Light and Charge yield study in LAr for energies from 100 eV to 1 MeV: A first principles approach

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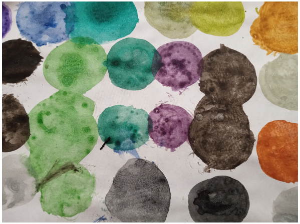
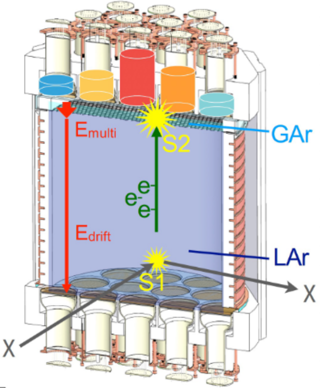
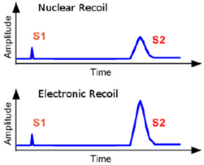


- Dual-phase Argon Time Projection Chamber (TPC).
- Light n_γ and Charge n_e detection combined to obtain Particle track.
- Primary scintillation (S1) from interaction in liquid.
- Secondary light signal (S2) from ionization electrons accelerated in gas chamber.
- Total quanta for electrons is constant in LAr (LXe): $n_q/E = 1/W = (n_e + n_\gamma)/E$.

$$W = (19.5 \pm 1)\ \text{eV in LAr}$$

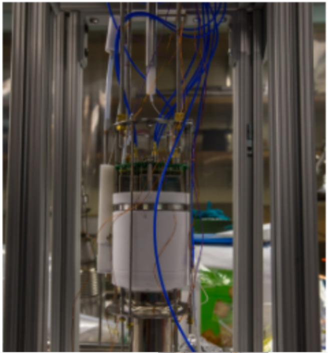


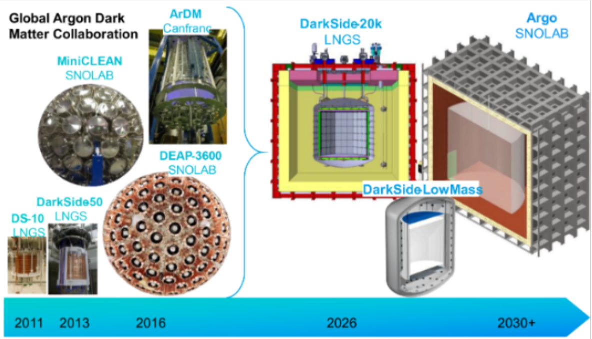


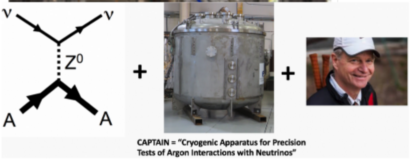
LAr Experiments now and future

ARIS experiment

Dark Side 20k experiment

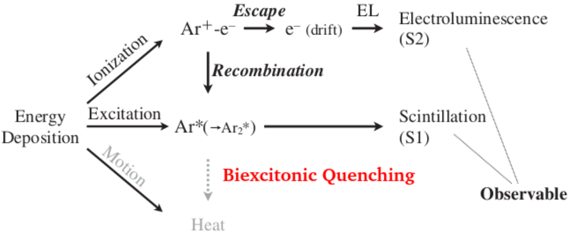






Nucl. Phys. B 1003 (2024) 116436

- Massive (nTon) detectors$\rightarrow$ larger signals $\rightarrow$ lower limits.
- Systematic fluctuations for S_1 and S_2 signals will limit this tendency.
- Hence the importance of having a first principles theory for energy reconstruction.
- In addition for LAr, charge and light recombination occur:



  - N_i: number of electron-ion pairs, $A+A \longrightarrow e+A^{+}+A^{*}$
  - N_{ex}: number of atoms excited, $A+A \longrightarrow A^{*}+A^{*}$
  - Biexcitonic Q, reduces two photons in to single photon (high energies).

Thomas-Imel box Model

- Diffusion equation for ions-electrons ($N_- \ N_+$) Jaffe model, [1].

$$\frac{\partial N_+}{\partial t} = -\alpha N_- N_+, \qquad \frac{\partial N_-}{\partial t} = \mu_e F \frac{\partial N_-}{\partial z} - \alpha N_+ N_-. \tag{1}$$

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

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

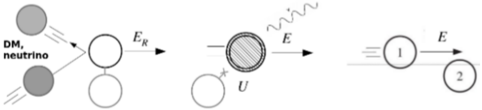
$$N_i = \frac{E_R \mathbf{f_n}}{W(1+\beta)}, \quad \text{Where } \beta = N_{ex}/N_i \text{ and } f_n = \frac{E_I}{E_R}.$$

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

Ionization Efficiency f_n

When a particle, (e.g. DM) interact with a nuclei the energy splits in

E_n : Nuclear collisions. [2] $(\bar{\nu} = C_0 E_n)$
E_I : Ionization (visible) energy $[\mathrm{keV_{ee}}]$ $(\bar{\eta} \to C_0 W(n_e + n_\gamma)_R)$.



- $\dfrac{\text{Ionization energy}}{\text{Deposited energy}} = \boxed{f_n = \dfrac{\bar{\eta}}{\varepsilon_R}.}$
- $\varepsilon_R = \varepsilon + u = \bar{\eta} + \bar{\nu}$, where ε_R is the recoil energy and
- u is the energy to disrupt the atomic electron cloud.
- This sets a cascade of slowing-down processes.
- DM or CEνNS searches are affected by quenching.

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

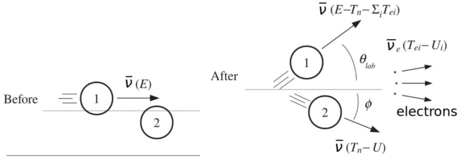
Basic Integral Equation and Approximations

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

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

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.

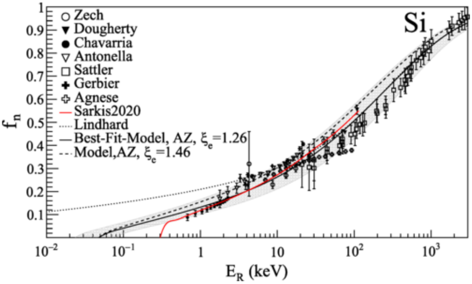


Simplified equation with binding energy

- We are going to use the integro-differential equation for atomic motion deduced in the past work for Si.[3].

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

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



- Electronic stopping S_e with Coulomb repulsion effects (Ziegler potential).
- Bohr electron stripping for ions.
- Electronic straggling effect.
- Scaling factor ξ_e from Pauli principle, instead of Lindhard semi-empirical factor $\xi_e \approx Z^{1/6}$.

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

Improvements for S_e

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

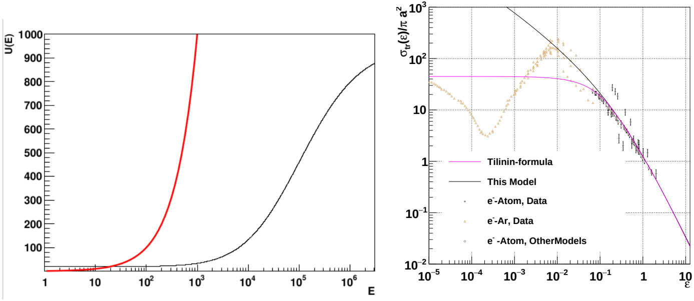


Figure 1: (left) Energy dependent binding energy, (right) σ_{tr} for Ar-e.

Physical interpretation of Scaling length ξ_e

- The scaling length measures how electrons are effectively excited, with energy Δ, in the cascade collision process.

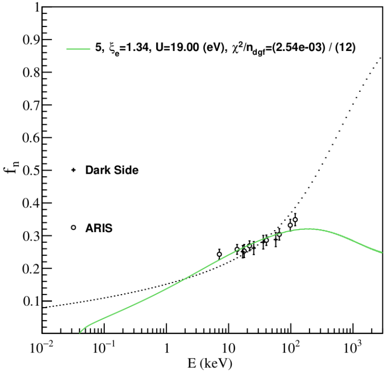
$$\xi_e^{2/3} \equiv \frac{5}{3}\frac{4\pi\int_{k_F-\Delta}^{k_F} E(k)k^2dk}{4\pi E(k_F)\int_{k_F-\Delta}^{k_F} k^2dk}, \; E(k) = \frac{(\hbar k)^2}{2m} \text{ and } E_F = U_{TF}/\xi_e^{2/3}.$$

- For $\Delta \to 0$ then $\xi_e \to (5/3)^{3/2} \approx 2.15$ (no electron excitation) and
- $\Delta \to \; k_F$ we have $\xi_e \to 1$ (total electron excitation).
- Both limits are assume to be physically unreachable.
- For Si, $\xi_e = 1.26$, this gives $\Delta = 88.0$ eV.
- **The cascade process and the recombination box are entangled by the scale length.**

Fit to LAr Data $\xi_e = 1.34$

- Biexcitonic processes reduce f_n^M (measure).
- Where $f_n^M = (n_e + n_\gamma)W/E_R \leq (n_e + n_\gamma/f_l)W/E_R$.

$$f_n^M = f_n f_l + (1 - f_l)(n_e/E_R)W, \; f_l = \frac{1}{1 + k_{Birks} S_e}.$$



- The Birks parameter can be deduced from

$$k_{Birks} = 1/ < S_e >= 4.19$$

.

- Where the average electronic stopping power.

Recombination Parameters from first principles

- Many authors [4], use **five to ten parameters** to describe charge and light data.
- **In this study we are just going to use ξ_e and the scale recombination probability α_0 (universal) as fit parameters.**

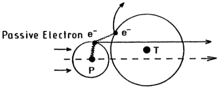
$$\alpha = \alpha_0 Z^3 (2r_W)^2 v_F, \quad \xi = \frac{\alpha_0 N_i Z^3 (2r_W)^2 v_F}{4\mu_e \boxed{(a^2 F)}}$$

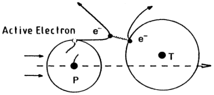
- In addition, the same inter-atomic potential used for f_n is going to be the main tool to explain:
  - The energy and field dependence of the ratio N_{ex}/N_i.
  - Biexcitonic quenching.
  - Box model length a, as function of external field.
  - Field dependence of Thomas-Imel Box model parameter: $\xi \propto F^{-\delta}$.
  - $\delta_{Ar} \approx (0.4 - 0.8)$ and $\delta_{Xe} \approx (0.04 - 0.12)$.

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

Bates-Griffing Process (BGP)

- For nuclear recoil $W_i = W(1 + N_{ex}/N_i)$ we can used the approach given by Bates-Griffing.
- *Passive electron*, remains in its ground state during the interaction with the target electron.
- The projectile electron acts as a part of the incident nucleus and appears to be a 'heavy' (classical) particle.

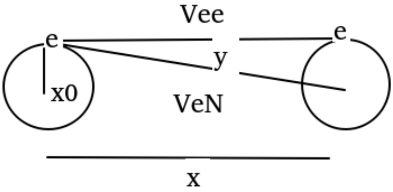




- *Active electrons,* the projectile electron is removed from its ground state.

Semi Classical approach

- We take the electron positioned at the top of valence orbital x_0, centered by the electron cloud distribution (nuclei $x \approx 0$).



- Electron-electron repulsion is given by Coulomb law, $\propto 1/x$.
- Attraction potential of electron of atom 1 with the atom 2, defined by distance (y).
- To estimate the effective number of electrons in the collision, Bohr stripping criteria ($v_{ion} \leq \sqrt{3}v_F$) is used to define $Z^* = N$.
- The total potential should be the average valence binding energy $E_{Ar} = 15.8$ eV.

Potential Model

We assume that the interaction potential energy is given by Ziegler semi-empirical potential

$$< \psi \mid V \mid \psi >= e\phi_Z(x,\xi_e) = \frac{Z_1 Z_2 e^2}{(\xi_e)^{2/3} ax}\chi_Z(x), \quad a = a_0 0.885/(Z_1^{0.23} + Z_2^{0.23}).$$

For the total energy the virial T. is used, $< \psi \mid (\bar{V} + \bar{T}) \mid \psi >= \frac{\phi_Z(x,\xi_e)}{2}$.

For an ion with N electrons, we used the TF-Amaldi approach, where the ion have a total positive charge $(Z - N)$,

$$e\phi_Z^e(x,\xi_e,N) = \frac{-Ze^2}{(\xi_e)^{2/3} ax}\left[\chi_Z(x) + \frac{(Z-N)}{Z}(1-\chi_Z(x))\right], \; a = a_0 0.885/N^{1/3}.$$

The equilibrium equation for BGP is,

$$E_{Ar}/2 = e\phi_Z^e(y,\xi_e,N)/2 + \frac{e^2}{(\xi_e)^{2/3} ax}, \; y = \sqrt{x_0^2 + x^2}.$$

The energy of the two ions when the distance is x is,

$$E'/2 = e\phi_Z((1.4836)x,\xi_e)/2, \; E' = W_i/2 \text{ (Two atoms)}.$$

Results for Ar, $\xi_e = 1.343$

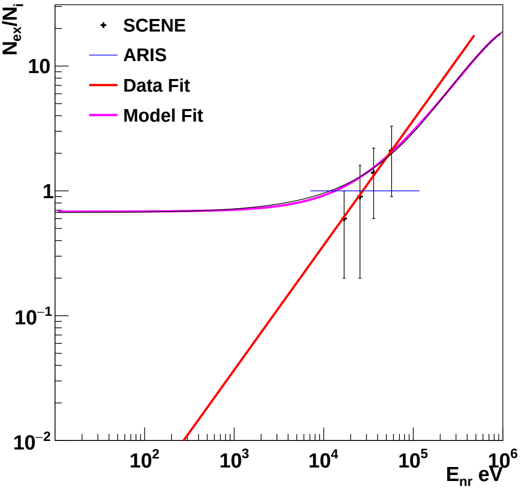
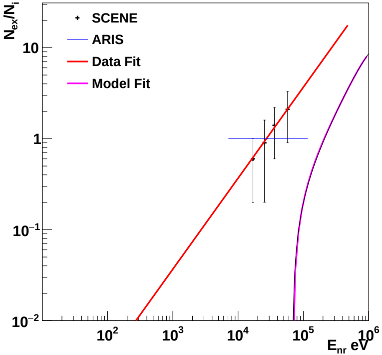


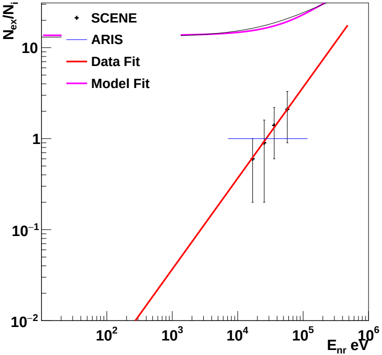
Figure 2: Ratio β for LAr as function of energy, $\chi^2/3 = 0.7$

Results for $\xi_e = 1$ and $\xi_e = 2.15$

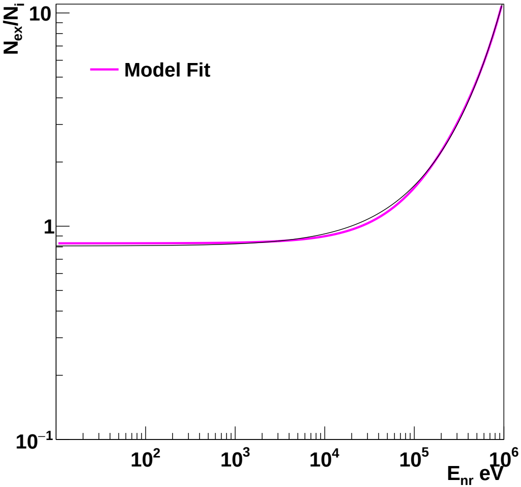
$\xi_e = 1$



$\xi_e = 2.15$

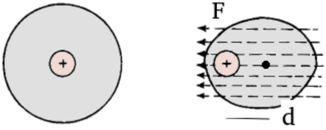


LXe $\xi_e = 1.189$



Stark Effect for Ions

- When an electric field F is applied to a TPC.
- Interacts producing a small deformation displacement d, of the outer electron orbitals.

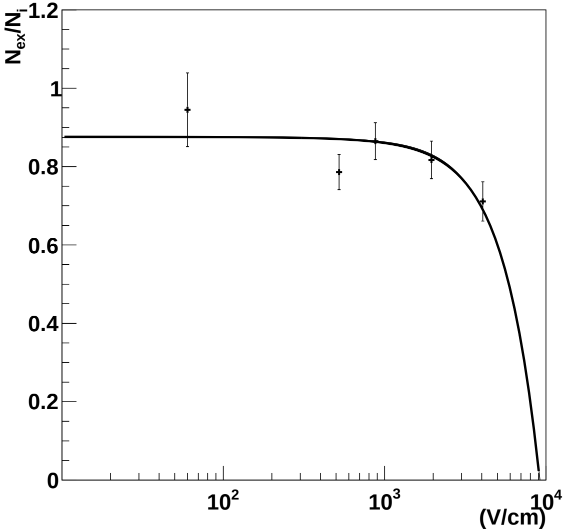


- By applying first order perturbation theory (no degenerate) we can compute the energy correction δ_1 to the potential $e\phi_Z(x,\xi_e) = <\psi \mid V \mid \psi>$,

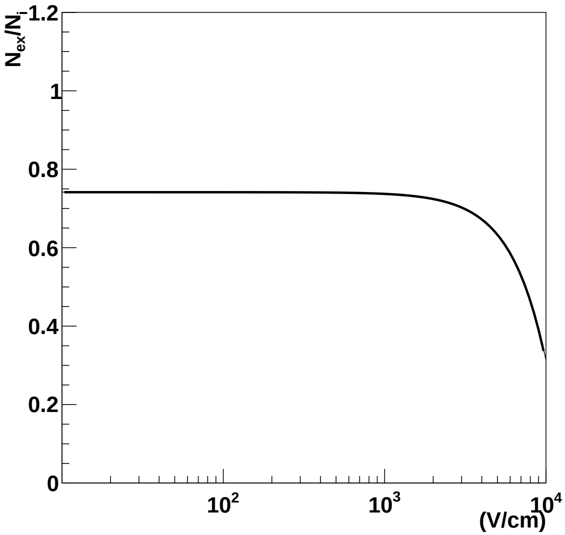
$$\delta_1 = <\psi \mid V_{ext} \mid \psi>, \; V_{ext} = \pm((\xi_e)^{2/3} a x_z eF) = \pm((\xi_e)^{2/3} axeF)cos(\theta).$$

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

Results for LXe $\xi_e = 1.189$

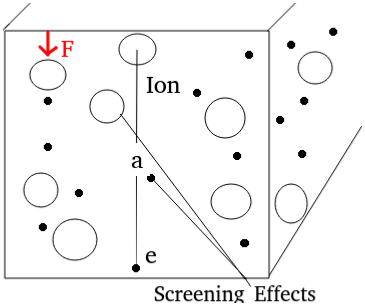


Results for LAr $\xi_e = 1.343$



Box Size

The box size is defined by electrostatic length scale (Dahl).



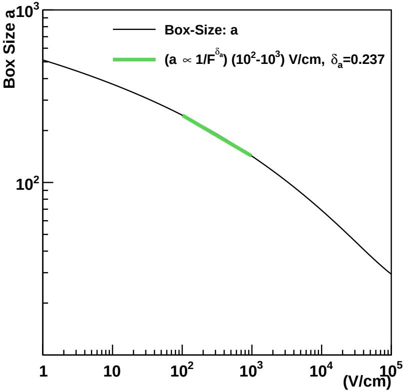
- The box size is much larger than the inter-atomic distance,
- Screening effects are considerable.
- We use Lindhard-Thomas-Fermi model $\varepsilon(k,0) = \varepsilon^0_{LAr}(1+\frac{\kappa^2}{k^2})$.
- This modify the potential is

$$\phi^e_{ZS}(x_a,\xi_e,N) = \phi^e_Z(x_a,\xi_e,N)e^{-\kappa x a \xi_e^{2/3}}$$

$$\kappa^2 = \frac{6\pi Z_{val} e^2 n_e(\Delta_{Ar})}{\varepsilon^0_{LAr}\Delta_{Ar}}.$$

- Hence the box size is defined by $\phi^e_{ZS}(x_a,\xi_e,N) = \xi_e^{2/3} eaxF$.

Results for LAr $\xi_e = 1.343$



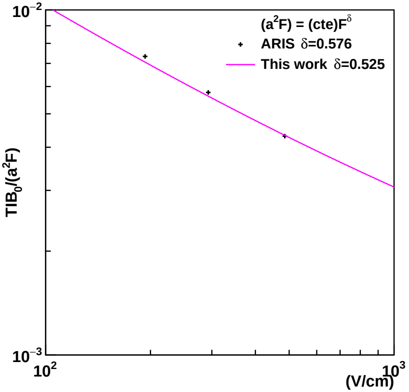


Figure 3: (left) Box size as function of the external TPC field, (right) TIB parameter as function of the field.

Results for LXe $\xi_e = 1.189$

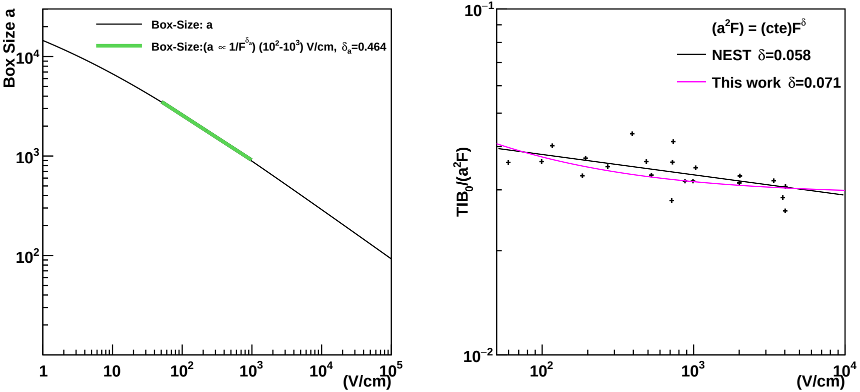
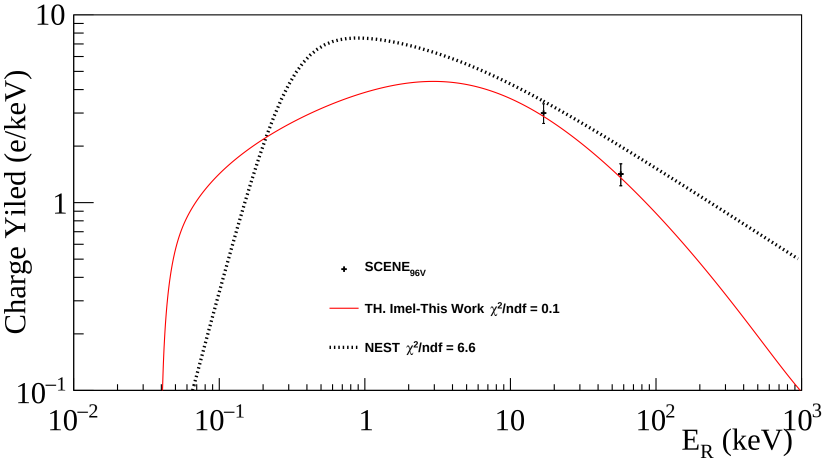
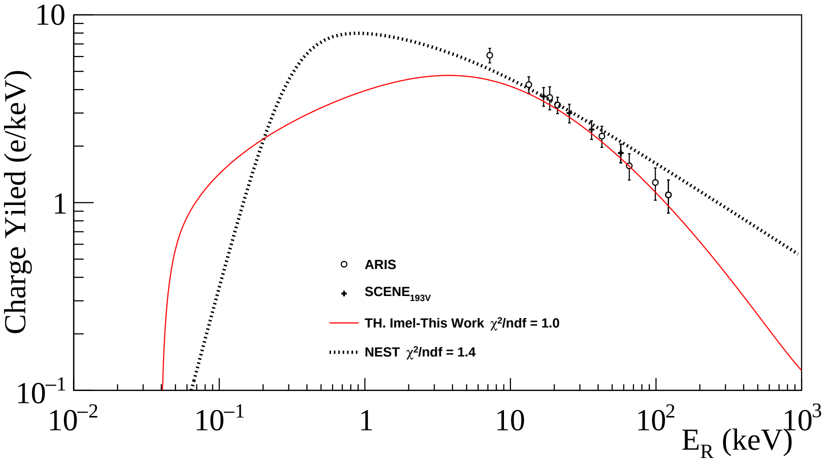


Figure 4: (left) Box size as function of the external TPC field, (right) TIB parameter as function of the field.

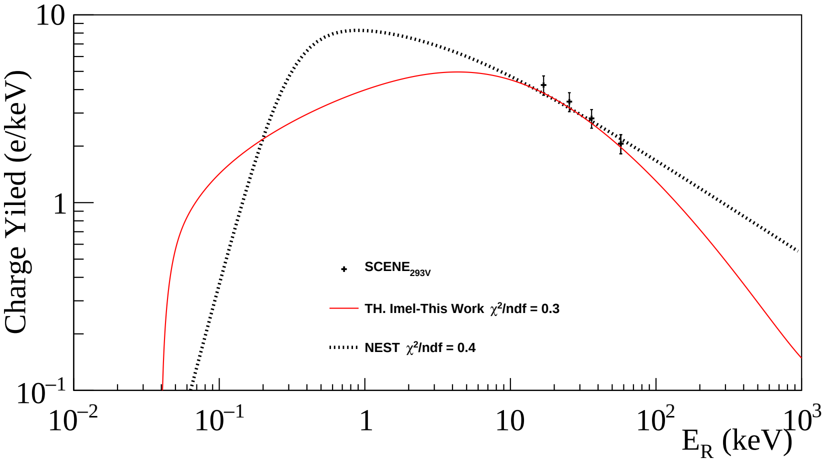
Charge Yield LAr (96 V/cm)



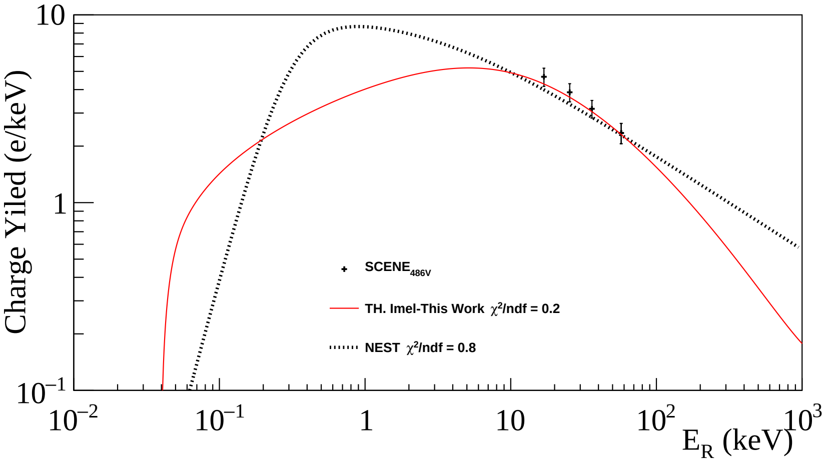
Charge Yield LAr (193 V/cm)



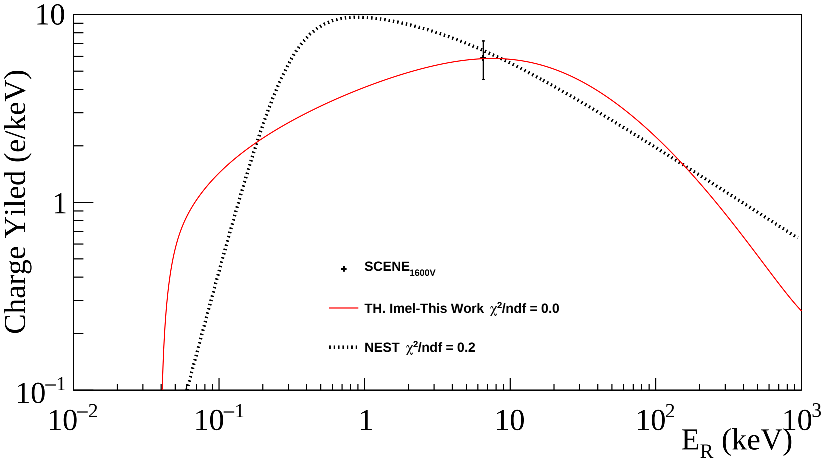
Charge Yield LAr (293 V/cm)



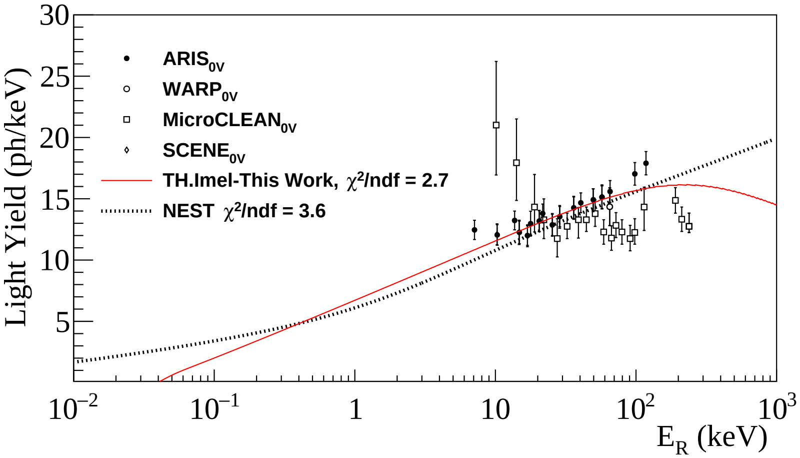
Charge Yield LAr (486 V/cm)



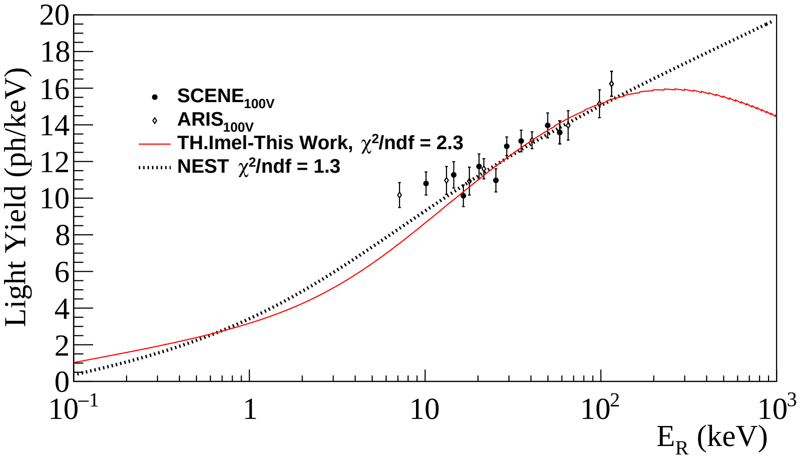
Charge Yield LAr (1600 V/cm)



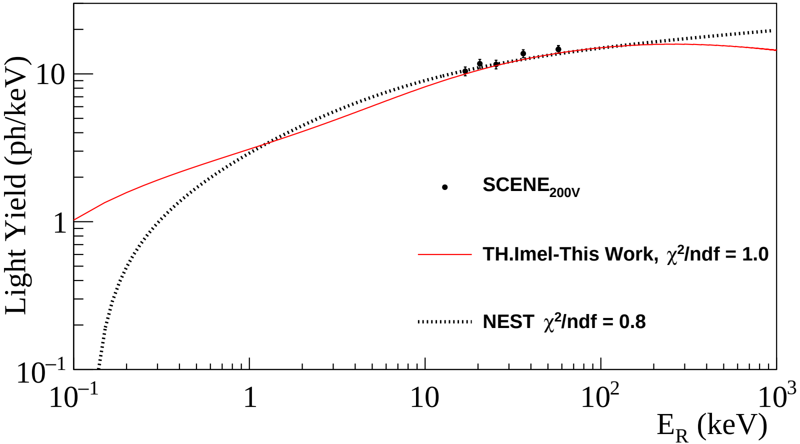
Light Yield LAr (0 V/cm)



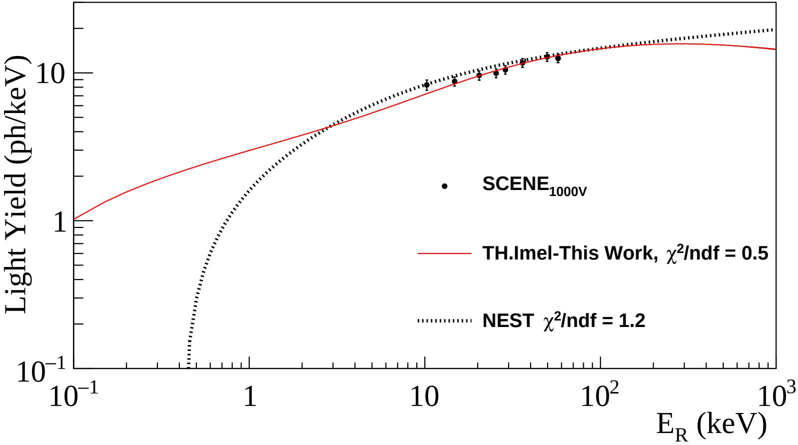
Light Yield LAr (100 V/cm)



Light Yield LAr (200 V/cm)



Light Yield LAr (1000 V/cm)



Conclusions

1. *We present a first principles approach study based on an integral equation for interactions in pure LAr.*

2. *Incorporating the same procedure to compute the ionization efficiency for Si, we get also a reasonable description for LAr.*

3. *We give a physical interpretation of ξ_e that allow to describe the N_{ex}/N_i ratio as function of energy and field.*

4. *With just two parameters, $\xi_e = 1.343$ and $\alpha_0 = 1.4 \times 10^{-11}$ we can describe the complete recombination model and prove to be consistent with data.*

5. *The model for Charge yield have a better match with data than NEST, thanks to Bates-Griffing process.*

6. *This work can be useful as a prelude to study the Ge ionization efficiency at low energies.*

Thank You!

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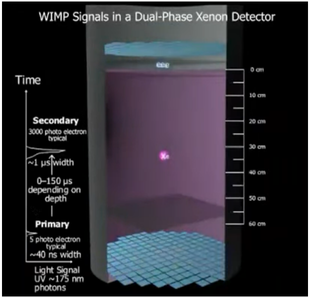
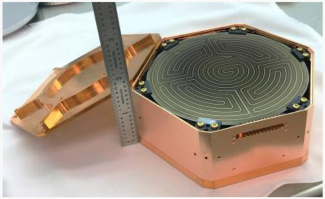
❈ *This research was supported in part by DGAPA-UNAM grants PAPIIT-IT100420 and PAPITT- IN106322, SNI, and CONAHCYT grant CB2014/240666..*

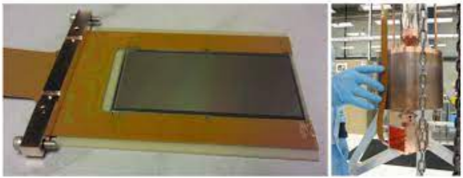
Backup

Relevant DM Experiments

- TPC's detectors: LUX, XeNT, ZEPLIN, etc.
- Bolometers: Super CDMS, EDELWEISS, etc.
- CCD's: DAMIC and OSCURA.



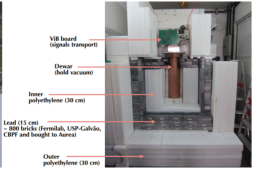


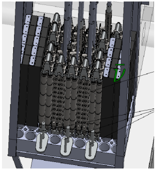


These detectors detect signals by ionization due to WIMP's that produce NR's in the material.

Figure 5: Credit images:M. Szydagis 2021 SCU AAP Conference https://damicm.cnrs.fr/en/detector/, https://supercdms.slac.stanford.edu/overview

- CCD's: CONNIE.
- Ge detectors: CoGeNT, TEXONO, νGeN , CONUS.
- Low-temp. bolometers: RICOCHET, MINER, ν-cleus.
- Noble liquid detectors: LAr Livermore, LXe, ITEP& INR, LXe ZEPLIN-III.
- Neutron Spallation: COHERENT.





CAPTAIN = "Cryogenic Apparatus for Precision Tests of Argon Interactions with Neutrinos"

https://coherent.ornl.gov/,Coherent Captain Mills: The Search for Sterile Neutrinos Ashley Elliott et al, https://indico.cern.ch/event/MINER_MI_workshop.pdf,http://icra.cbpf.br/twiki/bin/login/CONNIE

- Higher-dimensional Lagrangian effective operators.

$$\mathscr{L}_{\mathrm{NSI}} \supset -2\sqrt{2}G_F \sum_{\alpha,\beta} \sum_{P,q} \varepsilon_{\alpha\beta}^{q,P} \left(\bar{\nu}_\alpha \gamma^\mu P_L \nu_\beta\right) \left(\bar{q}\gamma_\mu P q\right) \tag{4}$$

- CEνNS experiments are primarily sensitive to light vector and scalar mediator models.

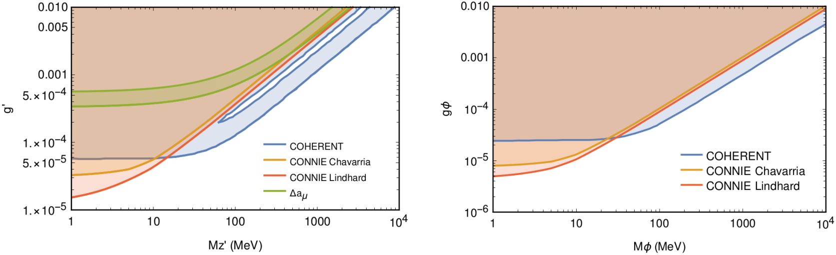
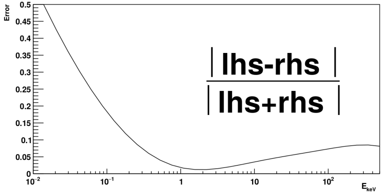


Figure 6: JHEP04(2020)054

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 [5], 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.

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

- The high energy cutoff is due to the limitations of the constant binding energy model.

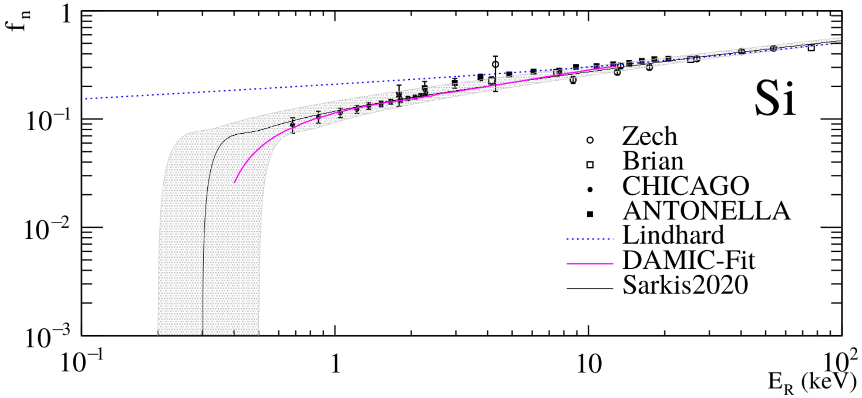


Figure 7: QF measurements for Si, compared with Lindhard model, the ansatz, and the numerical solution; U = 0.15 keV y k = 0.161.

Ge with recent data.

Results (Band is build to cover data)

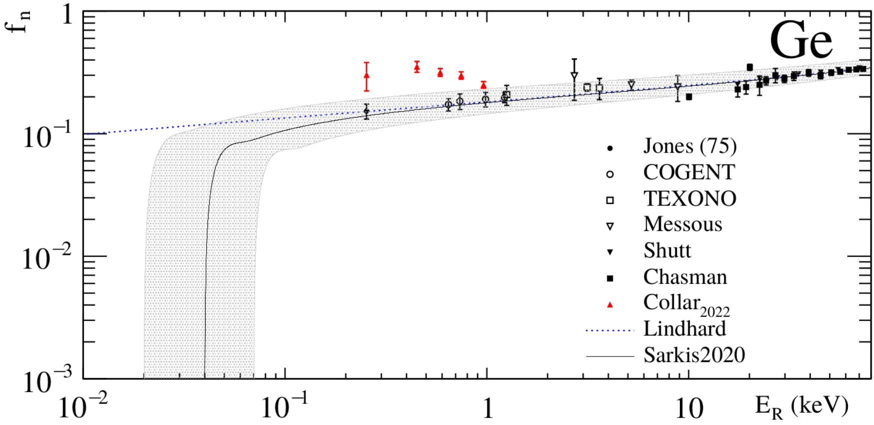


Figure 8: QF measurements for Ge, compared with Lindhard model, the ansatz, and the numerical solution; U = 0.02 keV y k = 0.162.

Low Energy Effects for S_e

§ Coulomb repulsion effects

- At low energies S_e departures from velocity proportionality.
- Colliding nuclei will partially penetrate the electron clouds.

$$S_e = (\Xi)Nmv \int_0^\infty v_F \sigma_{tr}(v_F) N_e dV \rightarrow (\Xi)Nmv \int_R^\infty v_F \sigma_{tr}(v_F) N_e dV$$

R distance closest approach and Ξ is a geometrical factor[4] , negligible for $Z < 20$.

- Three models will be considered; **Tilinin**[6]**, Kishinevsky**[7] **and Arista**[8]
- Models change details of the inter-atomic potential.
- Hence affect $f(t^{1/2})$ and S_e at low energies.

[6] I.S.Tilinin Phys. Rev. A 51, 3058 (1995)

[7] Kishinevsky, L.M., 1962, Izv. Akad. Nauk SSSR, Ser. Fiz. 26, 1410.

[8] J.M. FernÃ¡ndez-Varea, N.R. Arista, Rad. Phy. and C.,V 96, 88-91, (2014),

Exciton-Ion Behavior

- Exciton to ion fraction $\beta = \frac{N_{ex}}{N_i}$ usually is modeled by a constant.
- With our formalism, we can built an Int.Diff. equation taking in to account the excitation and ionization cross sections (work in progress).
- A preliminary study justify that $\frac{N_{ex}}{N_i}$ changes slowly for energies > 1 keV.
- So if the total quanta $N_i + N_{ex} = N$ with $N = E_{er}/W$, hence $E_{er} = WN_i(1+\beta)$.
- If $N_{er} = f_n E_R$ then, $N_i = f_n(\frac{E_R}{W(1+\alpha)})$, where f_n can be computed with our model. spatially small tracks.

- In the following we show the Charge and Light Yiels for Ar and Xe, using the constant binding energy model and $S_e = k\varepsilon^{1/2}$.
- Where also we are taking β and $\frac{\alpha}{4a^2v} \equiv \gamma$ as constants.