Recent study and results for ionization efficiency theory in pure materials

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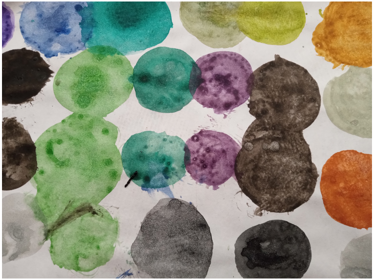
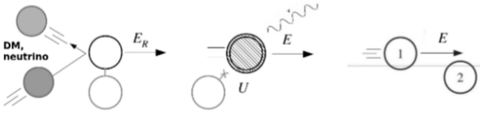
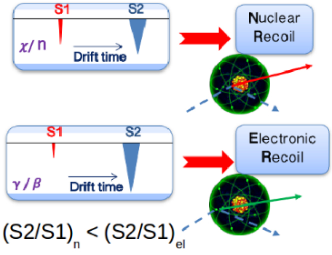


Nuclear Ionization Efficiency

When a particle interact with a nuclei the energy splits:

E_n : Nuclear collisions. ($\bar{\nu} = C_0 E_n$[1])
E_I : Ionization (visible) energy $[\mathrm{keV_{ee}}]$ ($\bar{\eta}$).





- *Quenching* $= \dfrac{\text{ionization energy}}{\text{deposited energy}} = \boxed{f_n = \dfrac{\bar{\eta}}{\varepsilon_R}.}$
- $\varepsilon_R - \bar{\eta} = \bar{\nu}$, energy lost to atomic motion
- u is the energy to disrupt the atomic bonding.
- This sets a cascade of slowing-down processes.
- For TPC $(S2/S1)_n < (S2/S1)_e$: $f_n = \dfrac{(n_e + n_\gamma)_R W}{\varepsilon_R}$

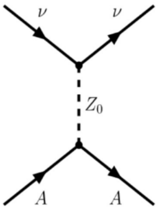
[1] Using dimensionless units ($C_0 = 16.26(1/\mathrm{keV})/\mathrm{Z_1 Z_2}(\mathrm{Z_1^{0.23}} + \mathrm{Z_2^{0.23}})$)

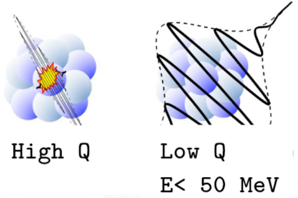
Coherent elastic Neutrino Nuclear Scattering [2]

1. Neutral-current process mediated by the Z-boson.
2. Low momentum transfer.

$$\frac{\mathrm{d}\sigma}{\mathrm{d}T} = \frac{G_F^2 M}{4\pi}\left(1 - \frac{MT}{2E_\nu^2}\right) Q_{\mathrm{w}}^2 \left[F_{\mathrm{w}}\left(q^2\right)\right]^2 \tag{1}$$

3. G_F Fermi constant, $T = E_\nu - E'_\nu$ NR energy, $F_w^2(q^2)$ weak Form Factor, M target mass and $Q_{\mathrm{w}} = Z\left(1 - 4\sin^2\theta_W\right) - N$.





[2] D.Z. Freedman, Coherent effects of a weak neutral current, Phys. Rev. D 9 (1974) 1389.

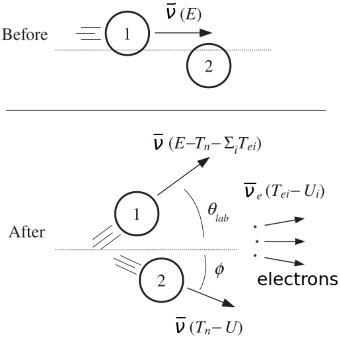
Lindhard Integral Equation

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

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

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.



Lindhard model

Lindhard's first order approximation.

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

1. Neglects binding energy $u = 0$.
2. Only valid for $\varepsilon \gg u$.
3. Electronic stopping power assume bare ions.
4. $k\varepsilon^{1/2} > S_e$ for energies $\varepsilon < 1$.

1. $u \neq 0$ implies a second order solution.
2. Threshold expected at $\varepsilon = u$.
3. Coulomb repulsion effect for S_e at low energies.

Lindhard formula[3] is valid for $\varepsilon > 1$

LXe $E_R^{LXe} \approx 1$ MeV and $E_R^{LAr} \approx 77$ keV

[3] J. Lindhard, et al, Mat. Fys. Med. 33 (1963)

- We use Tilinin model to compute the electronic stopping power.

$$S_e = (\xi_e) N m v \int_R^{\infty} v_F \sigma_{\mathbf{tr}}(v_F) N_e dV, \quad E = \phi_Z(R)$$

- We use data for $e-$ atom Momentum Transfer Cross Section (hard-Sphere energy dependent potential model)
- Valid for lower energies compare to Tilinin semi-classical approach.

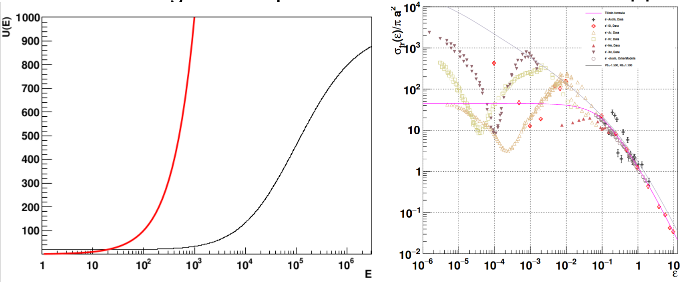


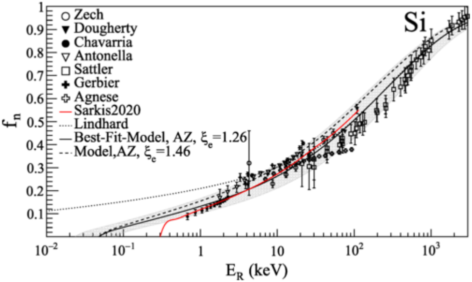
Figure 1: (left) Energy dependent binding energy, (right) σ_{tr} for Ar-e.

Simplified equation with binding energy

- We are going to use the integro-differential equation for atomic motion deduced in the past work for Si.[4].

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

This work have been used for **Skipper CCD's: (DAMIC) PRD 109 (2024) 6, 062007 and (CONNIE) e-Print: 2403.15976.**



- ξ_e from Pauli principle, instead of semi-empirical factor $\xi_e \approx Z^{1/6}$.

$$\xi_e^{2/3} \equiv \frac{5}{3}\frac{\int_{k_F-\Delta}^{k_F} E(k)k^2 dk}{E(k_F)\int_{k_F-\Delta}^{k_F} k^2 dk},$$

- $1 < \xi_e < 2.2$

[4]Sarkis, Y. and Aguilar-Arevalo, A. and D'Olivo, J. C, PRA.107.062811

For LXe the total quanta to low, this motivates new research!

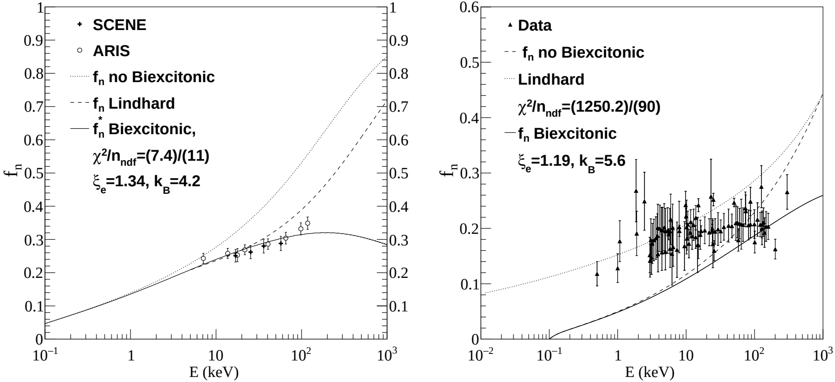
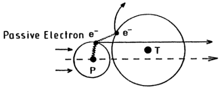
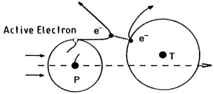


Figure 2: LAr (left) and LXe (right) total quanta.

Bates-Griffing Process (BG)

- For two atoms collision we take for outer electrons:$\psi(x_1', x_2')_\pm = (\psi_1(x_1')\psi_2(x_2') \pm \psi_1(x_2')\psi_2(x_1'))/\sqrt{2}$.
- This leads to exchange electron non classical potential.
- $\psi(x_1', x_2')_-$ (triplet): **Passive electrons**, remains in its ground state.





- $\psi(x_1', x_2')_+$ (singlet): **Active electrons,** electrons are removed.
- Average energy to create an electron from nuclear recoil $W_i^R = W(1 + N_{ex}/N_i)$ (explain $W_i^\alpha \neq W_i$).

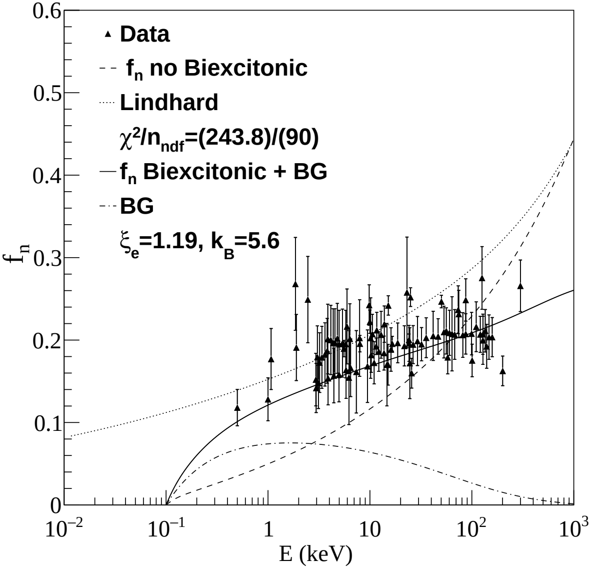


Figure 3: LXe total quanta with BG active effect.

Thomas-Imel box Model

- Diffusion equation for ions-electrons (N_- N_+) Jaffe model, [5].

$$\frac{\partial N_+}{\partial t} = -\alpha N_- N_+, \qquad \frac{\partial N_-}{\partial t} = \mu_e F \frac{\partial N_-}{\partial z} - \alpha N_+ N_-. \tag{4}$$

- Where α is the recombination factor, μ_e electron mobility and F the TPC electric field.
- Each excited or ionized atom leads to one photon or electron.
- $\Rightarrow N_i + N_{ex} = n_\gamma + n_e$,
- $n_e = (1-r)N_i$ and $n_\gamma = N_{ex} + rN_i$.
- Hence, the fraction of ionizations predicted is

$$\frac{n_e}{N_i} = \frac{1}{\xi}\ln(1+\xi), \quad 1-r = \frac{1}{\xi}\ln(1+\xi), \quad \xi = \frac{N_i \alpha}{4a^2 \mu_e F}.$$

$$N_i = \frac{E_R \mathbf{f_n}}{W(1+\beta)}, \quad \text{Where } \beta = N_{ex}/N_i \text{ and } f_n = \frac{E_{ee}}{E_R}.$$

- This recombination model depends on **four parameters for each noble liquid.**

[5] Ann.Phys.IV, V42, pp.303 – 344, (1913). PRA 36, 614 (1987)

Recombination Parameters from first principles

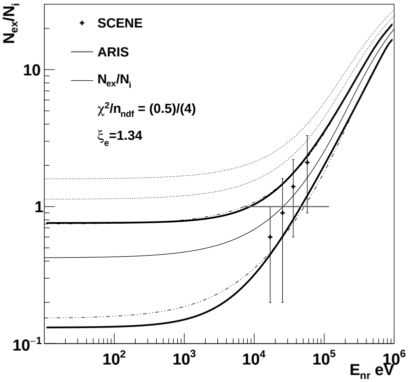
- Usually [6], **five to ten parameters** are need.
- **We are just going to use ξ_e and the scale recombination probability α_0 (universal) as fit parameters.**

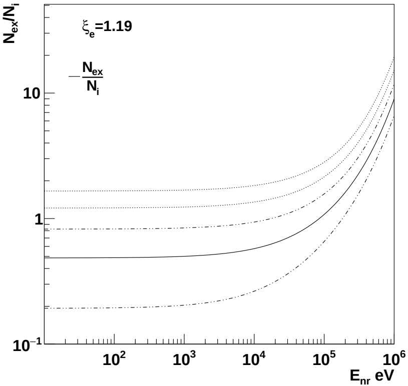
$$\alpha = \alpha_0 Z (2r_W)^2 v_0, \quad \xi = \frac{\alpha_0 N_i Z (2r_W)^2 v_0}{4\mu_e \boxed{(a^2 F)}} \tag{5}$$

- The same inter-atomic potential used for f_n will explain:
  - Energy and field dependence of the ratio N_{ex}/N_i.
  - Biexcitonic quenching.
  - Box model length a, as function of external field.
  - Field dependence of Thomas-Imel Box model parameter: $\xi \propto F^{-\delta}$.
  - $\delta_{Ar} \approx (0.4 - 0.6)$ and $\delta_{Xe} \approx (0.04 - 0.12)$.

[6] PRD 100,032002(2019),PRD 91,092007(2015)

We use BG to compute: $W_i^R = W(1 + \frac{N_{ex}}{N_i})$.





Stark Effect for Ions

Stark Effect for ions inside the Box

- Electric field F applied to a TPC.
- During recombination we have plasma formed by ions-electrons.
- The polarizability increase significantly $\varepsilon(k) \gg \varepsilon$
- We can compute the energy correction δ_1 to the potential $e\phi_Z(x,\xi_e) =< \psi \mid V \mid \psi >$,

$$\delta_1 =< \psi \mid V_{ext} \mid \psi >, \; V_{ext} = \pm((\xi_e)^{2/3} a x_z eF) = \pm((\xi_e)^{2/3} axeF) cos(\theta).$$

- Where $V_{ext} \ll \phi_Z(x,\xi_e)$ and $r \approx r_0 + dcos(\theta)$.
- We define the new electron-atom disturbed potential, $\phi_Z^e(x,\xi_e,Z,F) = \phi_Z^e(x,\xi_e,Z,0) - \delta_1$.

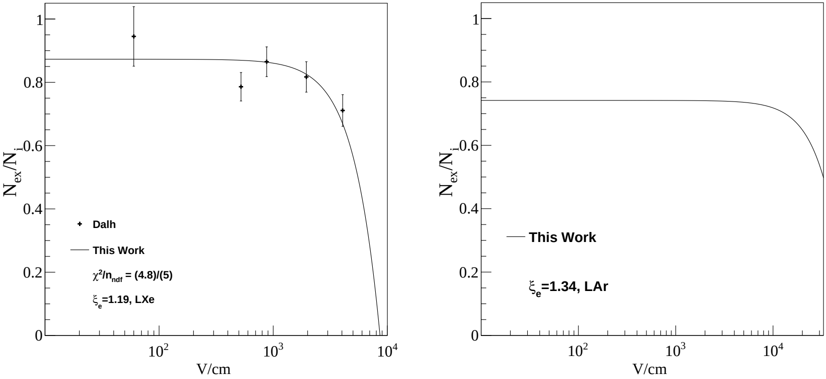
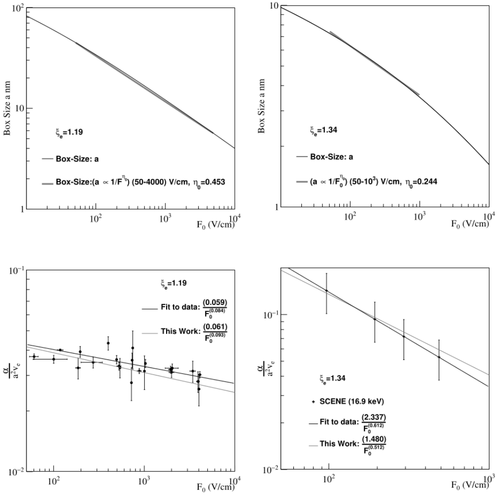


Figure 4: N_{ex}/N_i for LXe and LAr as function of the electric field. In LAr predict a breakdown voltage of $60\,\mathrm{kV/cm}$

Box size



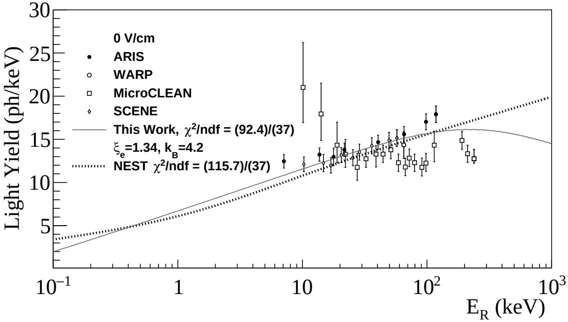
- Using the screen atom potential for ions,

$$-e\phi_Z^e(x',\xi_e,N) = \frac{Ze^2}{bx'}\left[\left(\frac{N}{Z}\right)(\chi_Z(x')-1)+1\right].$$

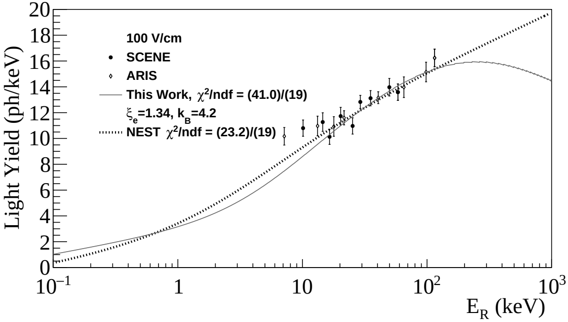
- We can use Dahl electrostatic interpretation for Box size determination,

$$-bzF = (\phi_Z^e(z,\xi_e,N))_{\rm sc},$$

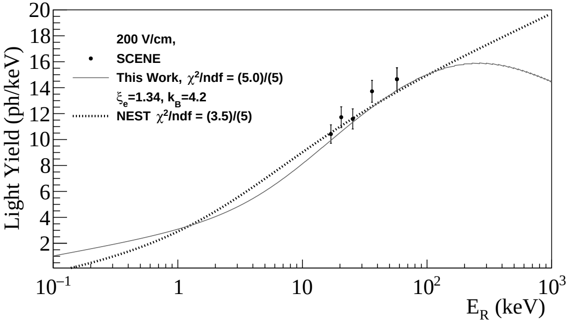
- Box size, depends weakly of electric field for high Z.
- For LNe, LAr, LKr and LXe we have **16 parameters reduced to 1!**

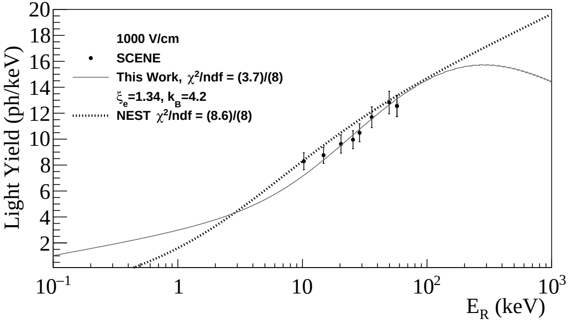


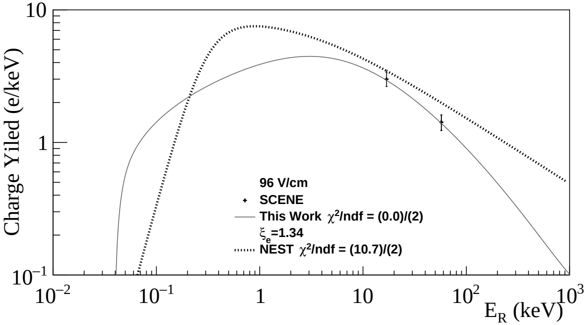
0 V/cm
ARIS
WARP
MicroCLEAN
SCENE
This Work, χ^2/ndf = (92.4)/(37)
ξ_e=1.34, k_B=4.2
NEST χ^2/ndf = (115.7)/(37)
Light Yield (ph/keV)
E_R (keV)

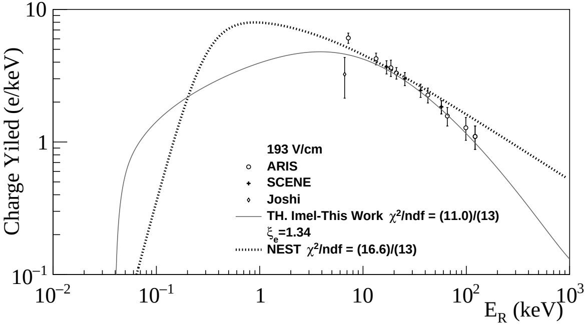


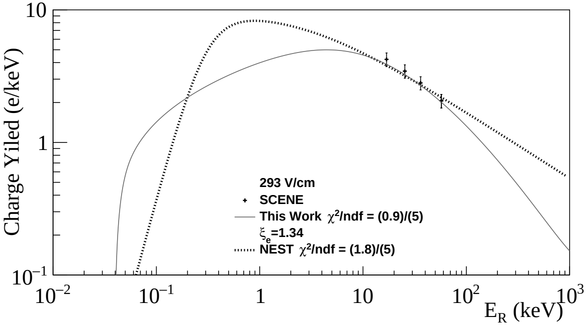
100 V/cm
SCENE
ARIS
This Work, χ^2/ndf = (41.0)/(19)
ξ_e=1.34, k_B=4.2
NEST χ^2/ndf = (23.2)/(19)
Light Yield (ph/keV)
E_R (keV)


200 V/cm,
SCENE
This Work, χ^2/ndf = (5.0)/(5)
ξ_e=1.34, k_B=4.2
NEST χ^2/ndf = (3.5)/(5)
Light Yield (ph/keV)
E_R (keV)
10^{-1}
1
10
10^2
10^3

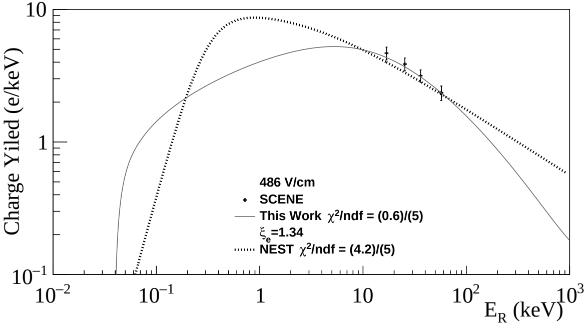

1000 V/cm
SCENE
This Work, χ^2/ndf = (3.7)/(8)
ξ_e=1.34, k_B=4.2
NEST χ^2/ndf = (8.6)/(8)
Light Yield (ph/keV)
E_R (keV)
10^{-1}
1
10
10^2
10^3


Charge Yiled (e/keV)
96 V/cm
SCENE
This Work χ^2/ndf = (0.0)/(2)
ξ_e=1.34
NEST χ^2/ndf = (10.7)/(2)
E_R (keV)


Charge Yiled (e/keV)
193 V/cm
ARIS
SCENE
Joshi
TH. Imel-This Work χ^2/ndf = (11.0)/(13)
ξ_e=1.34
NEST χ^2/ndf = (16.6)/(13)
E_R (keV)



Charge Yiled (e/keV)
E_R (keV)
293 V/cm
SCENE
This Work χ^2/ndf = (0.9)/(5)
ξ_e=1.34
NEST χ^2/ndf = (1.8)/(5)



Charge Yiled (e/keV)
E_R (keV)
486 V/cm
SCENE
This Work χ^2/ndf = (0.6)/(5)
ξ_e=1.34
NEST χ^2/ndf = (4.2)/(5)

Conclusions

- We present a first principles approach study based on an integral equation.
- We give a physical interpretation of ξ_e that allow to describe the N_{ex}/N_i ratio as function of energy and field.
- With just one parameter, α_0 to describe data in LAr and LXe. **Usufull for phenomenology studies.**
- The model for Charge yield have a better match with data at high energies.
- The publications will be available soon with a software to produce outputs too.

Thank you for listening!
Your feedback will be highly appreciated

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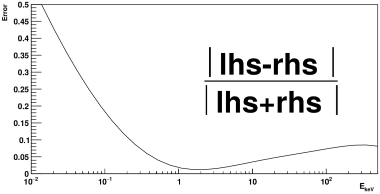
Backup

Lindhard QF and Other Works

- Lindhard used a primitive computer(DASK).
- His formula just solved approximately Eq. (3).



- Using Lindhard formula $\Rightarrow$ Systematic error, large at lower energies.
- Other authors [7], try to include binding energy.
- But fail to realize in changing the integration limit, reporting nonphysical results.
- One of the achievements of this work is to include in a consistent mathematical and physical way the binding energy.

[7] PHYSICAL REVIEW D 91, 083509 (2015)

Simplified Integral Equation With Constant Binding Energy with no Straggling

A previous work[a] fail the to defined correctly the lower limit of integration ($\bar{v}(t/\varepsilon - u)$). We take this into account,

$$\boxed{-\frac{1}{2}k\varepsilon^{3/2}\bar{v}''(\varepsilon)} + \underbrace{k\varepsilon^{1/2}}_{S_e}\bar{v}'(\varepsilon) = \int_{\boxed{\varepsilon u}}^{\varepsilon^2} \underbrace{dt\frac{f\left(t^{1/2}\right)}{2t^{3/2}}}_{d\sigma_n}[\bar{v}(\varepsilon - t/\varepsilon) + \bar{v}(t/\varepsilon - \boxed{u}) - \bar{v}(\varepsilon)] \tag{6}$$

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

The equation admits a solution featuring a "kink" at $\varepsilon = u$ Lower limit of integration $\varepsilon u \leqslant t$, predicts channeling (no atomic movement),

$$\sin\theta/2 = \sin\psi_{lab} = \sqrt{\frac{U}{E}}.$$

[a] PhysRevD 91 083509 (2015)

LIDINE2022[8] (Constant Binding Model and $S_e = k\varepsilon^{1/2}$)

Y. Sarkis et al 2023 JINST 18 C03006

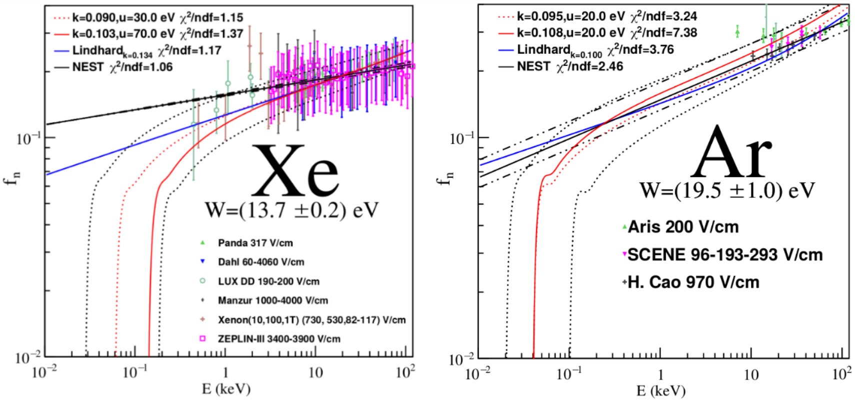


Figure 5: Total quanta for LXe and LAr as a function of the recoil energy.

[8] AstroCeNT (CAMK PAN), Poland