# Quenching factor for low energy nuclear recoils in Si and Ge

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6th Colombian Meeting on

High Energy Physics
Nov 29 to Dec 3

Based on *'Study of the ionization efficiency for nuclear recoils in pure crystals'*, **Y.S**, A. Aguilar-Arevalo, J.C D'Olivo, Phys. Rev. D 101, 102001 (2020)

# Overview



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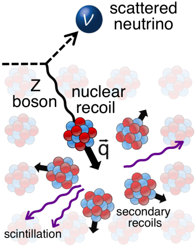
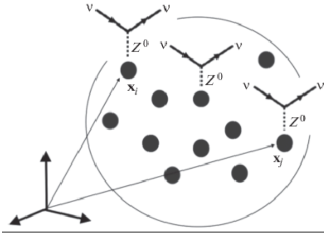
# Motivation




**CE$\nu$NS (Coherent Elastic Neutrino Nucleus Scattering):** neutrinos of $E_\nu < 1/R_{nuc}$ scatter off nucleus as a whole (recoil energy less than 1 keV). Measured by COHERENT (2017), usefull to study

- Anomalous neutrino magnetic moment
- Massive mediators
- Weinberg mixing angle
- Non standard interactions at low energy.
- Also important for Dark Matter searches.

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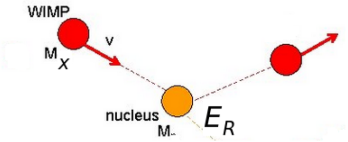
# Motivation

- Detection of nuclear recoils with $E_R < 10$ keV.
- For ionization-only detectors, the visible energy $E_v$ comes from electronic excitations.




$$E_{Rmax} = \frac{2E^2_{\bar{\nu}_e}}{M} \approx 10keV \text{ in Si.}$$

- Lindhard (1963) divided the deposited energy in electronic ionization ($H$) and nuclear movement ($N$); $E_R = H + N$.
  The *ionization efficiency* for nuclear recoils (quenching factor QF) is

$$\boxed{f_n = \frac{H}{E_R}}$$

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As experiments have lowered their detection thresholds well below 1 keV, understanding the quenching at those low energies has become important.

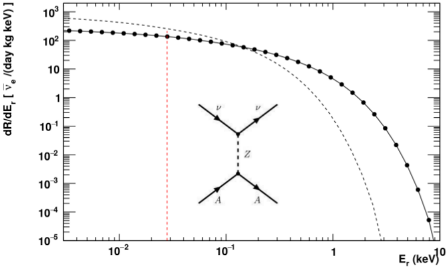
Suppose that the visible energy $E_v \approx H$.

Let $E_v = f_n(E_R)E_R$ be the visible energy reconstructed from the QF.

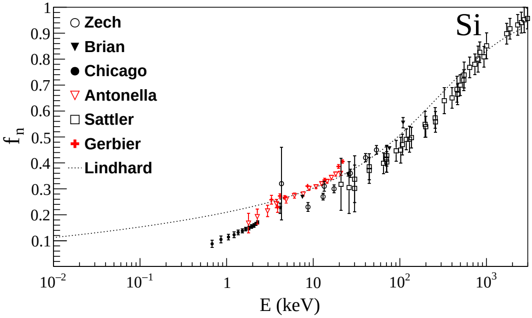
The visible energy spectrum is shifted to lower energies, due to the QF,

$$\frac{dR}{dE_R} = \frac{dR}{dE_v}\frac{dE_v}{dE_R} = \frac{dR}{dE_v}\left(f_n + E_R\frac{df_n}{dE_R}\right)^{-}$$

**QF moves events below threshold.**




CE$\nu$NS spectrum $\frac{dR}{dE_v}$ (dotted) and $\frac{dR}{dE_R}$ (solid).

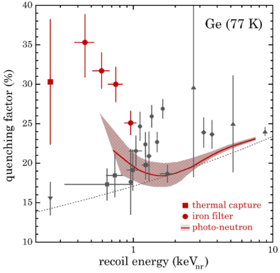



Si QF data from 0.69 keV to 3 MeV.

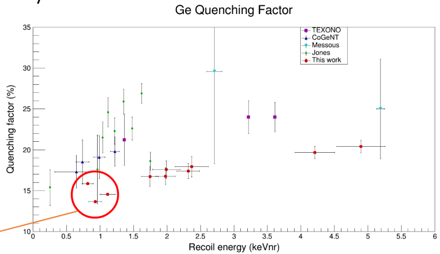
- Lindhard's model (LM) is expected to work only at high energies $> 10$ keV, where atomic binding energy (BE) can be neglected.
- For Si, LM fails below $\sim 5$ keV, where BE is relevant.
- Previous attempts to include BE had some problems.
- Our goal was to construct a mathematical consistent extension of LM with BE.

# Measurements of QF in Ge

- For Ge, Lindhard model works for high energies.
- Recent measurements (Collar'21) in disagreement with other data (COHERENT, SNL, Duke, TUNL, Jones'75).




Preliminary Results




Preliminary, no systematic errors

J.I.Collar, et al, PRD 103,122003 (2021), Long Li Duke University

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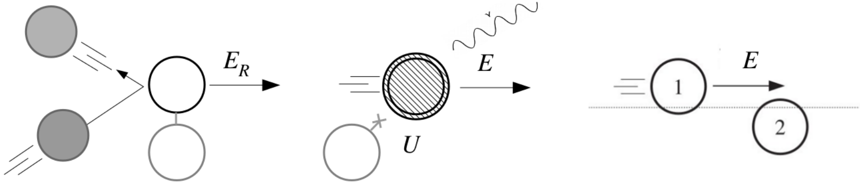
- Suppose that the ion recoils from the interaction with an energy $E_R$, after recoiling with an incident particle (e.g., a **neutrino**).
- Energy U is lost to some disruption of the atomic bonding, then $E_R = E + U$, then the ion moves with a kinetic energy $E$.
- The moving ion sets off a cascade of slowing-down processes that dissipate the energy $E$ throughout the medium.

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# Lindhard's model (LM)

- Lindhard's theory study the fraction of $E_R$ which is given to electrons, $H$, and that which is given to atomic motion, $N$, with $E_R = N + H$.
- Defining reduced dimensionless quantities, $\varepsilon_R = c_Z E_R, \eta = c_Z H, \nu = c_Z N$ where $c_Z = 11.5/Z^{7/3}\text{keV}$.
- The cascade process produce an average ionization $\bar{\eta}$.
- This separation is written as $\varepsilon_R = \bar{\eta} + \bar{\nu}$.
- The quenching factor ($f_n$) for a nuclear recoil is then defined as the fraction of $E_R$ which is given to electrons ($u = c_Z U$):

$$\boxed{f_n = \frac{\bar{\eta}}{\varepsilon_R} = \frac{\varepsilon + u - \bar{\nu}}{\varepsilon + u}} \tag{1}$$

When $u = 0$ one recovers the usual definition.

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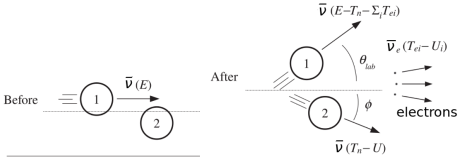
# Basic integral equation and approximations

($T_n$ : Nuclear kinetic energy and $T_{ei}$ electron kinetic energy.)

$$\underbrace{\int d\sigma_{n,e}}_{\textit{total cross section}} \left[ \underbrace{\bar{\nu}\left(E - T_n - \sum_i T_{ei}\right)}_{\text{A}} + \underbrace{\bar{\nu}\,(T_n - U)}_{\text{B}} + \underbrace{\bar{\nu}(E)}_{\text{C}} + \underbrace{\sum_i \bar{\nu}_e\,(T_{ei} - U_{ei})}_{\text{D}} \right] = 0 \quad (2)$$

**Lindhard's (five) approximations**

- I Neglect contribution to atomic motion coming from electrons.
- II **Neglect the binding energy, U = 0. (Now taken into account)**
- III Energy transferred to electrons is small compared to that transferred to recoil ions.
- IV Effects of electronic and atomic collisions can be treated separately.
- V $T_n$ is also small compared to the energy $E$.

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- Using these approximations Lindhard deduced a simplify integral equation,

$$\underbrace{\left(k\varepsilon^{1/2}\right)}_{S_e}\bar{\nu}'(\varepsilon) = \int_0^{\varepsilon^2} \underbrace{dt\frac{f\left(t^{1/2}\right)}{2t^{3/2}}}_{d\sigma_n}\left[\bar{\nu}(\varepsilon - t/\varepsilon) + \bar{\nu}(t/\varepsilon) - \bar{\nu}(\varepsilon)\right], \quad (3)$$

- Since binding energy was neglected, it is only valid at high energies.
- On the one hand $\bar{\nu}(\varepsilon \to 0) \to \varepsilon$, but according to Eq.(3) predict $\bar{\nu}'(0) = 0$.
- Lindhard gave a parametrization for $\bar{\nu}$, which only works for $\varepsilon_R \gtrsim 0.1$

$$\bar{\nu}_L(\varepsilon) = \frac{\varepsilon}{1 + kg(\varepsilon)},$$
$$g(\varepsilon) = 3\varepsilon^{0.15} + 0.7\varepsilon^{0.6} + \varepsilon.$$

- First principles elec. stopping power.
  $S_e = k\varepsilon^{1/2}$, $k = 0.133Z^{2/3}/A^{1/2}(\approx .15)$.

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# Approximation to LM with binding energy.

In order to compute a solution for $\bar{\nu}$ that includes the binding energy, we do the following

1. Neglect atomic motions caused by electrons, because they are negligible at low energies $\bar{\nu}_e = 0$.
2. Energy transferred to ionized electrons is small compared to that transferred to recoiling ions .
3. Effects of electronic and atomic collisions can be treated separately.
4. $T_n$ is also small compared to the energy E.
5. Expand the terms in Eq. 2 up to **second order** in $\boxed{\Sigma_i T_{ei}/(E - T_n)}$.

The first four are the same approximation used by Lindhard.

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# Simplified integral equation with binding energy

In a previous work on the subject it was not noticed[a] the necessity to change the lower limit of integration in order to be consistent with the term $\bar{\nu}(t/\varepsilon - u)$. We take this into account and, consequently, so Eq.2 becomes:

$$\boxed{-\frac{1}{2}k\varepsilon^{3/2}\bar{\nu}''(\varepsilon)} + \underbrace{k\varepsilon^{1/2}}_{S_e}\bar{\nu}'(\varepsilon) = \int_{\boxed{\varepsilon u}}^{\varepsilon^2} \underbrace{dt\frac{f\left(t^{1/2}\right)}{2t^{3/2}}}_{d\sigma_n}\left[\bar{\nu}(\varepsilon - t/\varepsilon) + \bar{\nu}(t/\varepsilon - \boxed{u}) - \bar{\nu}(\varepsilon)\right] \tag{4}$$

This equation can be solved numerically from $\varepsilon \geqslant u$. It predicts a threshold energy $\varepsilon_R^{threshold} = 2u$.

The equation admits a solution featuring a "kink" at $\varepsilon = u$ (discontinuous 1st derivative). We assume that the binding energy is a constant $u = u_0$

[a] PhysRevD 91 083509 (2015)

To solve the Eq.(4), the following parametrization is required

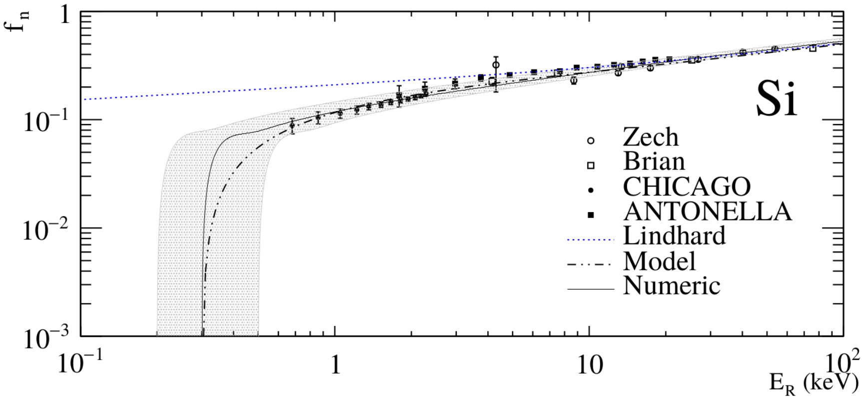
$$\bar{\nu}_u(\varepsilon) = \begin{cases} \varepsilon + u_0 & \varepsilon < u_0 \\ \varepsilon + u_0 - \lambda(\varepsilon) & \varepsilon \geq u_0 \end{cases} \tag{5}$$

where $\lambda$ has to be a continuous function, but must have a discontinuity in its first derivative at $\varepsilon = u_0$.

$$\begin{array}{ll} \lim_{\zeta\to 0} \lambda'(u+\zeta) = \alpha_1, & \lim_{\zeta\to 0} \lambda''(u+\zeta) = \alpha_2 \\ \lim_{\zeta\to 0} \lambda'(u-\zeta) = 0, & \lim_{\zeta\to 0} \lambda''(u-\zeta) = 0 \end{array} \tag{6}$$

with $\alpha_1 \neq 0$ and $\alpha_2 \neq 0$. Where can be determined by a shooting method.

# First Result for Si (PRD 101, 102001 (2020)).




Measurements of the QF in Si (points with error bars) compared to the Lindhard model (dot-dashed line), the fitted ansatz, and the numerical solution with $U = 0.15$ keV and $k = 0.161$.

- Straggling $\Omega^2 = \langle \delta E - \langle \delta E \rangle \rangle^2$, is an inherent feature of stopping.
- In dimensionless units[1]: $\frac{d\Omega^2}{d\rho} \equiv W = \frac{C^2}{\pi a^2} \int_0^E T_n^2 \sigma(T_n) dT_n$.
- Straggling appears when approximation (III) is relaxed up to second order in $(\Sigma_i T_{ei})$.
- Assuming a general electronic stopping power $S_e(\varepsilon)$, the integro-differential equation can be written,

$$\boxed{\begin{aligned} -\frac{1}{2}\varepsilon S_e(\varepsilon)\left(1 + \frac{W(\varepsilon)}{S_e(\varepsilon)\varepsilon}\right)\bar{\nu}''(\varepsilon) + S_e(\varepsilon)\bar{\nu}'(\varepsilon) = \\ \int_{\varepsilon u}^{\varepsilon^2} dt \frac{f\left(t^{1/2}\right)}{2t^{3/2}}[\bar{\nu}(\varepsilon - t/\varepsilon) + \bar{\nu}(t/\varepsilon - u) - \bar{\nu}(\varepsilon)], \end{aligned}} \tag{7}$$

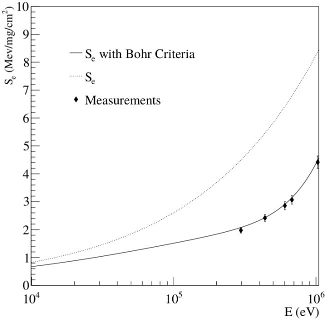
**Goes beyond than using the ratio $\xi(\varepsilon) = S_e(\varepsilon)/S_n(\varepsilon)$ as a measure of the energy dissipation, consider by Lindhard and Bezrukov.**

[1] $C = 11.5/Z^{7/3}[\frac{1}{\mathrm{keV}}]$

# High energy effects ($> 10$ keV) for $S_e(\varepsilon)$

## § *Bohr Stripping*

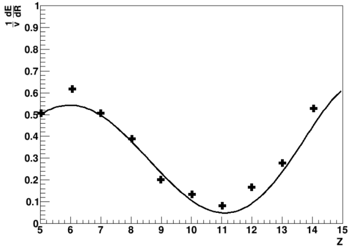
- Electrons can be lost according to momentum transferred.
- The effective number of electrons obeys $Z^\dagger \approx Z e^{-v/Z^{2/3} v_0}$.
- $S_e \propto Z^\dagger$, this leads to damping.




- $S_e$ vs data

## § *Z oscillations*

- When the ion charge changes, the transport cross section changes.
- Phase shift appear to maintain the neutrality of the electron Fermi gas.

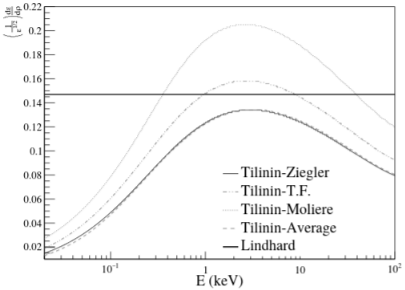



- Z oscillation for Si.

# Low energy effects for $S_e$

§ *Electronic stopping power*

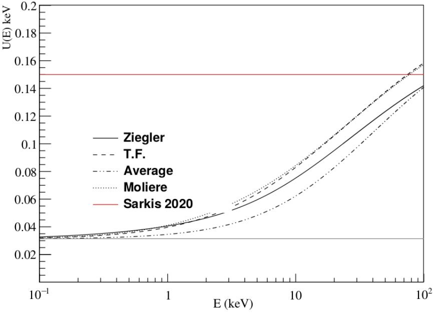
- Coulomb repulsion effects, produces a damping in $S_e$ at low energies.
- Using different inter-atomic potentials and models (12 curves); Tilinin,Kishinevsky and Arista.



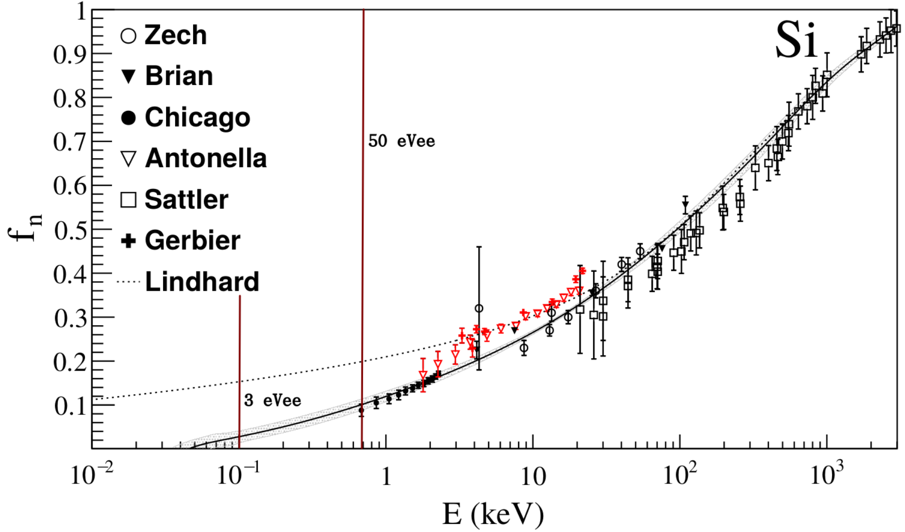

▫ $S_e/\sqrt{\varepsilon}$ for Tilinin model computed with four different inter-atomic potentials

§ *Binding energy*

- Frenkel pair creation energy.
- Atomic binding with T.F theory.

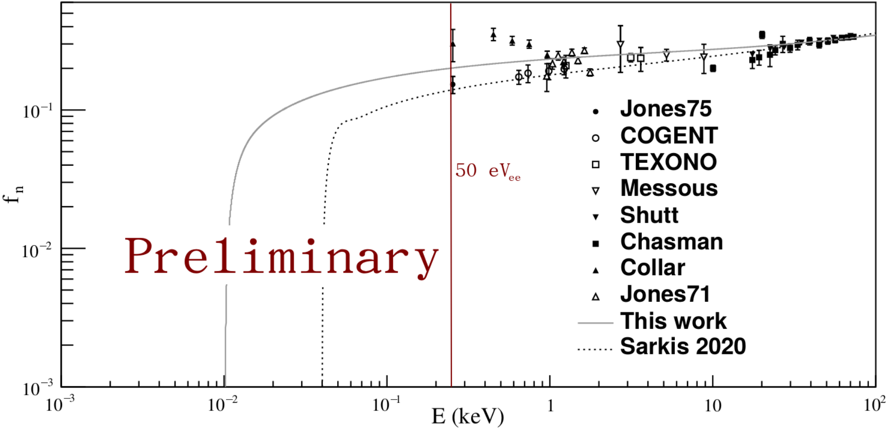



▫ Variable binding energy




Fit to all data except ANTONELLA and Gerbier. Band corresponds to twelve possible models. Fit deteriorates significantly if included.

**For Ge ($Z = 32$) we have to include a geometrical factor, mentioned by Tilinin and only significant for high Z ($Z > 20$).**




Germanium QF model with straggling, **geometrical factor**, low and high energy effects.

# Conclusions

1. We have improved our study of the basic integro-differential equation describing the energy given to atomic motion by nuclear recoils in pure crystals, based on Lindhard's theory.
2. Considering a variable binding energy and detail modeling of electronic stopping, we compute the QF in Si over nearly five orders of magnitude ($E_R \sim 50$ eV to 3 MeV).
3. The model describes all the silicon data well, except for ANTONELLA and Gerbier, which introduce some tension. The model shows potential to explain recent Ge measurements
4. A Si based experiment with a threshold of $E_{th} \approx 4 \,\mathrm{eV_{ee}}$ requires knowledge of the QF down to $E_R \approx 100$ eV. Needed for next generation CE$\nu$NS experiments, e.g. skipper CCD's.
5. Much work can be done from here, e.g directional quenching factor, straggling for $\bar{\nu}$, higher moments study, etc.

# Thanks

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# Backup

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# QF Measurements in Silicon

A series of experiments contrasted Lindhard model in different materials, using neutron beams produced in accelerators they measured QF for energies above 20 keV.

After 1965 other low energy measurements were made using mono energetic neutron beams from $^{3}\mathrm{H}(\mathrm{p},\mathrm{n})^{3}\mathrm{He}$ reaction and a Si detector.

Other technique implemented in 1990 (Gerbier) consist in using a broad spectrum neutron beam and, using nuclear resonance properties of Si and neutrons to make measurements.

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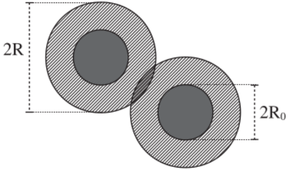
The lower integration limit in Eq. (4) can be motivated, for example, considering collisions between semi-hard spheres.

Lindhard used hard spheres in the collisions, so the minimum scattering angle was zero ($t_{min} = 0$). Semi-hard sphere model can take in to account the binding energy, and give $t_{min} = \varepsilon u$,

$$V(r) = \begin{cases} 0 & \text{for } \mathrm{r} \in [R, \infty] \\ -u & \text{for } \mathrm{r} \in [R_0, R] \\ \infty & \text{for } \mathrm{r} \in [0, R_0] \end{cases} \quad (8)$$




Where $R_0 \propto a_0/Z$ and $R \approx 2a_0$ ($R \gg R_0$). In order to estimate the $t$ value we use as an approximation the classical formula for the scattering angle.

# Numerical solution

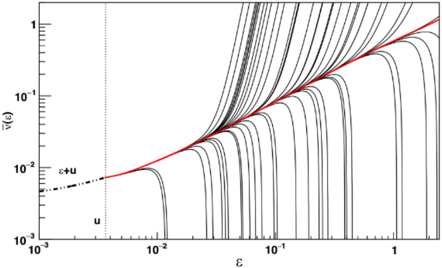
We first notice that the QF depends only of $\boldsymbol{k}$ and $\boldsymbol{u}$.

## Shooting method

We have the boundary condition (BC) $\bar{\nu}''(\varepsilon \to \infty) \to 0$.
Now, since the R.H.S of Eq. 4 is zero at $\varepsilon = u$ and lower, we impose that the L.H.S to be zero at this point, this gives the relation

$$\alpha_1 = 1 + \frac{1}{2} u_0 \alpha_2$$

So we give an initial try of $\alpha_2$ to hit the BC, we shoot in this way until the BC is satisfy.




# WHEN SHOOTING ENDS $\bar{\nu}''(\varepsilon \to \infty) \to 0$

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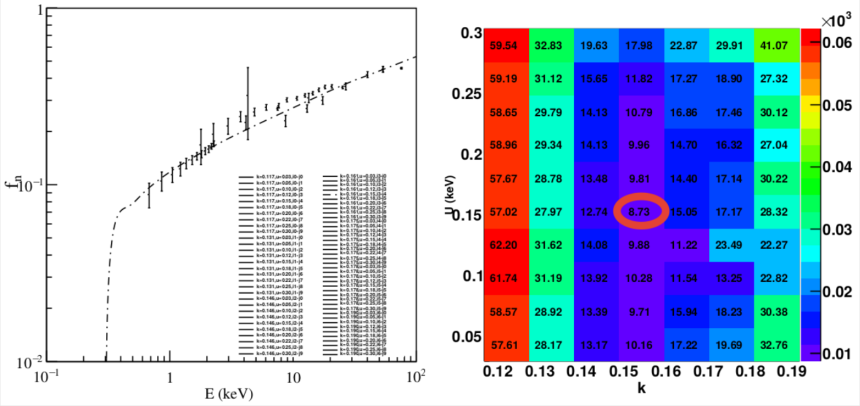
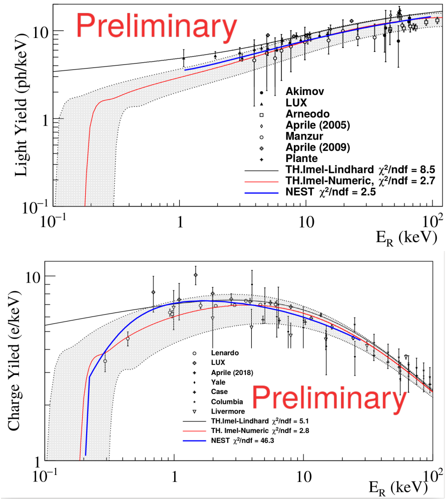
# Fits to data

To find $U$ and $k$ we make a fit over a coarse grid shown here. And find a solution that describes the available data using a $\chi^2$ to determine the optimal value. We do this for Si and Ge.



## Xe Light and Charge yields



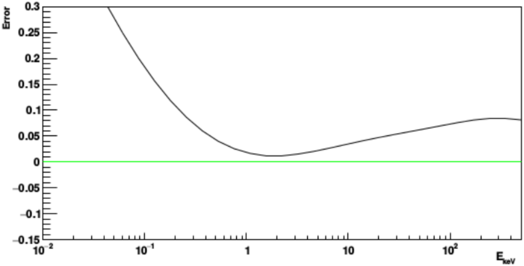

- The Ligh Yield and Charge Yield in noble gases are proportional to $f_n$.
- We can compute the total quanta $(N_e + N_{ex})$ ($N_e$ : electrons and $N_{ext}$ : excitons).
- Using the Thomas-Imel[a] box model its possible to obtain the **Charge** and **Light** Yields.
- Its also possible to add Penning effect directly.
- The binding energy obtained is compatible with the bindings for Xe atomic shells.

[a] Phys. Rev. A36, 614, 1987

# Lindhard Parametrization

Lindhard's parametrization solve aproximatle the simplify integral equation, just well at high energies ($\varepsilon > 1$).

$$\bar{\nu}_l(\epsilon) = \frac{\epsilon}{1+kg(\epsilon)}$$
$$g(\epsilon) = 3\epsilon^{0.15} + 0.7\epsilon^{0.6} + \epsilon \tag{9}$$




The parametrization doesn't solve the Equation at low energies.

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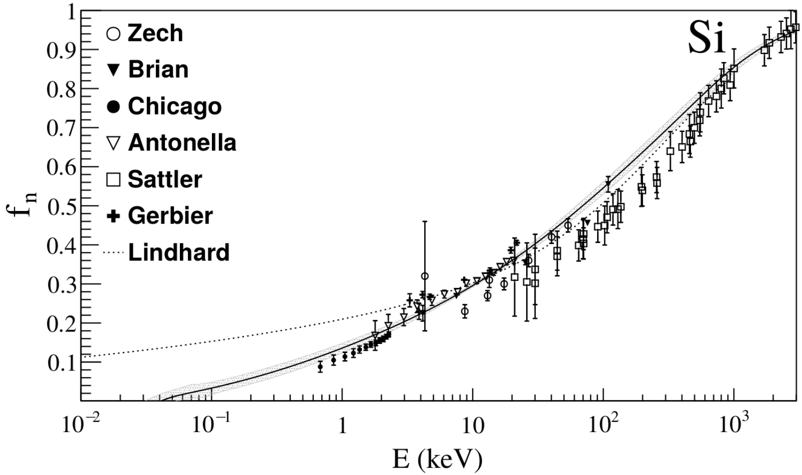
# QF with all data

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