Dechanneling of Positrons by Dislocations: Effects of Anharmonic Interactions

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Plan of the talk

- → Introduction to channeling
- → Channeling Radiation
- → Effects of Dislocations on Positron Planar channeling
- → Effects of Anharmonicity
- → Conclusions

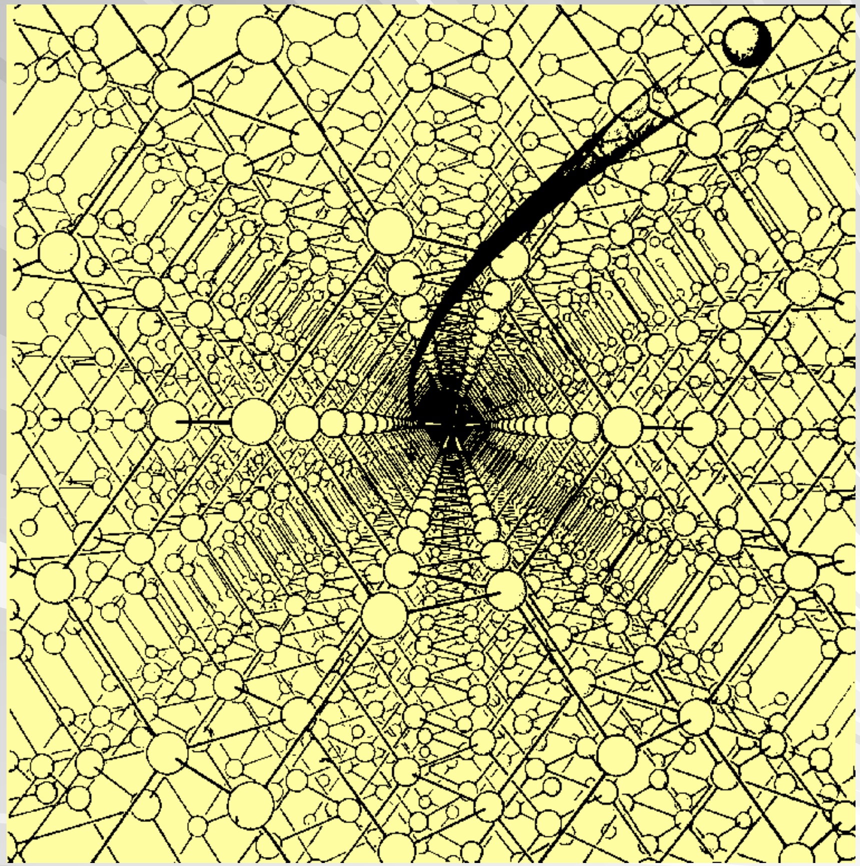
Introduction to Channeling

Channeling

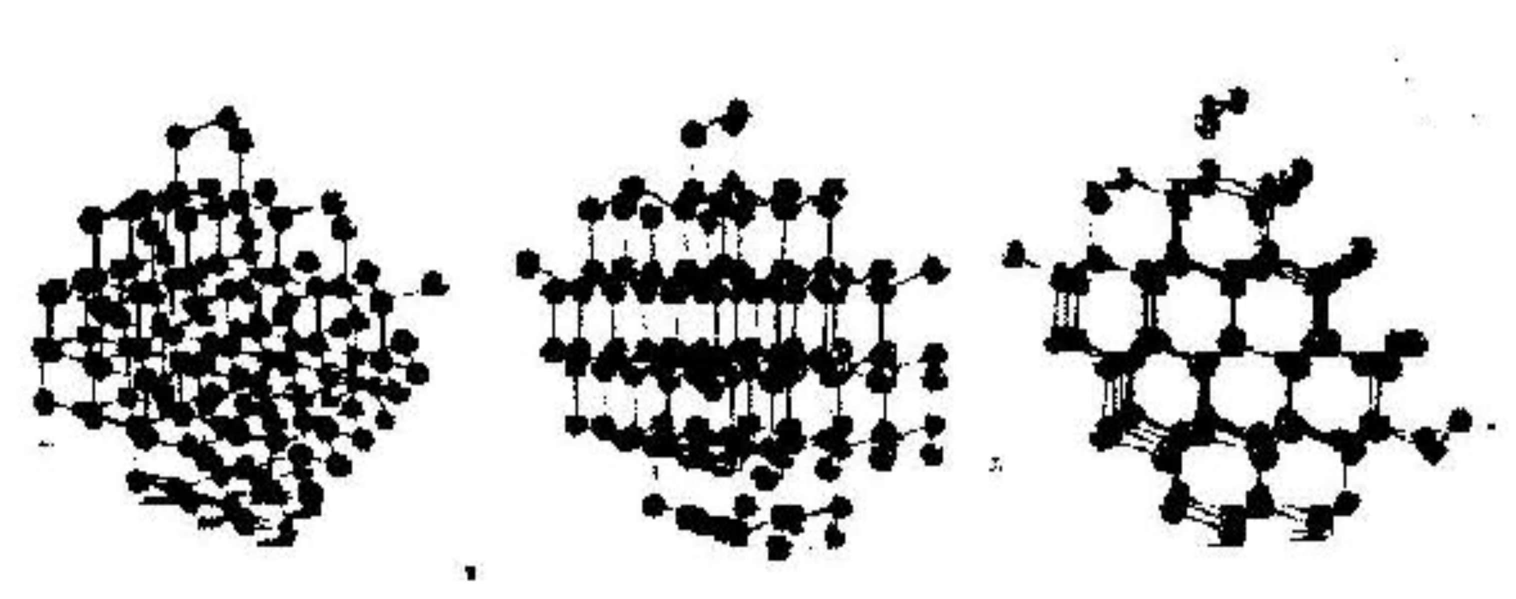
- The influence of the crystal lattice on the trajectories of ions penetrating into the crystal is known as channeling.

- The term Channeling visualizes the atomic rows and planes as guides that steer energetic ions along the channels between rows and planes

- Channeling of energetic ions occurs when the beam is carefully aligned with a major symmetry direction of a single crystal.

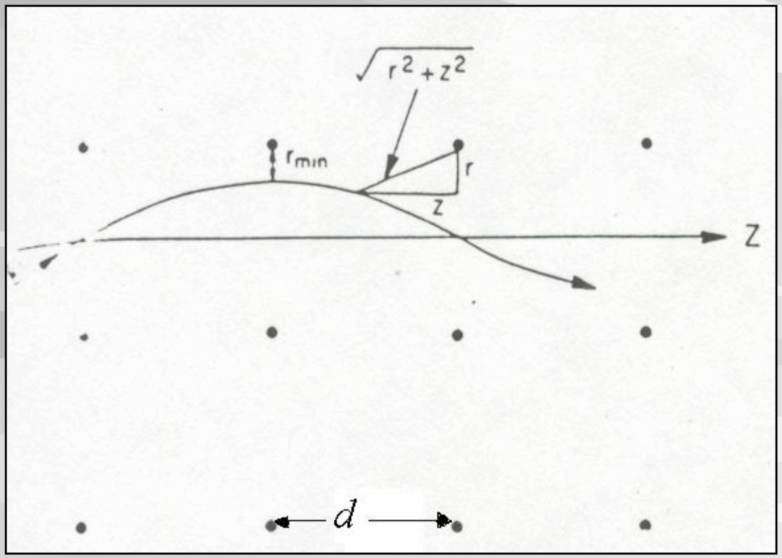


Channeling along <110> axis in a diamond structure



(a) Random **(b) Planar** **(c) Axial**

Continuum Model

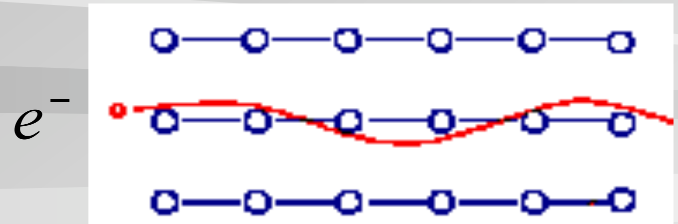


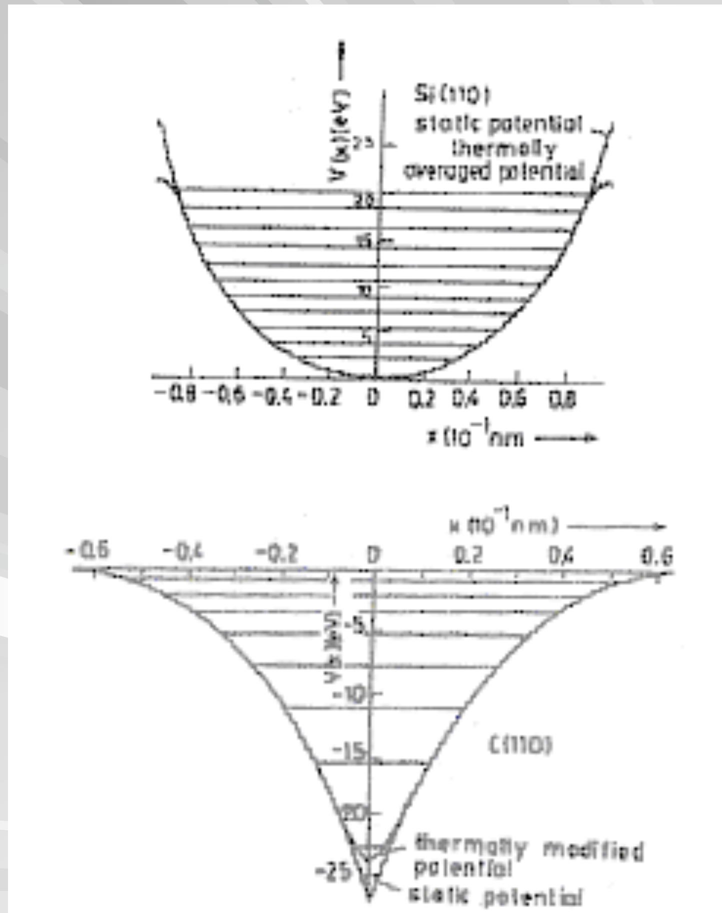
$$\frac{r_{\min}}{v\sin\psi} > \frac{d}{v\cos\psi}$$

Electron and Positron Channeling

- ➔ **For planar channeling, the motion of positrons in the transverse motion can be described by harmonic oscillator potential.**

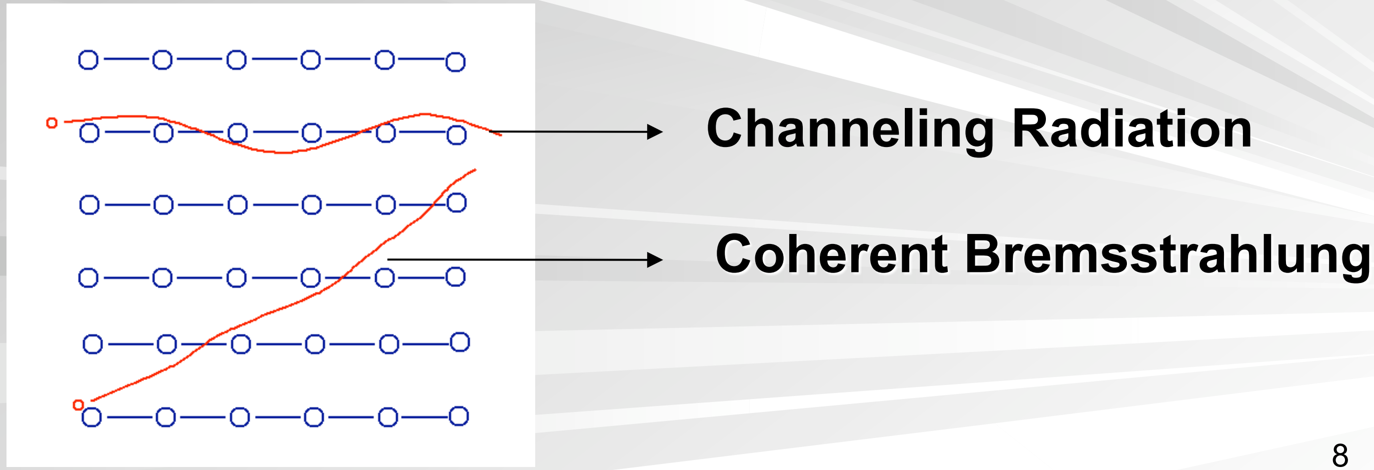
- ➔ **In the case of electrons, the continuum potential is simply the negative of that governing the motion of positrons.**





Channeling Radiation

- ➔ When light charged particles like electrons or positrons move along major crystallographic planes or axes, they experience force due to planes or axes, and as a result acceleration or deceleration occurs which gives rise to the emission of bremsstrahlung.
- ➔ Normal bremsstrahlung originates from uncorrelated deflections by atoms.
- ➔ The deflections in distant collisions are highly correlated resulting in coherent bremsstrahlung, and the trajectories are nearly straight lines.
- ➔ For very small angles of incidence however, the projectile motion is governed by the correlated deflections. The particle is channeled, and the radiation associated with the confinement in the transverse motion perpendicular to a plane or axis is called "channeling radiation" (due to quantization of transverse energy levels and spontaneous transitions among these levels)

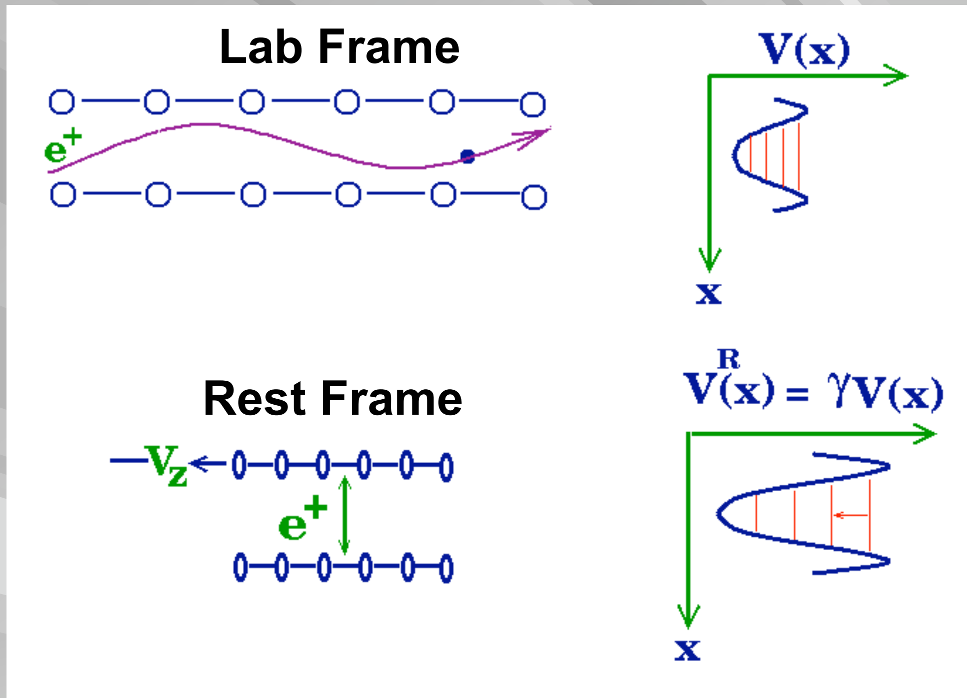


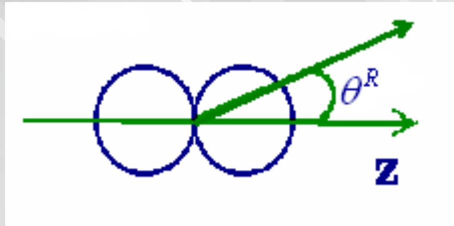
→ **For a relativistic particle, the emission process is considered in the rest frame of the particle moving through the crystal.**

$$d^R = \frac{d}{\gamma}$$

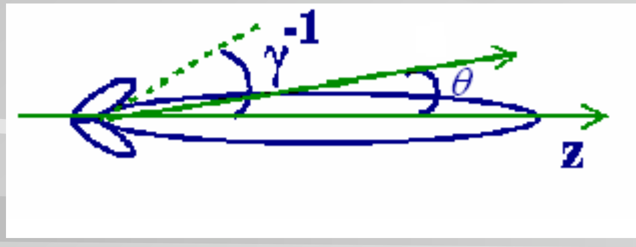
$$E_\perp^R = \gamma E_\perp$$

$$V^R = \gamma\, V$$





$$\omega^R = \gamma \omega_0$$



$$\omega^L = \frac{\omega_0}{1 - \beta \cos\theta}$$

The maximum frequency is in the forward direction, i.e., at θ = 0 (β =1)

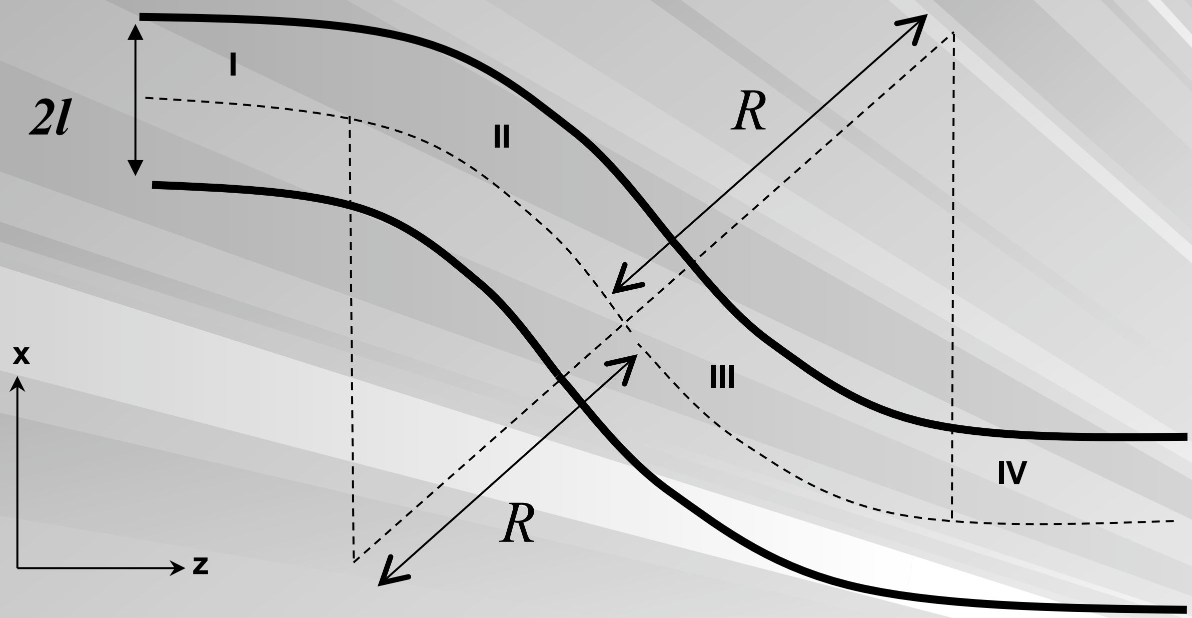
$$\omega_m = 2\gamma^2 \omega_0$$

Effects of Dislocations on Positron Planar channeling

Dislocation

- The most important example of defects that produce distortion in the channel is dislocation.
- Around dislocation the atomic rows and planes exhibit curvature which will alter the trajectory of the channeled particle and can dechannel the particle altogether if the curvature is large enough to severely modify the trajectory.
- This distortion is at a maximum near the dislocation core and decreases as one moves away from the core.
- Thus one can think of a cylindrical region around the dislocation axis, called "dechanneling cylinder".
- The effects of dislocations are introduced through the curvature of the channels.
- The effect of this curvature is to introduce a transverse centrifugal force on the propagating particles; this force should therefore be combined with the force due to the continum potential (longitudinal).

➔ The Model



The effective potential in the distorted part of the channel

$$V_{eff} = \frac{4V_0 L a_{TF}}{L^2 - x^2} - \frac{2E}{R}x$$

The shifted potential minima due to distortion,

$$a_r = \sqrt{\left(\frac{B}{L}\right)^2 - \frac{L^2}{2}} - \frac{B}{L}$$

$$B = \frac{RV_0 a_{TF}}{E}$$

The effective force constant

$$k_1^{eff} = \frac{8V_0 a_{TF} L}{(L^2 - a_r^2)^3}[L^2 + 3a_r^2]$$

The maximum number of bound states

$$j_{max} = \frac{1}{2}\left[\sqrt{\frac{\gamma m 8V_0 a_{TF} L}{(L^2 - a_r^2)^3}[L^2 + 3a_r^2]}\ \frac{(l - a_{TF} - a_r)^2}{\hbar} - 1\right]$$

Due to the change in the force constant, the coupling constant α gets modified to α'

$$\alpha'^2 = \sqrt{\gamma m 8 V_0 a_{TF} L \frac{L^2 + 3a_r^2}{(L^2 - a_r^2)^3}} = \sqrt{\frac{\gamma m 8 V_0 a_{TF}}{L^3} \left\{ \frac{1 + 3(a_r/L)^2}{1 - (a_r/L)^2} \right\}}$$

$$\alpha'^2 = \tau^2 \alpha^2$$

$$\alpha^2 = \sqrt{\frac{\gamma m 8 V_0 a_{TF}}{L^3}}$$

The distortion parameter $\tau = \alpha'/\alpha$

$$\tau^2 = \sqrt{\frac{1 + 3(a_r/L)^2}{1 - (a_r/L)^2}}$$

The wavefunction of particle in the four regions,

$$\begin{aligned}
\psi_i &= \left(\frac{\alpha}{\sqrt{\pi}2^i i!}\right)^{1/2} exp\left\{\frac{-\alpha^2 x^2}{2}\right\} H_i(\alpha x) \\
\psi_j^{(1)} &= \left(\frac{\alpha'}{\sqrt{\pi}2^j j!}\right)^{1/2} exp\left\{\frac{-\alpha'^2 (x+a_r)^2}{2}\right\} H_j(\alpha' x + \alpha' a_r) \\
\psi_k^{(2)} &= \left(\frac{\alpha'}{\sqrt{\pi}2^k k!}\right)^{1/2} exp\left\{\frac{-\alpha'^2 (x-a_r)^2}{2}\right\} H_k(\alpha' x - \alpha' a_r) \\
\psi_f &= \left(\frac{\alpha}{\sqrt{\pi}2^f f!}\right)^{1/2} exp\left\{\frac{-\alpha^2 x^2}{2}\right\} H_f(\alpha x)
\end{aligned}$$

The transition probability across the first interface,

$$p_{i\to j} = |\langle \psi_j^{(1)} | \psi_i \rangle|^2$$

$$\begin{aligned}
|\langle j^{(1)} | i \rangle|^2 &= \left(\frac{\alpha\alpha'}{\pi 2^{j+i} j!\, i!}\right) exp\left\{-\left(\frac{\alpha'^2}{\alpha^2+\alpha'^2}\right)\alpha^2 a_r^2\right\} \\
&\times \left| \int_{-\infty}^{\infty} exp\left\{-\frac{1}{2}(\alpha^2+\alpha'^2)\left[x+\frac{\alpha'^2}{\alpha^2+\alpha'^2}a_r\right]^2\right\} H_j(\alpha' x+\alpha' a_r)\ H_i(\alpha x)\right|^2
\end{aligned}$$

The total probability of the particle in the initial state $|i>$ to occupy any of the final states $|j>$ in the first region

$$p_i^I = \sum_{j=0}^{j_{max}} |\langle j^{(1)}|i\rangle|^2$$

With dechanneling probability

$$\chi_i^I = 1 - p_i^I$$

For the II and III regions,

$$\begin{aligned} p_{j^{(1)}}^{II} &= \sum_{k=0}^{k_{max}} |\langle k^{(2)}|j^{(1)}\rangle|^2 \\ \chi_j^{II} &= 1 - p_{j^{(1)}}^{II} \\ p_{k^{(2)}}^{III} &= \sum_{f=0}^{f_{max}} |\langle f|k^{(2)}\rangle|^2 \\ \chi_j^{III} &= 1 - p_{k^{(2)}}^{III} \end{aligned}$$

The total channeling probability of the particle

$$p_{i\to f} = \sum_{k^{(2)}=0}^{k_{max}^{(2)}} \left(p_{k^{(2)}\to f} \left[\sum_{j^{(1)}=0}^{j_{max}^{(1)}} p_{i\to j^{(1)}} \times p_{j^{(1)}\to k^{(2)}} \right] \right) = p_{f\to i}$$

Effects of anharmonic interactions

$$V(x) = U_0 + \frac{1}{2}k_1 x^2 + \frac{1}{4}k_2 x^4$$

with

$$U_0 = \frac{4V_0 a_{TF}}{L}$$

The effective potential

$$V_{eff}(x) = V_{eff}(a_r) + \frac{1}{2}(x-a_r)^2 \frac{d^2V_{eff}}{dx^2}\bigg|_{x-a_r} + \frac{1}{4}(x-a_r)^4 \frac{d^2V_{eff}}{dx^4}\bigg|_{x-a_r}$$

The force constants

$$k_1^{eff} = 8V_0 a_{TF} L \left[\frac{L^2 + 3a_r^2}{(L^2 - a_r^2)^3}\right]$$

$$k_2^{eff} = 8V_0 a_{TF} L \left[\frac{60a_r^4 + 12a_r^2 L^2 12L^2}{(L^2 - a_r^2)^5}\right]$$

The energy spectrum including the anharmonic term

$$E_n = \hbar\omega_0\left[(n+1/2) + \frac{\varepsilon}{4}(2n^2+2n+1)\right]$$

$$\varepsilon = \frac{3\hbar k_2}{4\gamma m\omega_0 k_1}$$

And the frequency of oscillations changes to

$$\omega_{ah} = \omega_0\left[1+\frac{\varepsilon}{4}\right]$$

The distortion parameter

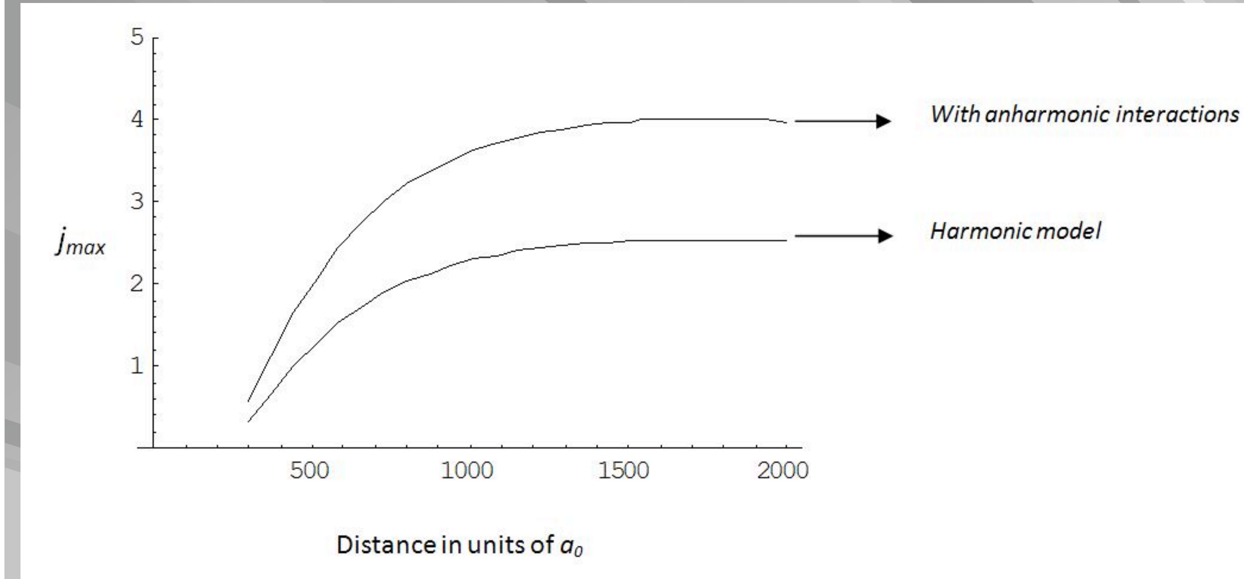
$$\tau^2 = \sqrt{\frac{k_1^{eff}}{k_1}\frac{\left(1+\frac{\varepsilon^{eff}}{4}\right)}{\left(1+\frac{\varepsilon}{4}\right)}}$$

$$\varepsilon^{eff} = \frac{3\hbar k_2^{eff}}{4\gamma m\omega_0 k_1^{eff}}$$

Maximum number of bound state

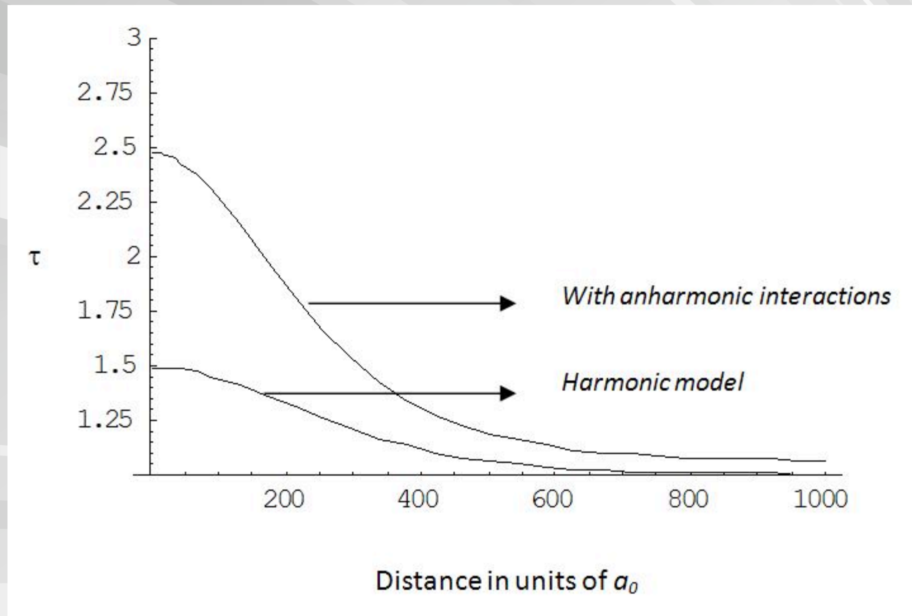
$$j_{max} = \left(\frac{1}{2}+\frac{1}{\varepsilon^{eff}}\right)\left[-1+\left(1-\frac{2\varepsilon^{eff}}{\varepsilon^{eff}+2}+\frac{4\varepsilon^{eff}}{(\varepsilon^{eff}+2)^2}\,\frac{k_1^{eff}x_{max}^2+1/2k_2^{eff}x_{max}^4}{\hbar\omega_0}\right)^{1/2}\right]$$

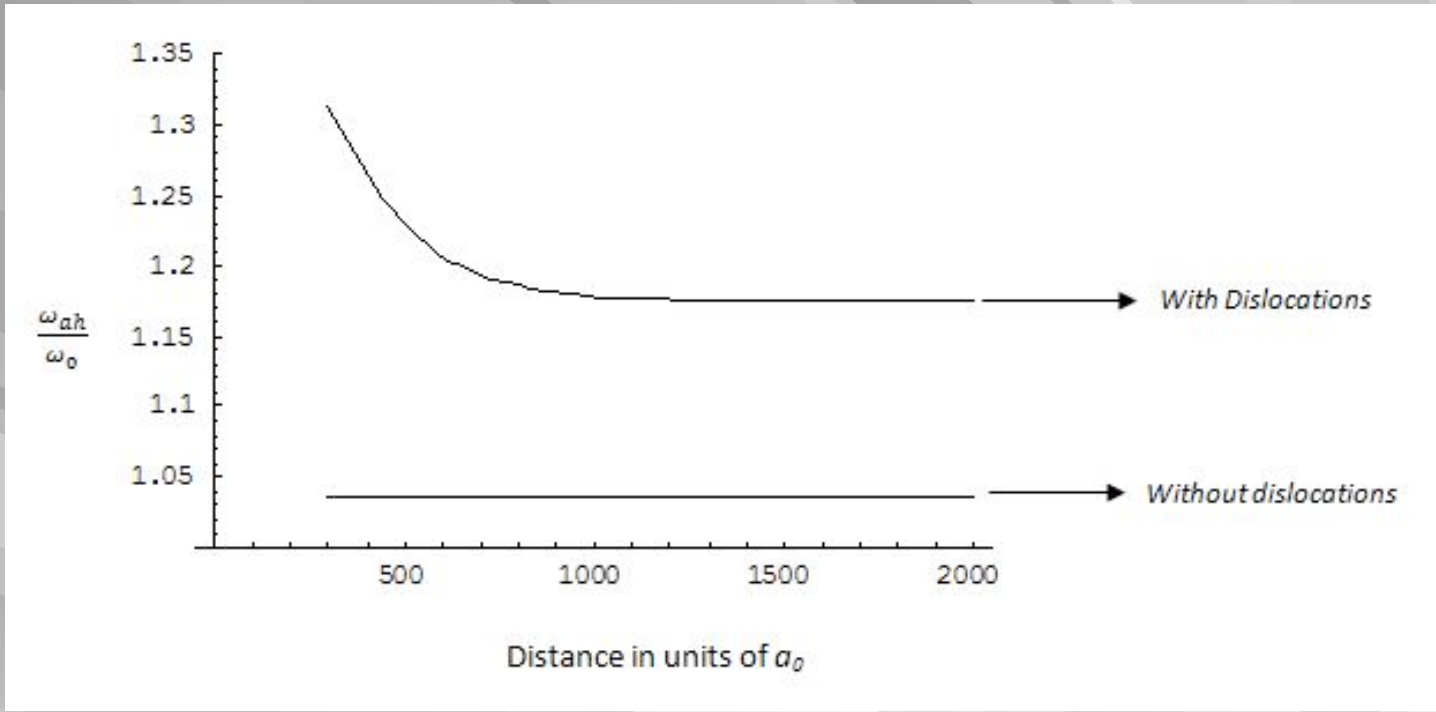
$$x_{\max} = d_p/2 - a_{T.F.}$$



Change in the maximum number of bound states.

Change in the distortion parameter





Anharmonicity increases the frequency of oscillations by 3.5%

With Dislocation the total increase the frequency is by 17%

The first order perturbed wave function

$$
\begin{aligned}
|\psi\rangle = |n\rangle + \frac{\varepsilon^{eff}}{48} \Big[& \sqrt{n(n-1)(n-2)(n-3)}|n-4\rangle \\
+ & \ 4(2n-1\sqrt{n(n-1)}|n-2\rangle) \\
- & \ 4(2n+3)\sqrt{(n+1)(n+2)}|n+2\rangle \\
- & \sqrt{(n+1)(n+2)(n+3)(n+4)}|n+4\rangle \Big]
\end{aligned}
$$

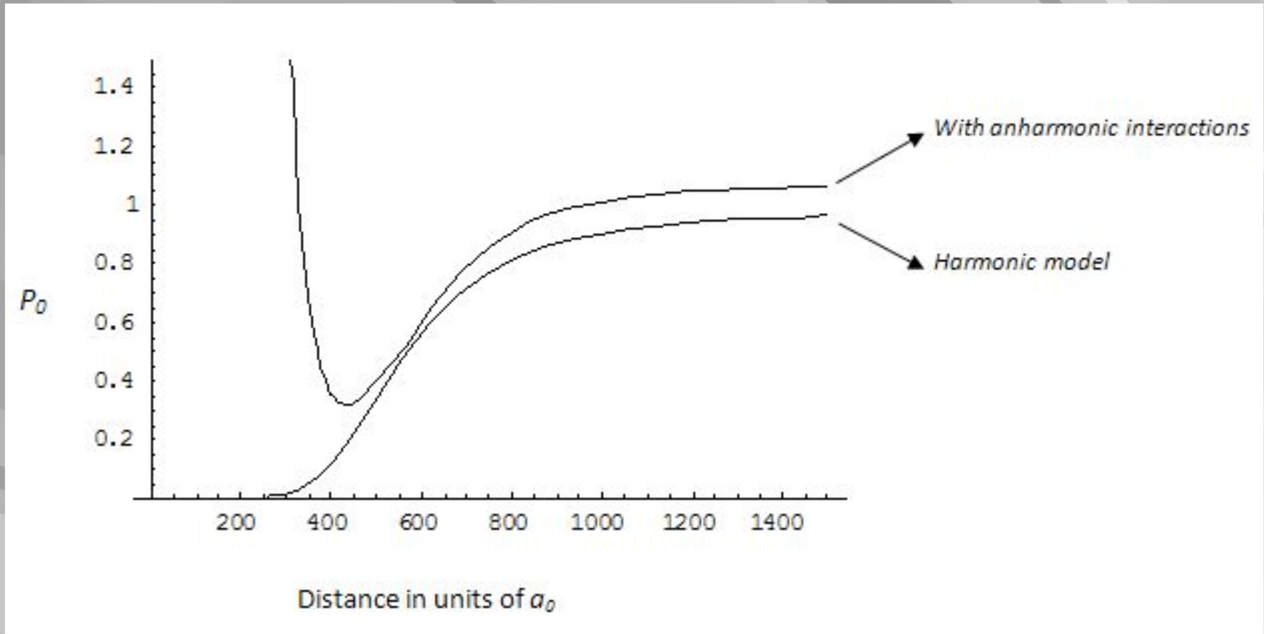
Introducing constants,

$$
\begin{aligned}
A_n &= \sqrt{n(n-1)(n-2)(n-3)} \\
B_n &= 4(2n-1)\sqrt{n(n-1)} \\
C_n &= 4(2n+3)\sqrt{(n+1)(n+2)} \\
D_n &= \sqrt{(n+1)(n+2)(n+3)(n+4)}
\end{aligned}
$$

The overlap integral corresponding to the anharmonic potential

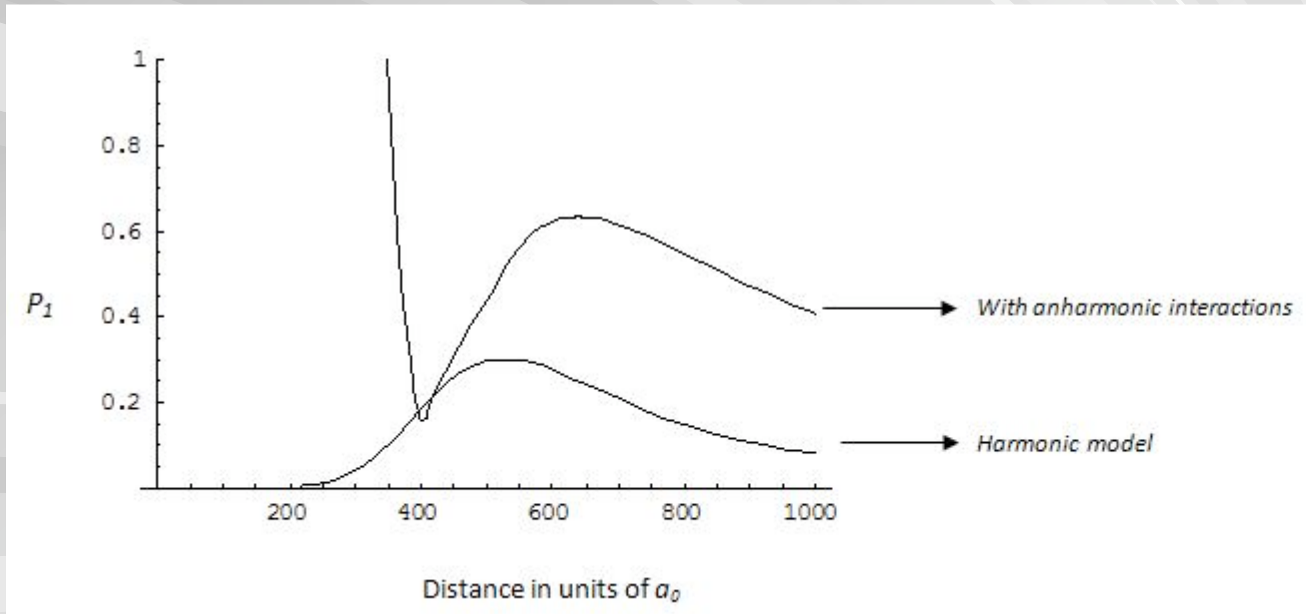
$$
\begin{aligned}
\langle \psi_m | \psi_n \rangle \;=\; & \langle m|n\rangle + \frac{\varepsilon^{eff}}{48}\Big[A_n\langle m|n-4\rangle + B_n\langle m|n-2\rangle - C_n\langle m|n+2\rangle - D_n\langle m|n+4\rangle\Big] \\
+\; & \frac{\varepsilon^{eff}}{48}\Big[A_m\langle m-4|n\rangle + B_m\langle m-2|n\rangle - C_m\langle m+2|n\rangle - D_m\langle m+4|n\rangle\Big] \\
+\; & \left(\frac{\varepsilon^{eff}}{48}\right)^2\Big[A_nA_m\langle m-4|n-4\rangle + B_nA_m\langle m-4|n-2\rangle - C_nA_m\langle m-4|n+2\rangle - D_nA_m\langle m-4|n+4\rangle\Big] \\
+\; & \left(\frac{\varepsilon^{eff}}{48}\right)^2\Big[A_nB_m\langle m-2|n-4\rangle + B_nB_m\langle m-2|n-2\rangle - C_nB_m\langle m-2|n+2\rangle - D_nB_m\langle m-2|n+4\rangle\Big] \\
+\; & \left(\frac{\varepsilon^{eff}}{48}\right)^2\Big[A_nC_m\langle m+2|n-4\rangle + B_nC_m\langle m+2|n-2\rangle - C_nC_m\langle m+2|n+2\rangle - D_nC_m\langle m+2|n+4\rangle\Big] \\
+\; & \left(\frac{\varepsilon^{eff}}{48}\right)^2\Big[A_nD_m\langle m+4|n-4\rangle + B_nD_m\langle m+4|n-2\rangle - C_nD_m\langle m+4|n+2\rangle - D_nD_m\langle m+4|n+4\rangle\Big]
\end{aligned}
$$

Change in the channeling probabilities.



Initially well channeled particle.

Particle with an initial state |1> .



Conclusions

- A quantum theory of dechanneling due to dislocations with the effects of anharmonic term in the positron planar potential is developed.

- The effective potential due to dislocations and anharmonicity are found in the regions affected by dislocation.

- The maximum number of bound states are calculated and is found to increase from 3 to 5 due to anharmonicity.

- The effect of anharmonicity on the distortion parameter is also found and compared with that of the harmonic case.

- The overlap integral is written and the channeling probabilities are found for initially well-channeled particle and particle with an initial state |1> and are compared with the harmonic case.

- We found the change in frequency of oscillation due to anharmonicity and compared that of the without dislocation case. We found an increase of 17% in oscillation frequency as against the 3.5% increase in the case of without dislocation.

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Thank You