

VIIIth International Conference

Channeling 2018

Sept. 23-28. Ischia (NA), Italy

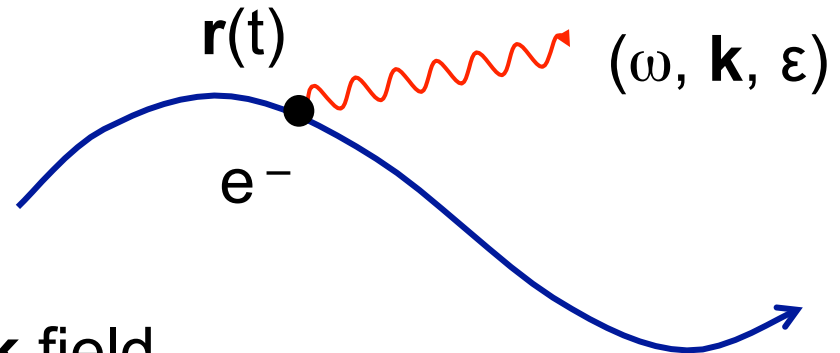
On the validity of the Baier-Katkov formula

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Classical radiation formula in vacuum (1/2)

applies to :



- Synchrotron radiation in **weak** field,
e.g. in undulator
- **Soft** Compton effect (Thompson regime)
- **Soft** coherent Bremsstrahlung ($\omega \ll \gamma m$)
- Channeling Radiation (classical trajectory .and. $\omega \ll \gamma m$)

Natural units systems $\hbar = c = 1$; $\alpha = 1/137$

$$m = 511 \text{ KeV} \quad p^0/m \equiv \gamma = (1-v^2)^{-1/2} \quad (v \equiv \beta)$$

$$\lambda_c = \text{Compton wavelength} = 1/m = 386 \text{ fermi}$$

Classical radiation formula (2/2) :

Spectral-angular distribution : $dN(\boldsymbol{\epsilon}) / (d\omega d\Omega) = (\alpha\omega/4\pi^2) |\mathbf{a} \cdot \boldsymbol{\epsilon}^*|^2$

$\boldsymbol{\epsilon}$ = photon polarization

Right circular polarization (helicity $\Lambda = +1$) : $\boldsymbol{\epsilon}_{(+)} = (1, i) / \sqrt{2}$

Left circular polarization (helicity $\Lambda = -1$) : $\boldsymbol{\epsilon}_{(-)} = (1, -i) / \sqrt{2}$

$$\mathbf{a} = \int \exp(i\phi) d\mathbf{r}_{\perp} ;$$

$$\phi = \mathbf{k} \cdot \mathbf{X}$$

$$\mathbf{r}_{\perp} = \text{perpendicular to } \mathbf{k} ; \quad \mathbf{v}_{\perp} = d\mathbf{r}_{\perp} / dt$$

4-vectors :

$$\mathbf{X} = (t, \mathbf{r})$$

$$\mathbf{k} = (\omega, \mathbf{k})$$

$$\mathbf{p} = (\gamma m, \gamma m \mathbf{v})$$

Ultrarelativistic approximation : $\phi = (\omega/2) \int^t (\gamma^{-2} + \mathbf{v}_{\perp}^2) dt'$

*The classical theory is **Spin-blind** and without **recoil effect***

Recoil and spin effects

... become important when $\omega/\gamma m$ is not small. It can happen in :

- fast varying field: $|F|^{-1} |dF/dt| \sim m$ in the instantaneous electron frame, where $F = F^{\mu\nu} = \{\mathbf{E}, \mathbf{B}\}$. Examples:

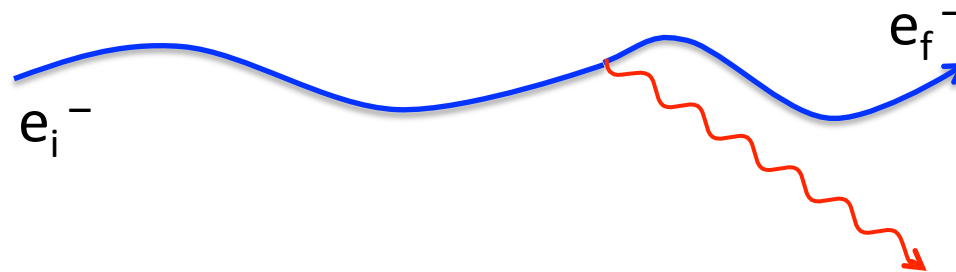
- hard Compton effect ($p.k \sim > m^2$)
- bremsstrahlung at impact parameter $b < \sim \gamma \lambda_C$

- *Strong Field*, i.e., $|F| \sim > \mathbf{E}_{\text{crit}} = m^2/e = 1,32 \cdot 10^{18}$ volt/m in the electron frame. Examples:

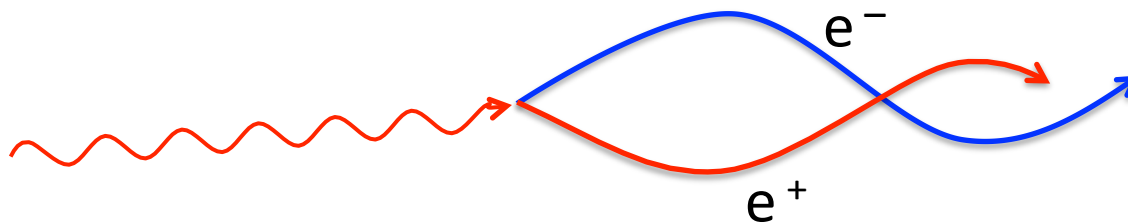
- near neutron stars,
- in channeling of electrons of energy $\sim > 100$ GeV
- in very intense laser fields.

The "magic" Baier-Katkov formula (1/5)

... is a modification of the classical radiation formula which takes **recoil** and **spin** effects into account.



Using crossing symmetry, it can also apply to pair creation in strong field.



The "magic" Baier-Katkov formula (2/5)

1) *Recoil effect* : replace $\phi = k \cdot X$
by $\phi' = (\gamma/\gamma') k \cdot X$

2) *Spin dependence* : replace $\mathbf{a} \cdot \mathbf{e}^*$ by $\langle \lambda' | a_\Lambda | \lambda \rangle$
 $\lambda, \lambda' = \text{electron helicities} = \pm 1/2$
 $\Lambda = \text{photon helicity}.$

After summation over spins :

$$dN / (d\omega d\Omega) = (\alpha\omega/8\pi^2) \left\{ (1 + \gamma^2/\gamma'^2) \left| \int \exp(i\phi') dr_\perp \right|^2 + (1/\gamma' - 1/\gamma)^2 \left| \int \exp(i\phi') dt \right|^2 \right\}$$

The "magic" Baier-Katkov formula (3/5)

Helicity *non-flip* amplitudes

$$\begin{aligned} \langle + | a_- | + \rangle &= \int \exp(i\phi') (dx + idy) / \sqrt{2} \\ \langle - | a_+ | - \rangle &= \int \exp(i\phi') (dx - idy) / \sqrt{2} \end{aligned} \quad \left. \vphantom{\int} \right\} = \text{as classical, but with } \phi'$$

$$\langle - | a_- | - \rangle = (\gamma/\gamma') \langle + | a_- | + \rangle$$

$$\langle + | a_+ | + \rangle = (\gamma/\gamma') \langle - | a_+ | - \rangle$$

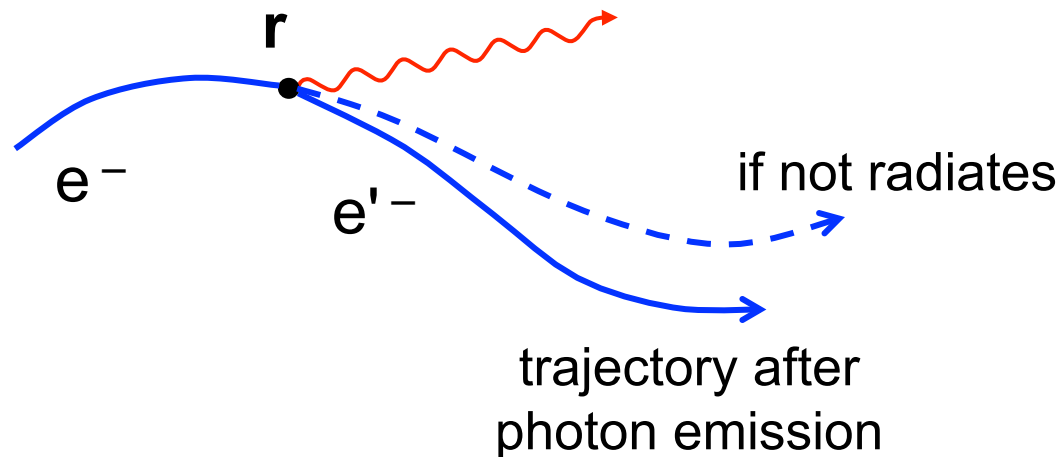
Helicity-*flip* amplitudes

$$\langle - | a_+ | + \rangle = - \langle + | a_- | - \rangle = 2^{-1/2} (1/\gamma' - 1/\gamma) \int \exp(i\phi') dt$$

$$\langle - | a_- | + \rangle = - \langle + | a_+ | - \rangle = 0 \text{ (too much imbalance of helicity !)}$$

The "magic" B-K formula (4/5)

« magic » because it does not depend on the final electron trajectory !



. . . whereas the quantum formula involves *both* the initial and final wave functions :

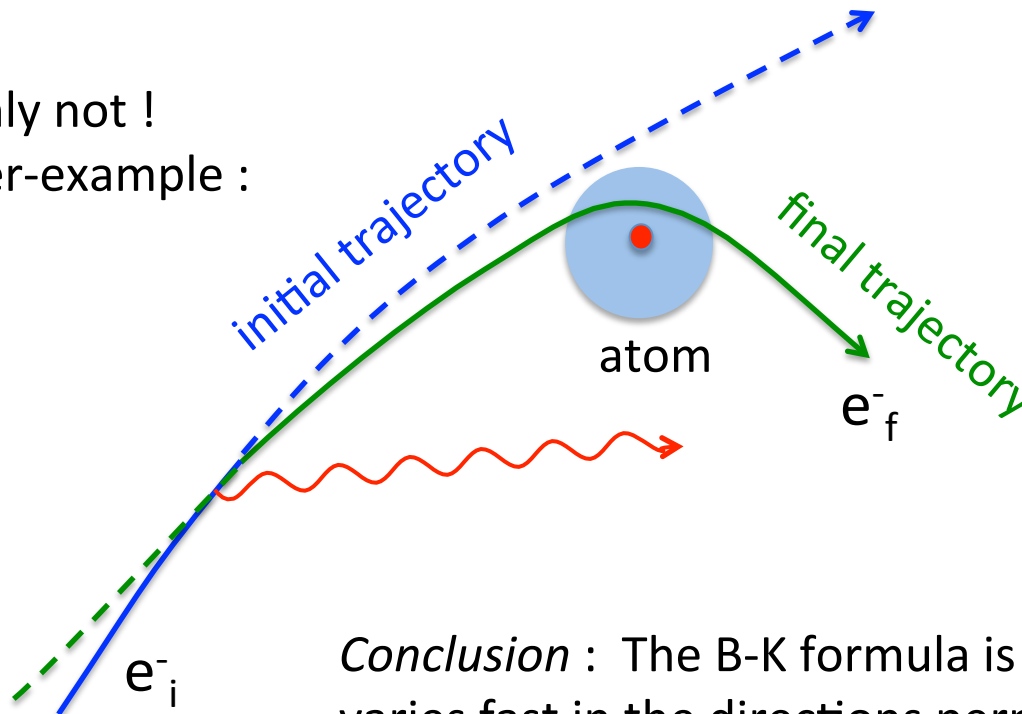
$$\langle f|a|i\rangle = \int d^3\mathbf{r} \, \psi_f^*(\mathbf{r}) \, \boldsymbol{\varepsilon}^* \cdot \boldsymbol{\alpha} \, \psi_i(\mathbf{r}) \, e^{i\mathbf{k} \cdot \mathbf{r}}$$

The "magic" B-K formula (5/5)

Should we conclude that the full information about the final trajectory is contained in the initial one ?

Certainly not !

Counter-example :

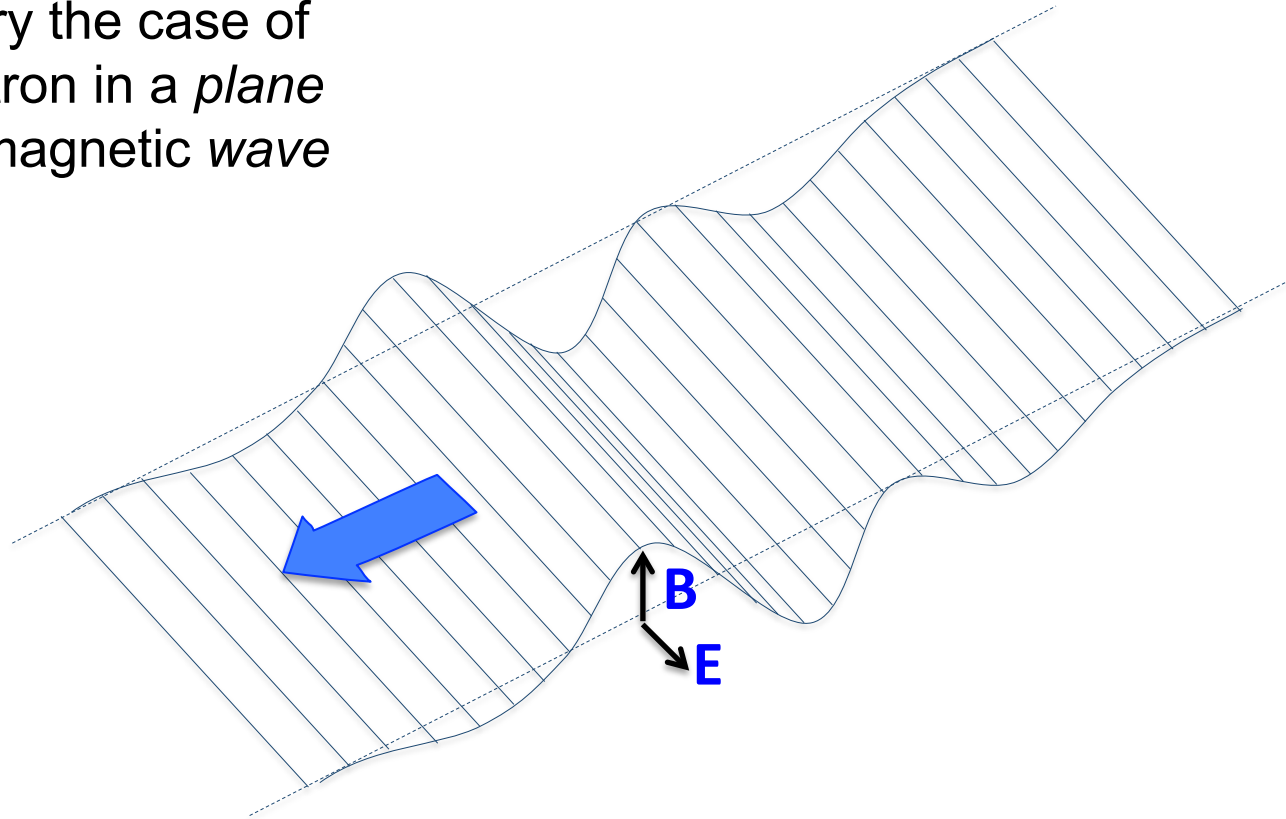


Conclusion : The B-K formula is inaccurate if the field varies fast in the directions perpendicular to the trajectory.

- Does the B-K formula becomes exact when the field is invariant along a plane ?

Plane wave external field

Let us try the case of
an electron in a *plane*
electromagnetic *wave*
packet :



Then the Dirac wave function of the electron
has a simple form, found by Volkov

Plane wave packet - Volkov wave function

Representation where α_z and Σ_z are diagonal: $\psi = (\chi, \xi) = (\chi_+, \chi_-, \xi_+, \xi_-)$

χ = component of $\alpha_z = +1$
 ξ = component of $\alpha_z = -1$

+ or - is the sign
of the *helicity* $\Sigma_z/2$

Light-like coordinates: $X = (\eta, \mathbf{r}_T, X^-)$ with $\eta = X^+ = t+z$ and $X^- = t-z$

Potential 4-vector of the wave packet: $(0, \mathbf{A}_T(\eta), 0)$

Mechanical $\mathbf{p}_T = \gamma m \mathbf{v}_T$

Canonical $\mathbf{P}_T = \mathbf{p}_T - e\mathbf{A}_T$ $P^+ = p^+ ; P^- = p^-$

Mass-shell condition:

$$p^+ p^- = m^2 + \mathbf{p}_T^2$$

Eigenstates of P^+ and \mathbf{P}_T :

$$\Psi(X) = \exp(-i p^+ X^- / 2 + i \mathbf{P}_T \cdot \mathbf{X}_T) \psi(\eta)$$

$$\mathbf{p}_T(\eta) = \mathbf{P}_T + e\mathbf{A}_T(\eta)$$

$$p^-(\eta) = [m^2 + \mathbf{p}_T^2(\eta)] / p^+$$

Solution of the Dirac equation:

$$\chi(\eta) = \chi(-\infty) \exp\left\{(-i/2) \int_{-\infty}^{\eta} d\eta' p^-(\eta')\right\}$$

$$\xi(\eta) = (1/p^+) [m + \boldsymbol{\sigma} \cdot \mathbf{p}_T(\eta) \sigma_z] \chi(\eta)$$

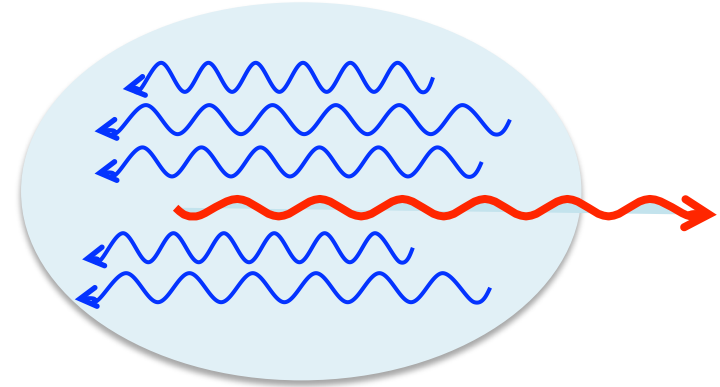
Volkov transition amplitude – 1) the phase factor

Photon momentum $k = (k^+, \mathbf{k}_T, k^-)$.

Frame where $\mathbf{k}_T = 0$, $k^- = 0$

Mom. conservation $P' + k = P$

$$p'^+ = p^+ - k^+ ; \quad \mathbf{P}'_T = \mathbf{P}_T ; \quad \mathbf{p}'_T(\eta) = \mathbf{p}_T(\eta)$$



$$\begin{aligned} \langle f | a | i \rangle &= \int d\eta \, \psi_f^*(\eta) \, \boldsymbol{\epsilon}^* \cdot \boldsymbol{\alpha} \, \psi_i(\eta) \exp(i k^- \eta / 2) \\ &= \int d\eta \exp[i \phi'(\eta)] \, \langle \lambda_f | Q(\boldsymbol{\epsilon}, \eta) | \lambda_i \rangle , \end{aligned}$$

The phase factor

$$\phi'(\eta) = (p^+ / p'^+) \int_{-\infty}^{\eta} d\eta' / 2 \, [m^2 + \mathbf{p}_T^2(\eta)] / (p^+)^2$$

equals the Baier-Katkov phase in the ultra-relativistic limit,

$$\omega \, dt \Rightarrow k^+ \, d\eta' / 2 ; \quad \gamma \Rightarrow p^+ / (2m) ; \quad \mathbf{v}_T(t) \Rightarrow 2 \, \mathbf{p}_T(\eta) / p^+ ; \quad \gamma / \gamma' \Rightarrow p^+ / p'$$

Transition amplitude – 2) the spin factor $\langle \lambda_f | Q(\boldsymbol{\epsilon}, \eta) | \lambda_i \rangle$

helicity $\lambda = \sigma_z / 2$ applied to the $\alpha_z = +1$ component χ

$$\langle + | Q(-, \eta) | + \rangle = \sqrt{2} [\mathbf{p}_x(\eta) + i \mathbf{p}_y(\eta)] / p^+$$

$$\langle - | Q(-, \eta) | - \rangle = (p^+ / p'^+) \langle + | Q(-, \eta) | + \rangle$$

$$\langle - | Q(+, \eta) | + \rangle = \sqrt{2} m (1/p'^+ - 1/p^+)$$

$$\langle - | Q(-, \eta) | + \rangle = 0, \text{ etc.}$$

Recall Baier-Katkov :

$$\langle + | a_- | + \rangle = \int \exp(i\phi') (\mathbf{dx} + i \mathbf{dy}) / \sqrt{2}$$

$$\langle - | a_- | - \rangle = (\gamma / \gamma') \langle + | a_- | + \rangle$$

$$\langle - | a_+ | + \rangle = 2^{-1/2} (1/\gamma' - 1/\gamma) \int \exp(i\phi') dt$$

$$\langle - | a_- | + \rangle = 0$$

Application of the B-K formula

- 'Exact' case : Compton back scattering on laser field
- Approximate cases : when the electron is ultra-relativistic so that in its frame the field of the radiator is nearly equivalent to a plane electromagnetic wave
- (Weizsäcker-Williams approximation). Examples:
 - > Undulator radiation
 - > Synchrotron radiation
 - > Coherent bremsstrahlung on planes
 - > Bremsstrahlung on a single atom

In these cases, the Baier-Katkov formula can also be obtained by the WKBJ method.

What about channeling radiation ?

B-K formula in channeling radiation

In channeling, the potential strongly depends on the transverse coordinates. The B-K formula is *a priori* inapplicable.

The spectral lines predicted by the B-K formula do not coincide with the ones of radiative transition between transverse states (X.A. in Channeling 2014).

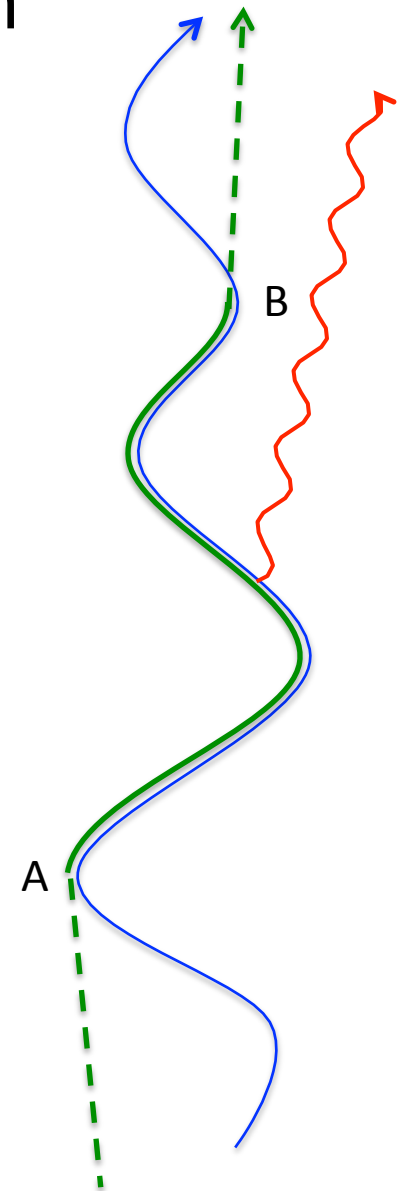
Radiative capture :

above-barrier state => channeled state

is certainly a bad case for the B-K formula: the final motion is too different from the initial one.

Nevertheless, B-K formula is usefull in channeling radiation, if one applies it by small parts of the trajectory, like **AB** here (completed by the 2 semi-infinite lines).

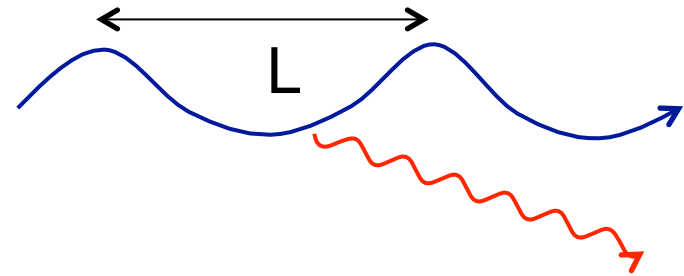
It makes the spectrum continuous, but provides an average energy loss. This is the method used in the Fortan program FOT.



----- Thank you ! -----

Fine test of the B-K formula in channeling radiation

- Assume periodic trajectories and compare the spectral lines predicted by B-K with "exact" spectral lines.



Conserv. of energy and P_L :

$$(\omega/\gamma\gamma' + \omega\theta^2)/2 = E_T - E'_T \quad (1)$$

B-K formula for the ν^{th} harmonic

$$(\omega/\gamma\gamma' + \omega'\theta^2)/2 = 2\nu\pi/L - \omega'\langle \mathbf{v}_T^2 \rangle /2 \quad (2)$$

$\nu = n - n' = \text{decrease of transverse quantum number}$

n is given by the Bohr quantization rule $L \cdot E \cdot \langle \mathbf{v}_T^2 \rangle = 2n\pi$

\Rightarrow The R-H-S of (1) and (2) are equal for $\omega \ll E$.

\Rightarrow B-K formula does not give the exact detailed spectrum in the hard region of CR.

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Quantum versus classical approach of dechanneling and other incoherent processes at high energy in aligned crystals

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(Axial channeling)

Continuous Lindhard potential:

$$V_{\text{Lin}}(\mathbf{r}_T) = \langle \langle V(t, \mathbf{r}_T, z) \rangle_t \rangle_z$$

created by the charge density

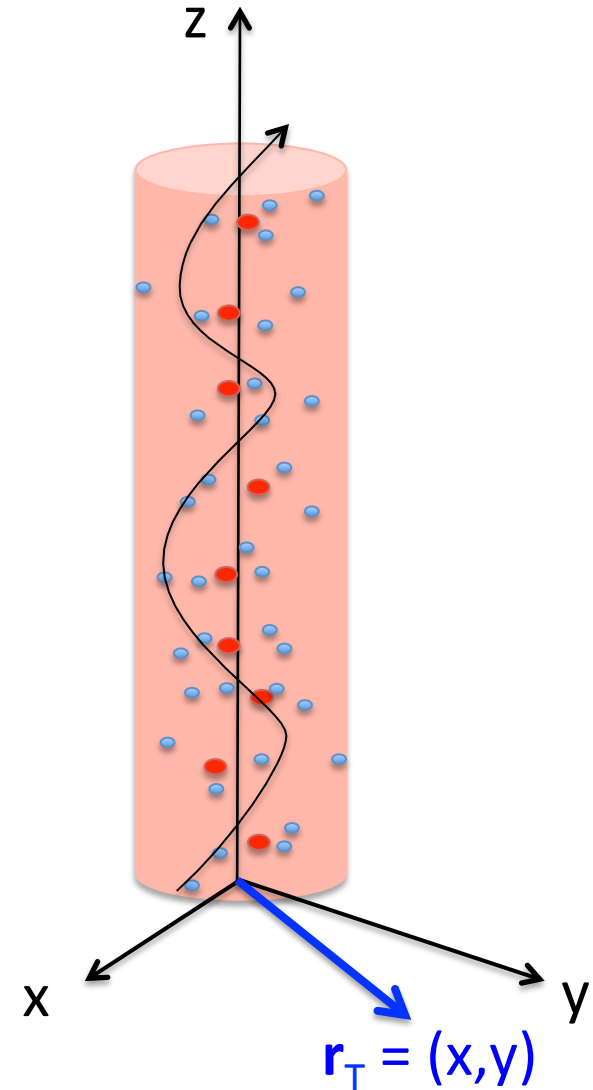
$$\rho_{\text{Lin}}(\mathbf{r}_T) = \langle \langle \rho(t, \mathbf{r}_T, z) \rangle_t \rangle_z$$

V_{Lin} conserves :

> the projectile energy ε ,

> the longitudinal momentum p_z

> the transverse energy $\varepsilon_T = \mathbf{p}_T^2 / (2\varepsilon) - e V_{\text{Lin}}(\mathbf{r}_T)$



Residual potential:

$$\delta V(t, \mathbf{r}_T, z) = V(t, \mathbf{r}_T, z) - V_{\text{Lin}}(\mathbf{r}_T)$$



- Breaks ε , p_z and ε_T .
- Responsible for *dechanneling* and *incoherent bremsstrahlung*.

Residual charge density

$$\delta \rho(t, \mathbf{r}_T, z) = \rho(t, \mathbf{r}_T, z) - \rho_{\text{Lin}}(\mathbf{r}_T)$$

Frozen approximation:

Neglect the t-dependence
of $\delta \rho$ and δV :

$$\delta \rho(\mathbf{r}_T, z) = \delta \rho(t, \mathbf{r}_T, z)_{t=0}$$

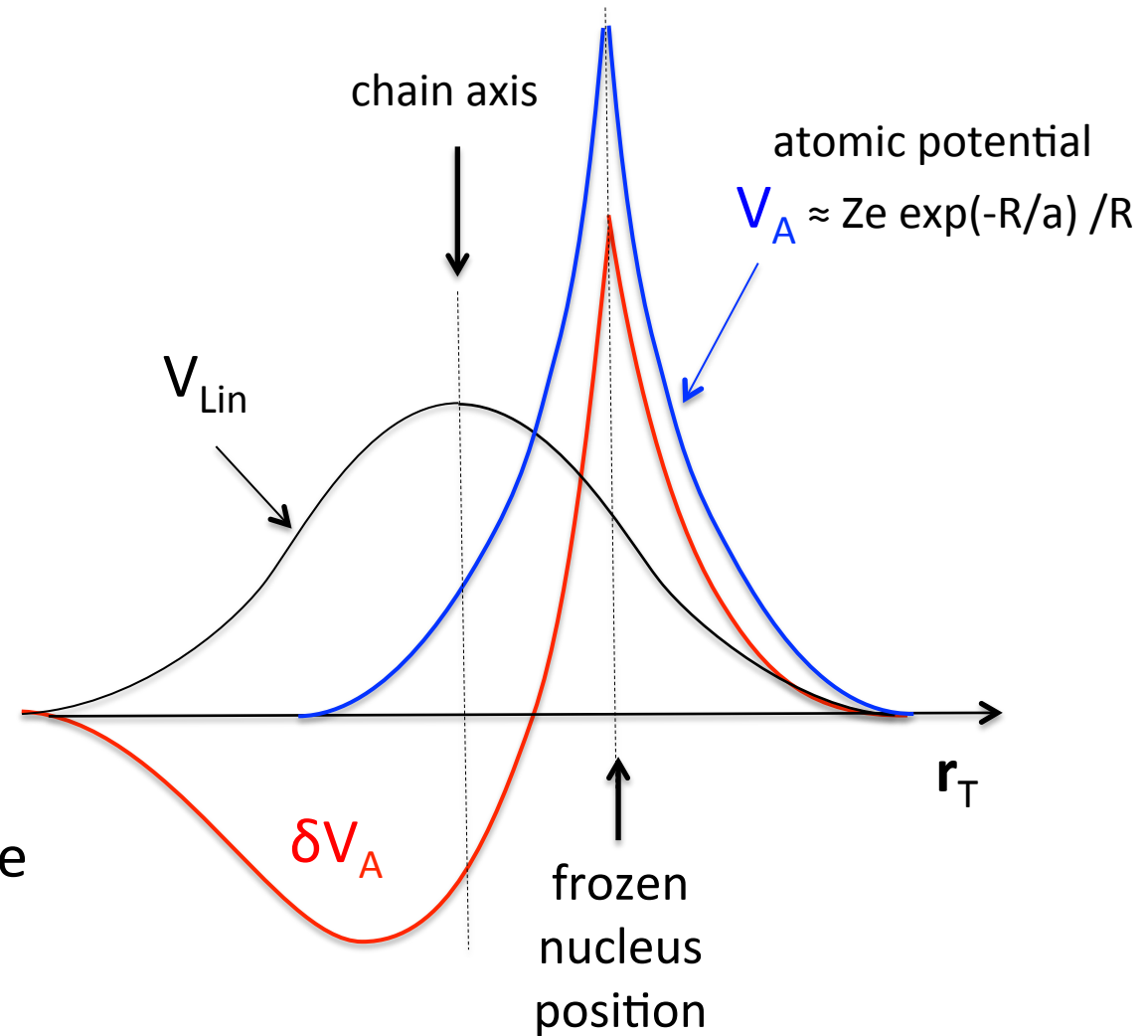
Justification : the projectile
moves much faster than the
crystal constituents

Three contributions to $\delta \rho$ and δV
(Beloshitsky, ...)

- 1) periodic modulation in z
(negligible effects)
- 2) vibrations of the atomic chain
(phonons)
- 3) electron motion inside the atoms

$$\delta V = \delta V_{\text{period}} + \delta V_A + \delta V_e$$

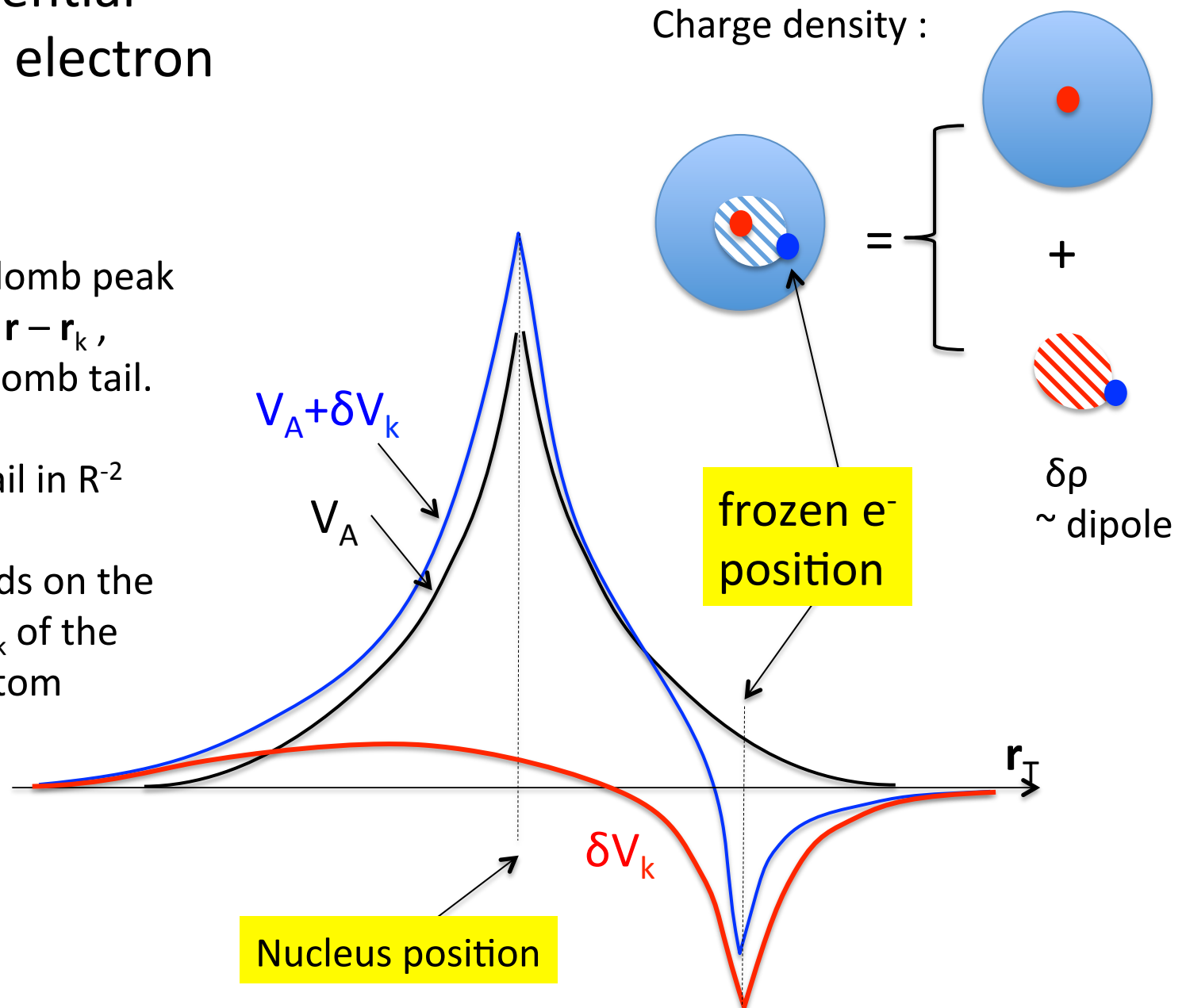
Residual potential δV_A from the vibrations of the atomic chain



- δV_A is of short range
- Its shape depends on the transverse position r_{NT} of the frozen nucleus
- It is generally dissymmetric
- zero mean value : $\int d^3r \delta V_A = 0$

Residual potential from the k^{th} electron of an atom

- δV_k has the Coulomb peak in $-e/R$ with $\mathbf{R} = \mathbf{r} - \mathbf{r}_k$, but not the Coulomb tail.
- It has a dipole tail in R^{-2}
- Its shape depends on the frozen position \mathbf{r}_k of the electron in the atom
- It is generally dissymmetric



Monte Carlo simulation - 1

Semi-quantum method :

Represent the effect of δV by *kinks* of the trajectory,
where \mathbf{p}_T receives a sudden jump \mathbf{q} ($= \mathbf{q}_T$)

- between two kinks: classical motion in V_{Lin} .
- kinks are generated at the rate

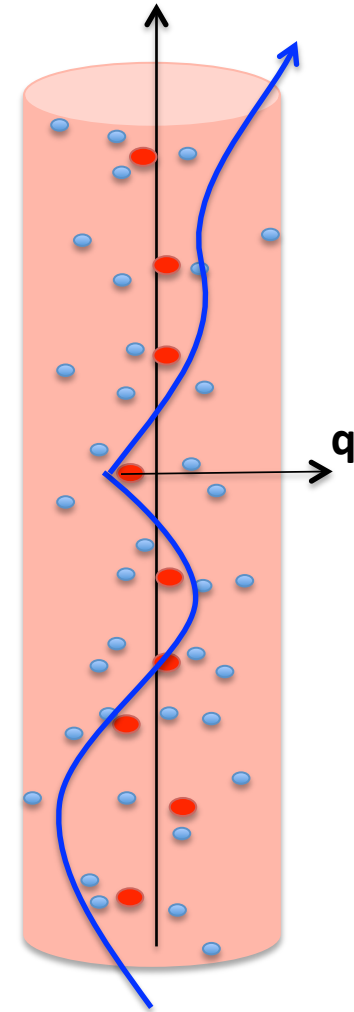
$$dN(\mathbf{q}) / (dz d^2\mathbf{q}) = \rho_N(\mathbf{r}_T) \cdot d\sigma_{N(\text{Qu})} / d^2\mathbf{q} + \rho_e(\mathbf{r}_T) \cdot d\sigma_{e(\text{Qu})} / d^2\mathbf{q}$$

where $\sigma_{(\text{Qu})}$ is the *quantum-mechanical cross section* on δV_k

$\rho_{e \text{ or } N}(\mathbf{r}_T)$ is the density of electrons or nuclei,
averaged on z

(the Lindhard charge density is $\rho_{\text{Linhard}} = Ze \rho_N - e \rho_e$)

- To simplify we ignore the shape dependence of the δV_k 's on the \mathbf{r}_k 's
- we ignore the correlations between the \mathbf{r}_k 's
- The random quantity is the vector \mathbf{q}



Monte Carlo simulation - 2

Classical method : “binary collisions”

Use the classical equation of motion in the full frozen potential

$$V(\mathbf{r}_T, z) = V_{\text{Lin}} + \delta V = \sum_k e_k / |\mathbf{r} - \mathbf{r}_k|$$

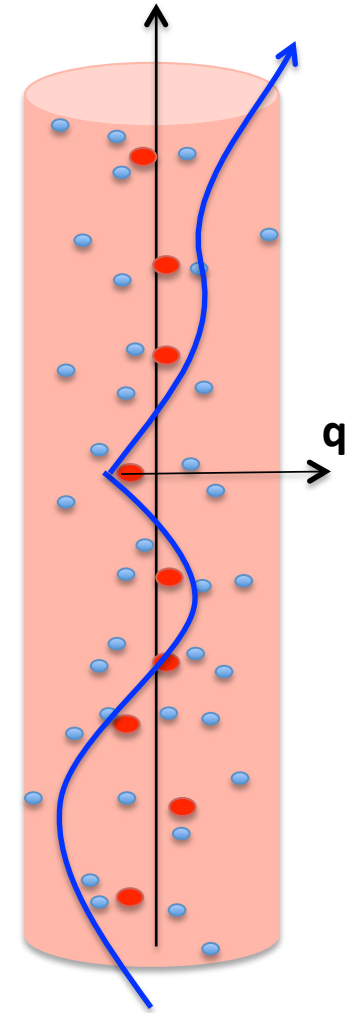
Each constituent k sitting near the trajectory changes \mathbf{p}_T by

$$\Delta \mathbf{p}_T = (e/v) \int dz \text{ grad}_{\mathbf{b}} V_k(\mathbf{b}, z)$$

(straight-line approximation). $\mathbf{b} = \text{impact parameter} = (\mathbf{r} - \mathbf{r}_k)_T$

$$\Delta \mathbf{p}_T = \underset{\substack{\uparrow \\ V_{\text{Lin}}}}{\Delta \mathbf{p}_{T(\text{continuous})}} + \underset{\substack{\uparrow \\ \delta V}}{\mathbf{q}}$$

- To simplify we ignore the correlations between the \mathbf{r}_k 's
- The random quantity is the vector $\mathbf{r}_{k,T}$



Classical vs. quantum cross sections on δV_k

We re-formulate the classical method like the semi-quantum one, *neglecting the variations of the density $\rho_k(\mathbf{r}_{k,T})$ of constituent k , near the trajectory* (at least within the range b_{\max} of δV_k).

This rough approximation gives

$$dN(\mathbf{q})/(dz d^2\mathbf{q}) \approx \rho_N(\mathbf{r}_T) \cdot d\sigma_N(\text{cl})/d^2\mathbf{q} + \rho_e(\mathbf{r}_T) \cdot D\sigma_e(\text{cl})/d^2\mathbf{q}$$

where $\sigma_{(\text{cl})}$ is the *classical cross section* on δV_k

Then it suffices to compare $d\sigma_{(\text{cl})}/d^2\mathbf{q}$ and $d\sigma_{(\text{Qu})}/d^2\mathbf{q}$.

Recall of the main properties of δV_k :

- Coulomb singularity at the origin, $-e \delta V_k \sim \alpha_k/r$ ($\alpha_k = 1/137$ or $-Z/137$)
- short range, or decreasing at least like r^{-2}
- dissymmetry in \mathbf{b}_T .

General comparison between **classical** and **quantum** cross sections

↑
(straight-line approximation)

↑
(Born approximation)

Average vector \mathbf{q} : $\int d^2\mathbf{q} \mathbf{q} \, d\sigma/d^2\mathbf{q} = 0$ (both in classical and quantum models)

Weighted cross sections: $M^{(n)} = \int d^2\mathbf{q} |\mathbf{q}|^n \, d\sigma/d^2\mathbf{q}$; $M^{(0)}$ = total cross section;

$M^{(n)}_{(\text{cl})}$ is better re-written as $\int d^2\mathbf{b} |\mathbf{q}_{\text{cl}}(\mathbf{b})|^n$

Examples :

- For a spherically symmetric and monotonic potential $V(r)$:

$$M^{(1)}_{(\text{cl})} = 2\pi^2 \int r \, dr \, V(r)$$

$$M^{(1)}_{(\text{qu})} = 4\pi^2 \int r^2 \, dr \, V^2(r)$$

- For any potential: $M^{(2)}_{(\text{cl})} = M^{(2)}_{(\text{qu})}$

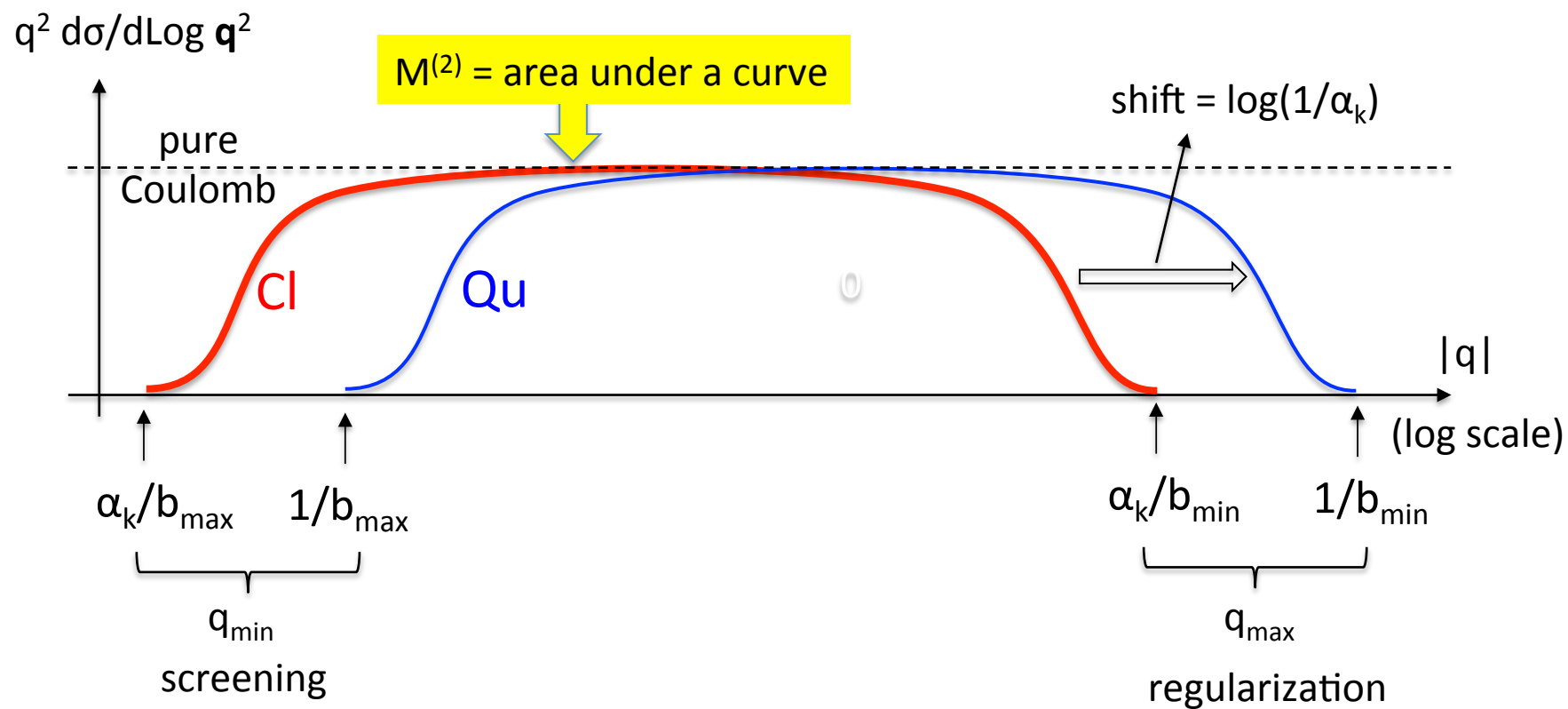
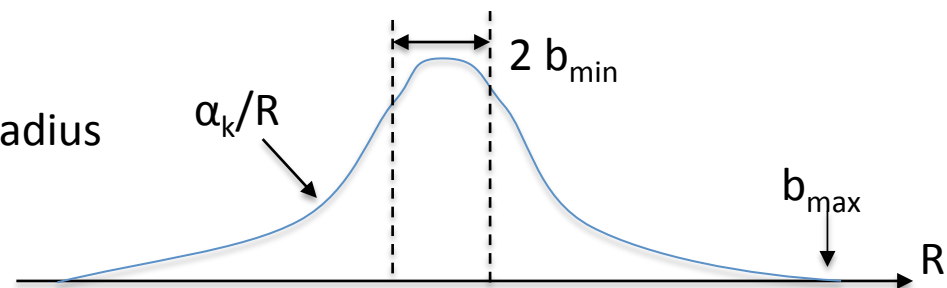
$M^{(2)}$ from δV_k governs the **rate of increase** of the **transverse energy**. Should we conclude that the classical and quantum models predict *the same dechanneling length* ?

Simple model
for δV_A :

$$\alpha_k = Z/137$$

$b_{\min} \sim$ nuclear radius

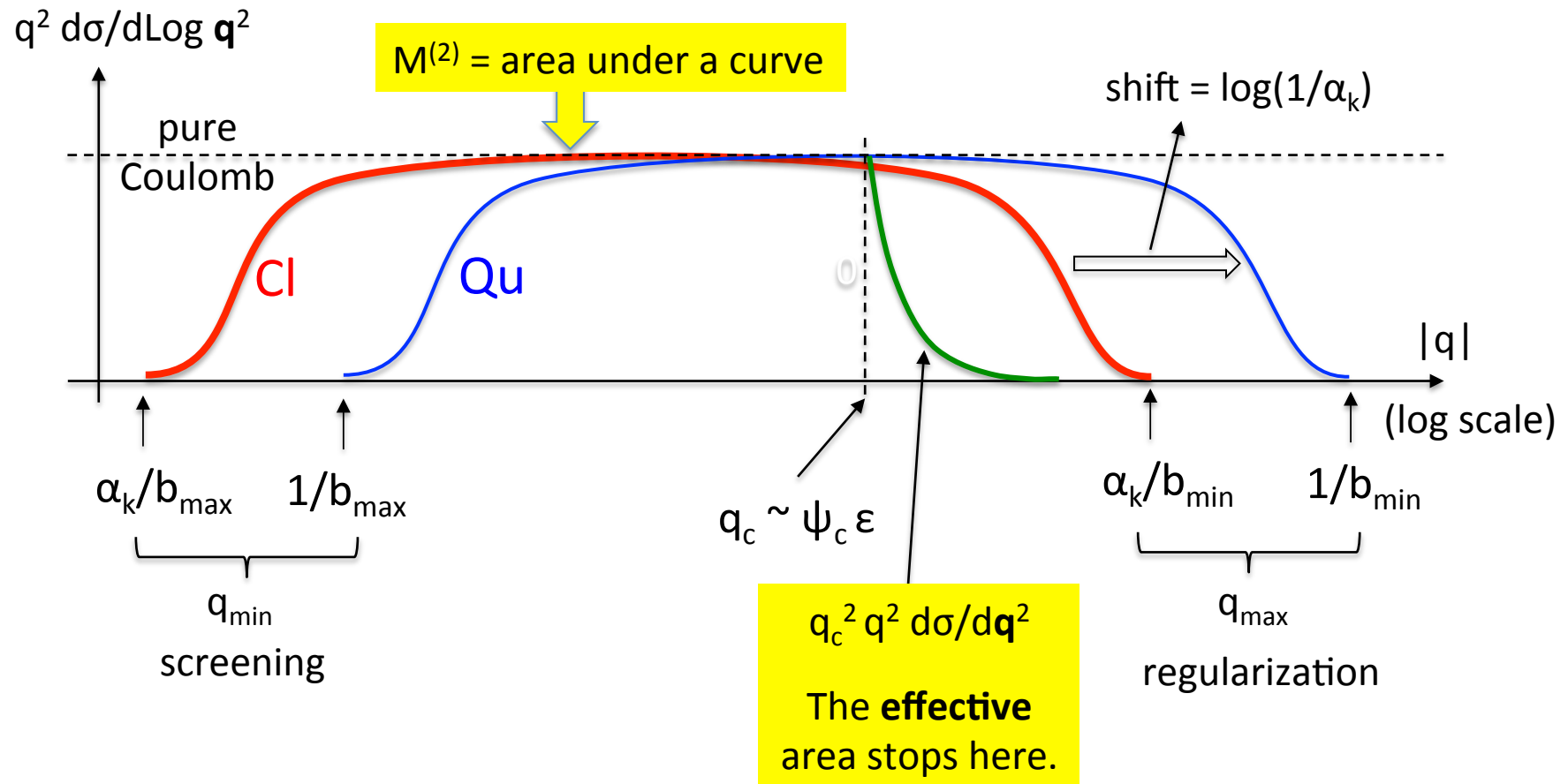
$b_{\max} \sim a_{\text{TF}}$



For $q > q_c \sim \psi_c \varepsilon$ dechanneling occurs at once, no matter the excess $q - q_c$.

Therefore the dechanneling rate is sensitive to $M_{\text{eff}}^{(2)} = \int d^2\mathbf{q} \cdot d\sigma/d^2\mathbf{q} \cdot \min(q^2, q_c^2)$

Conclusion: $M_{\text{eff}}^{(2)}(\text{Qu}) > M_{\text{eff}}^{(2)}(\text{Cl})$ (assuming $\alpha_k < 1$)



Rough estimation :

$$M_{\text{eff}}^{(2)}(\text{Cl}) / M_{\text{eff}}^{(2)}(\text{Qu}) = \log(q_c b_{\text{max}} / \alpha_k) / \log(q_c b_{\text{max}})$$

Typical order of magnitude

$$b_{\text{max}} \sim 1 \text{ \AA} = 1/(2\text{keV}) ; \alpha_k \sim 1/10 \text{ (Silicium)} ;$$

$$\varepsilon \sim 1 \text{ GeV} ; \psi_c \sim 1 \text{ mrad} \Rightarrow q_c \sim 1 \text{ MeV}$$

$$\Rightarrow M_{\text{eff}}^{(2)}(\text{Cl}) / M_{\text{eff}}^{(2)}(\text{Qu}) \approx 4/3$$

$$\text{For electrons, } \alpha_k = 1/137 \Rightarrow M_{\text{eff}}^{(2)}(\text{Cl}) / M_{\text{eff}}^{(2)}(\text{Qu}) \approx 5/3$$

Our final opinion :

The quantum method is *dirty* (full of approximations). The classical method is *cleaner* but far from reality. Neglecting quantum effects *underestimates* the dechanneling length.

Effects of correlations between the constituents

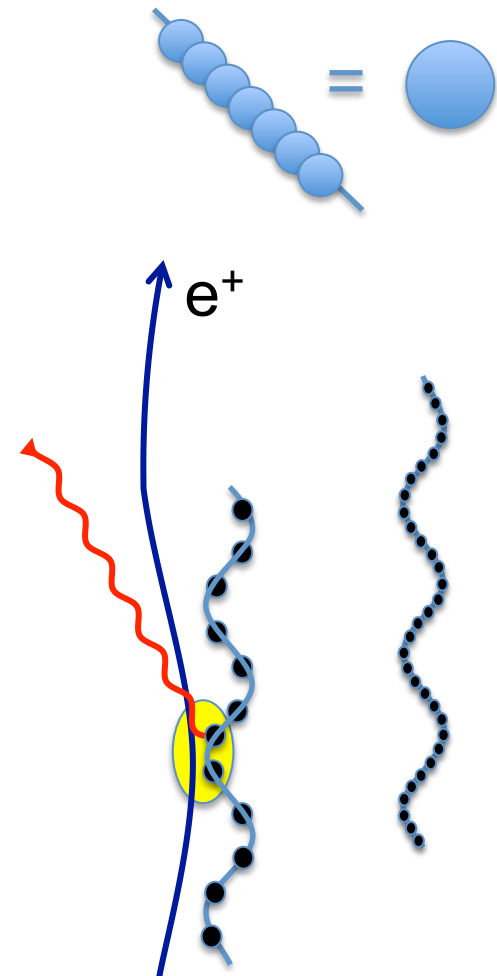
Roughly speaking, the Born approximation becomes bad, and the Classical scattering theory becomes good, when α_k becomes $> \sim 1$.

When a group of N successive atoms is nearly aligned along the particle trajectory, it acts like *one **super-nucleus** of charge NZ* . If $NZ / 137 > \sim 1$, coherent scattering on this group should be treated classically. This is the case of atoms displaced by a long-wavelength phonon.

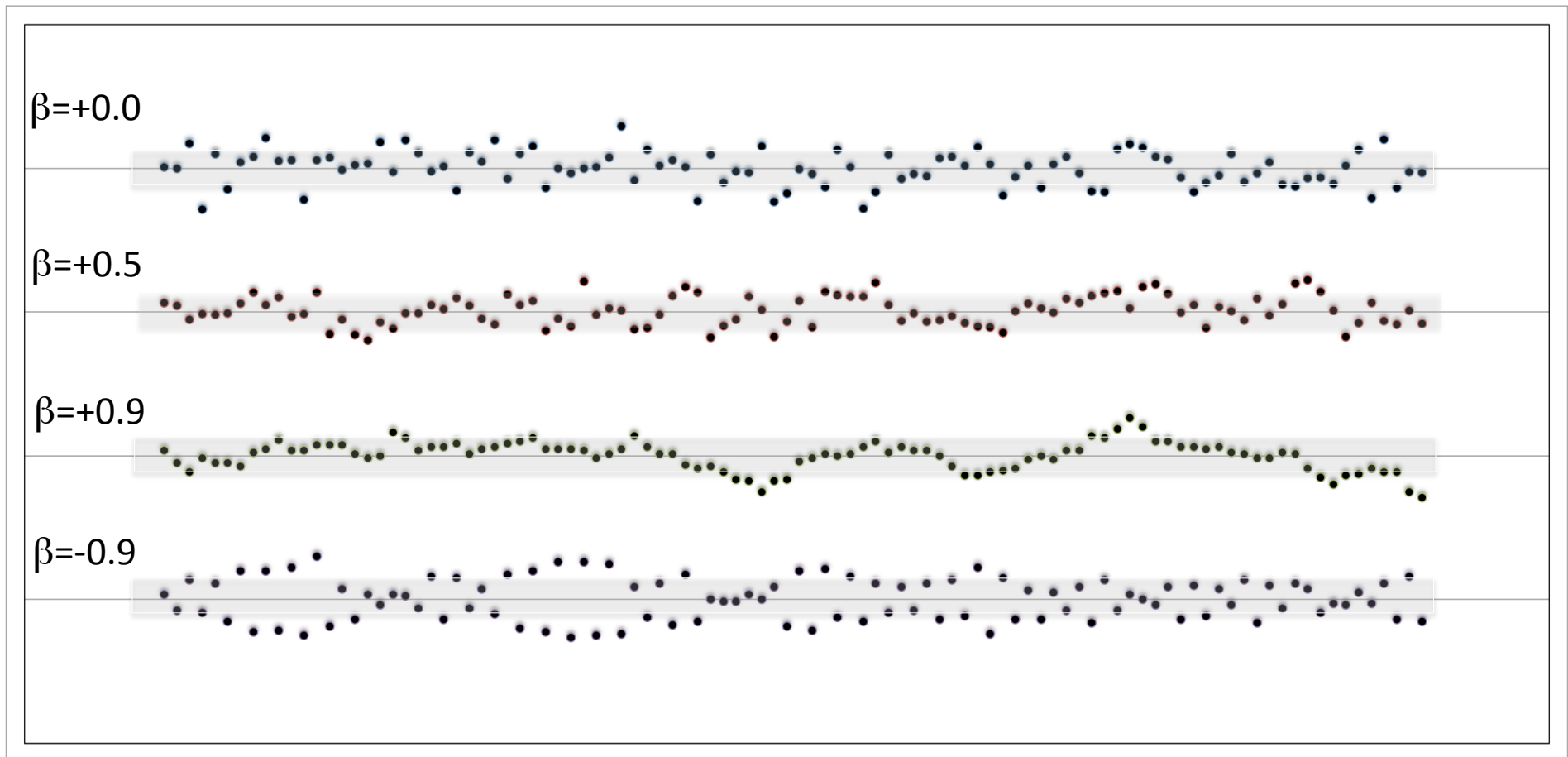
We obtain a 'semi-incoherent' process (X.A. Channeling 2016)

Thus, δV_A should be separated in two contributions:

- That produced by long-wavelength phonons, which can be treated classically,
- That produced by short-wavelength phonons, which must be treated quantum-mechanically.



Atomic chain vibration (simulated)



Conclusions

- The residual potential δV , responsible for incoherent processes, is usually of shorter range and weak ($\alpha_k \ll 1$). It should better be treated with the quantum Born approximation than treated classically.
- However, the inverse is true for the part of δV_A which is due to long-wavelength phonons.

Thank you !