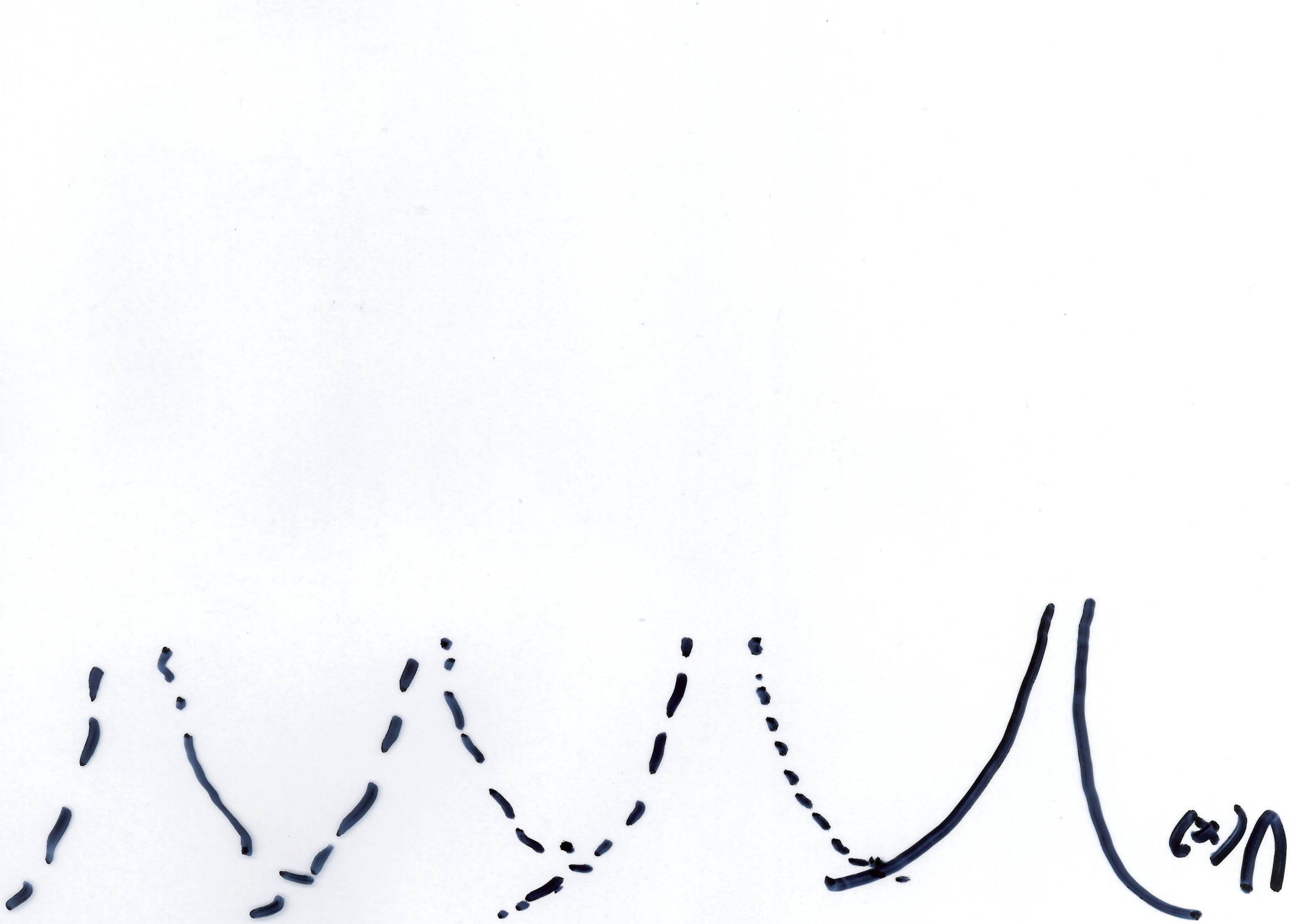
$$I^2 = \int_{x=-\infty}^{+\infty} \int_{y=-\infty}^{+\infty} e^{-(x^2+y^2)}\, dx\, dy$$

$$I^2 = \int_{r=0}^{\infty} \int_{\theta=0}^{2\pi} e^{-r^2}\, r\, dr\, d\theta$$

$$I^2 = 2\pi \int_{r=0}^{\infty} e^{-r^2}\, r\, dr$$

$$= 2\pi \left[\frac{-e^{-r^2}}{2} \right]_0^{\infty} = \pi$$

$$I = \sqrt{\pi}$$



Thermal Conductivity

Hot  Cold

$$j_{th} = - K_{th} \frac{\partial T}{\partial x}$$

j_{th}: $\dfrac{\text{energy}}{\text{Area} \cdot \text{time}}$

K_{th}: thermal conductivity

$\frac{\partial T}{\partial x}$: temperature gradient

$$\vec{J} = - \underline{K}_{th} \vec{\nabla} T(\vec{r})$$

Phonon Collisions

Normal : $\vec{k}_1 + \vec{k}_2 = \vec{k}_3$

conserves energy + momentum

Umklapp (Up conversion)

$$\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{G}$$

conserves energy

$$K_{th} = \frac{1}{3} C_v \bar{v} \ell$$

heat capacity — C_v

average speed of phonons — $\bar{v}$

mean free path between collisions* — ℓ

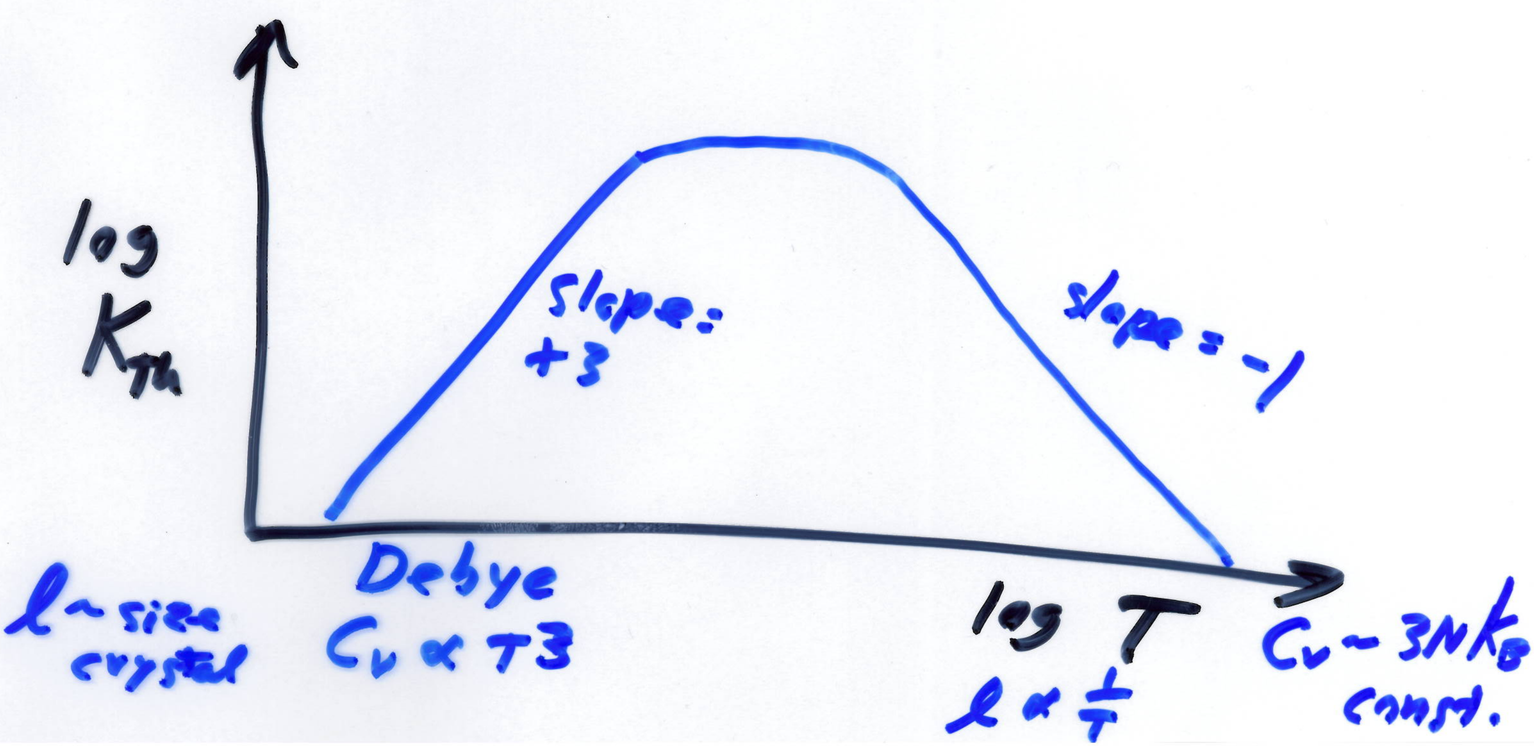
* Umklapp collisions

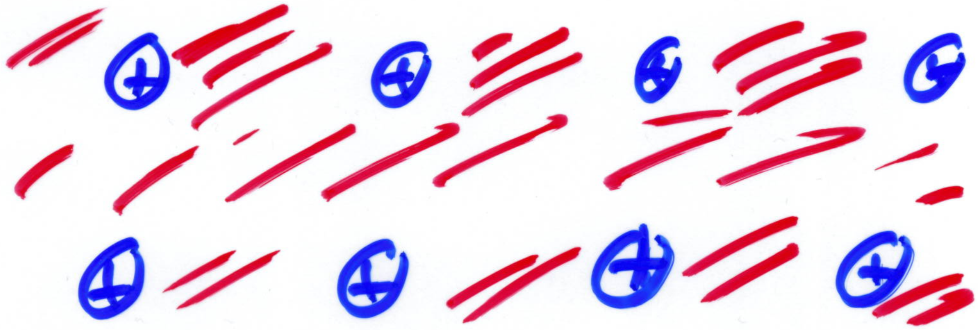
e.g. quartz

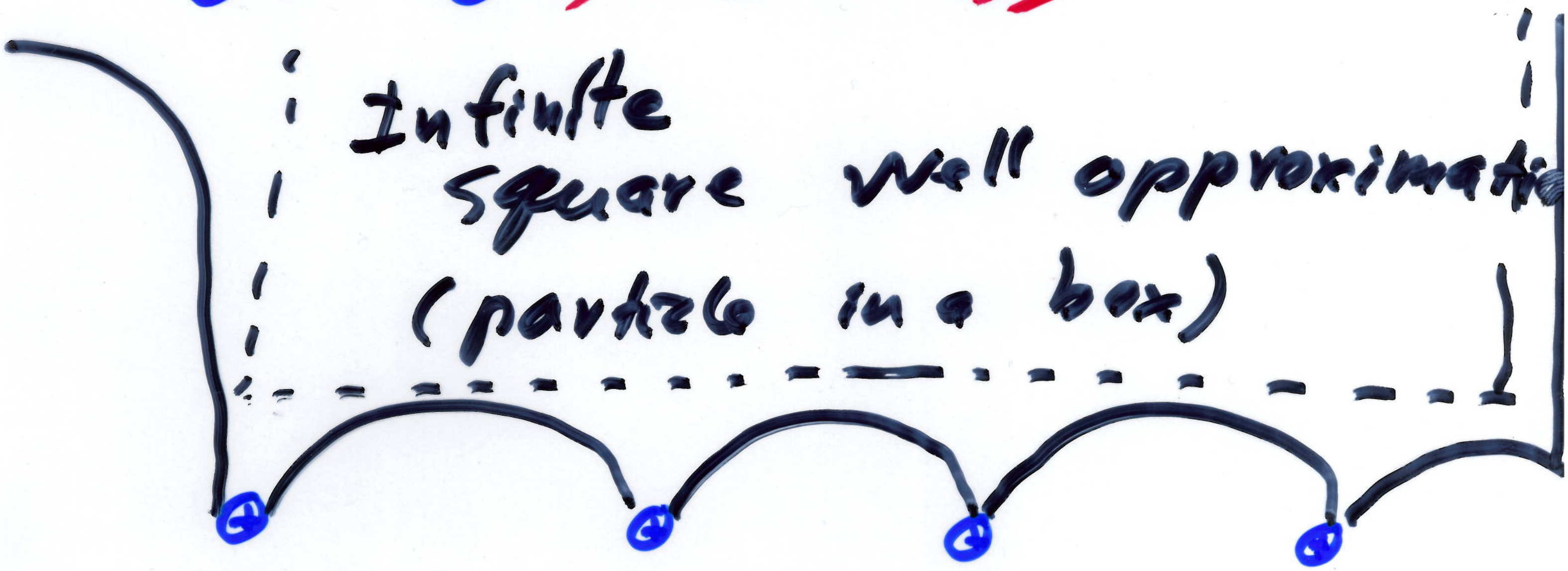
$T = 80K$ $\quad \ell = 540$ Å

$T = 270K$ $\quad \ell = 40$ Å

room temp







Na^+ e.g.

Schroedinger Equation is
non-relativistic, spin-zero

$$T + V = H$$

$$\frac{p^2}{2m} + V = H \qquad p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial}{\partial t}\psi$$

$H\psi = E\psi$ for stationary states