

LIGHT DETECTION IN NOBLE ELEMENTS (LIDINE 2025)

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## Light and charge yield in noble liquids from sub-keV to MeV: a first-principles approach beyond Lindhard

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**ABSTRACT:** We present a first-principles model of the total quantum (light + charge) production in liquid argon and xenon for nuclear recoils from sub-keV energies up to 1 MeV. The calculation extends Lindhard's framework by solving the second-order integro-differential equation for atomic motion, including electronic straggling, Coulomb repulsion, and inelastic electronic emission. A physically motivated electronic scale length, derived from Thomas-Fermi theory, is introduced as a key parameter governing the electronic response. The recombination process is modelled using an improved Thomas-Imel formalism with an electrostatic definition of the box size. The model yields consistent predictions for light and charge yield in all noble liquids without medium-specific tuning and improves agreement with low-energy data compared to empirical frameworks such as NEST.

**KEYWORDS:** Ionization and excitation processes; Liquid detectors; Charge transport and multiplication in liquid media; Scintillators, scintillation and light emission processes (solid, gas and liquid scintillators)

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**1 Introduction**

Liquid argon and xenon detectors are central to low-energy searches such as dark matter, double beta decay, and CE $\nu$ NS. The interpretation of nuclear recoils at sub-keV energies relies on the accurate prediction of total quanta production, defined as the sum of scintillation photons (S1) and ionization electrons (S2). Existing semi-empirical models, including Lindhard, become inaccurate at low energies where atomic binding, electron screening, and straggling effects become significant. We present a fully microscopic model that consistently describes energy deposition, ionization, excitation, and recombination for noble liquids using only atomic properties. This framework extends to all noble liquids and provides improved accuracy, especially in the sub-keV regime.

**2 Total quanta model**

The recoil energy is distributed among excitons, ions, and heat according to the Platzman equation [1]. The total quanta are

$$f_n(E_R) = \frac{N_q W}{E_R} = \frac{E_e}{E_R}, \quad (2.1)$$

where  $N_q = N_i + N_{\text{ex}}$  is the sum of ions  $N_i$  and excitons  $N_{\text{ex}}$ ,  $E_e$  is the electron equivalent energy and  $W$  the average energy required to create an exciton or ion in noble liquid [2, 3]. To determine  $f_n(E_R)$ , we calculate the energy that goes into atomic motion,  $E_v = E_R - E_e$ , by solving the second-order Lindhard integro-differential equation [4, 5], which in reduced units  $\nu = 8.13E_v[\text{keV}]/Z^{2.23}$ ,

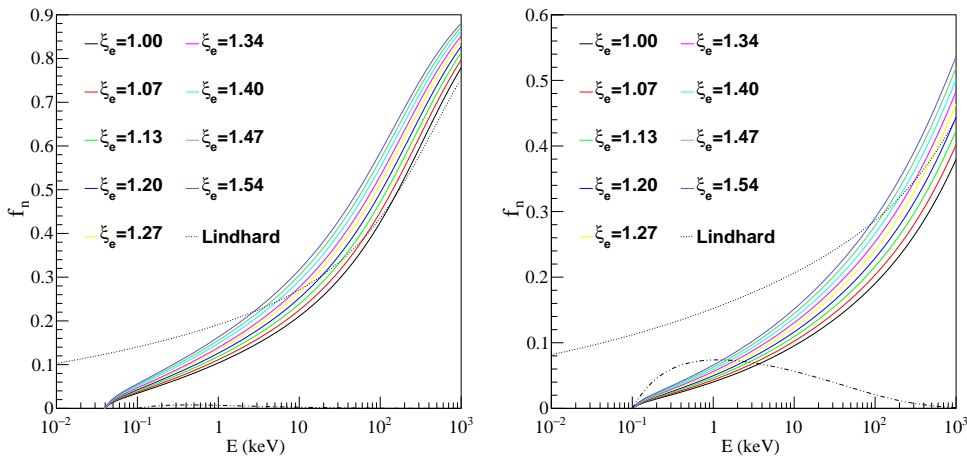
$$\begin{aligned} & -\frac{1}{2}\varepsilon S_e(\varepsilon) \left(1 + \frac{W(\varepsilon)}{S_e(\varepsilon)\varepsilon}\right) \bar{v}''(\varepsilon) + S_e(\varepsilon)\bar{v}'(\varepsilon) \\ & = \int_{\varepsilon u(\varepsilon)}^{\varepsilon^2} dt \frac{f(t^{1/2})}{2t^{3/2}} \times [\bar{v}(\varepsilon - t/\varepsilon) + \bar{v}(t/\varepsilon - u(\varepsilon)) - \bar{v}(\varepsilon)]. \end{aligned} \quad (2.2)$$

Here,  $\bar{v}$  is the average energy of atomic motion,  $S_e(\varepsilon)$  is the electronic stopping power,  $W(\varepsilon)$  the electronic straggling and  $f(t^{1/2})$  is a function related to nuclear stopping power.

The solution to eq. (2.2) incorporates atomic binding  $u$  via Thomas-Fermi potential and a realistic electronic stopping (Tilinin formalism) that consider Coulomb-repulsion effects [6]. In this study, only the energy associated with elastic electron momentum transfer was considered. To incorporate inelastic electron emission we use the Bates-Griffing (BG) formalism [7], with passive and active

channels for two approaching incoming atoms. In the passive channel, the outer electrons are assumed to remain in the ground state and act as a heavy particle (triplet) transferring momentum to the nuclei; whereas, in the active channel, the outer electrons interact directly (singlet) and can produce ionization. The active case occurs only when the energy  $W_i^R$  of both ions overcomes the valence binding energy, and electrons are emitted with an average energy according to the orbital momentum dispersion [8].

The probability of electron emission is related to its mean free path in the quasi-molecular system. This quantity is calculated as the sum of the elastic and inelastic electron cross-sections times the contribution to electron density by the electron exchange energy. If the two atoms are close enough to exceed  $W_i^R$ , the emission probability is maximal. Therefore, the probability of electrons transitioning to the triplet state decreases with increasing energy. We calculate this effect in terms of the valence binding energy, using a semiclassical model. This introduces an additional electronic energy contribution to  $f_n(E_R)$ , see figure 1.

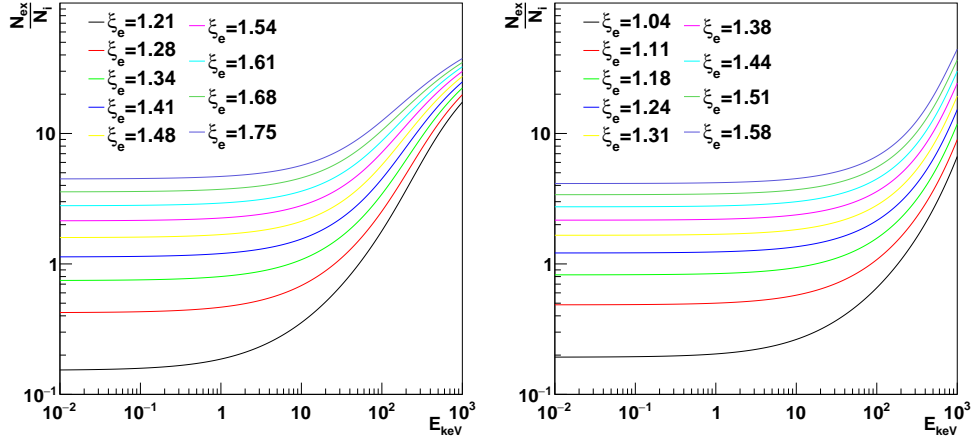


**Figure 1.** Total quanta for LAr (left) and LXe (right) for several scaling length with only Tulinin electronic stopping power. The (dash line) is the part related to the BG process. We show Lindhard formula (dotted) for comparison.

We introduce a fundamental parameter *electronic scaling length*  $\xi_e$ , linked to the Pauli exclusion principle during the cascade [5]. This parameter is associated to the electronic stopping power,  $S_e(E_R; \xi_e) = \xi_e S_e(E_R)$ , and explains the semi-empirical factor introduced by Lindhard ( $\xi_e \approx Z^{1/6}$ ). The value can also be used to set the average electron energy available in the plasma produced by the cascade process. Using density functional theory [9], we get,  $\xi_e = 1.34$  and  $\xi_e = 1.19$  for LAr and LXe respectively, in accord with the expected trend ( $Z \rightarrow \infty$  then  $\xi_e \rightarrow 1$  from Thomas-Fermi) that the scale parameter diminishes with atomic number.

### 3 Exciton to ion ratio

For liquid noble elements, the exciton to ion ratio produced in nuclear recoil signals is related to the energy required to ionize a pair of atoms in a collision,  $W_i^R = W(1 + N_{\text{ex}}/N_i)$ . To calculate  $W_i^R$ , a semiclassical implementation of the Bates-Griffing process is used, which depends on the interatomic potential (we use the ZBL potential), the average valence energy, and  $\xi_e$ . This gives an increasing function  $\beta(E_R, \xi_e) = N_{\text{ex}}/N_i$ , with minimum values consistent with previous measurements [10, 11], see figure 2. For values of  $\xi_e \rightarrow 2.15$ , only electrons near the Fermi level can be ionized, and  $\beta(E_R, \xi_e)$  reach a maximum.



**Figure 2.** Exciton to ion ratio for LAr (left) and LXe (right) computed for several scaling lengths.

#### 4 Recombination model

Recombination is described using a modified Thomas-Imel box model:

$$\frac{N_e}{N_i} = 1 - \frac{1}{\xi} \ln(1 + \xi) = 1 - r, \quad (4.1)$$

where  $N_e$  is the number of electrons and  $\xi = N_i \alpha / 4a_B^2 \mu_e F_0$  the recombination parameter. Here,  $\alpha$  is a constant recombination parameter,  $F_0$  is the external electric field,  $a_B$  is the recombination box size that depends on  $F_0$ , and  $\mu_e$  is the electron mobility. Scintillation is equal to exciton quanta plus the fraction of recombined ions:  $N_\gamma = N_{\text{ex}} + rN_i$  [12].

The box size is determined by the equilibrium distance at which the detector external field equals the electric field of an electron and an ion inside the box [13]. We implement a model with ions and electrons assumed to be a weak plasma gas restricted by  $F_0$ . Therefore the external potential energy  $-ea_B F_0$  must be equal to the electron-ion potential energy  $-e\phi(a_B; \xi_e, Z, \kappa_e)$ , given by the Ziegler screen potential modified by the attenuation length of the weak plasma  $\kappa_e$  [14]. From this relationship, we obtain that the box size is a decreasing function of  $F_0$ . The attenuation length  $\kappa_e$  increases with atomic number, so  $a_B$  exhibits less dependence on the electric field for low values of  $Z$ .

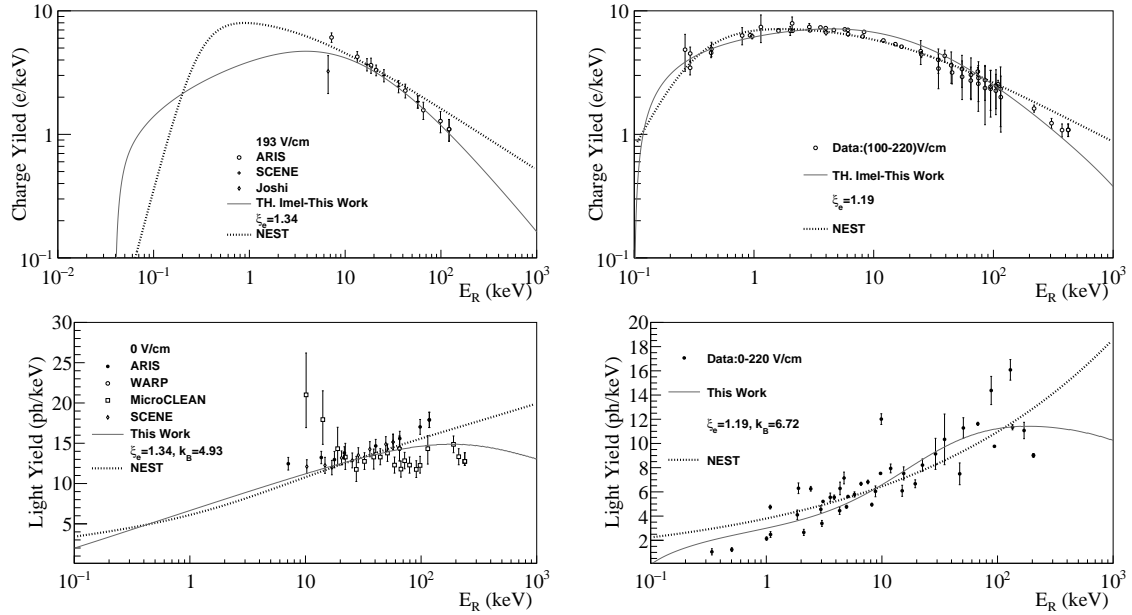
Furthermore, we need to consider biexcitonic extinction, that is, i.e.,  $Ar^* + Ar^* \rightarrow Ar + Ar + e$ . This mechanism is proportional to the deposited energy and produces light extinction in noble liquids [15].

We used Birks-Law [16] which reduces the light emission by a factor of  $(1 + k_B S_e(E_R))^{-1}$ , where  $k_B$  is the Birks constant. this constant can be estimating by assuming that  $k_B = S_e(E_0)^{-1}$ , where  $E_0$  is determined by  $\xi_e$  and correspond with the energy associated to electrons of inner orbitals of the plasma produced by the cascade process. For LAr and LXe, we obtained  $k_B = 4.93$  and  $k_B = 6.72$  respectively, which compares well to previous results [6, 17].

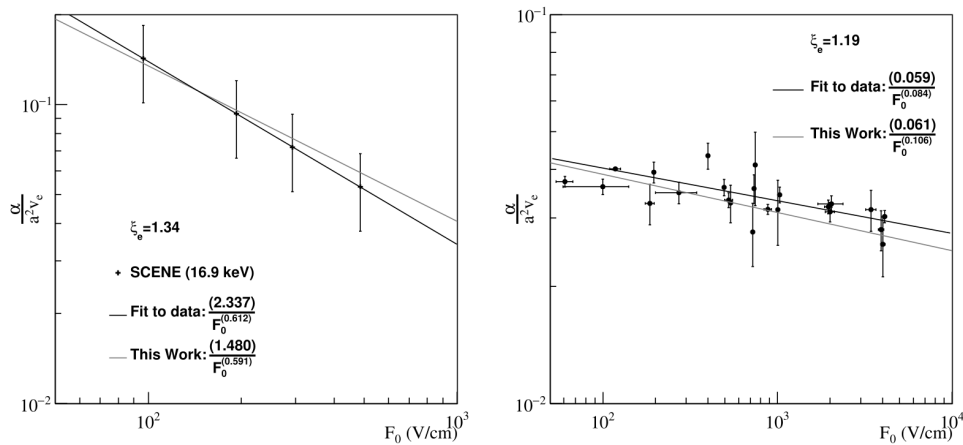
#### 5 Results

From the study described above we predict that, for any noble liquid,  $\xi/N_i = C_0 \Xi(Z, \xi_e)/F_0^\eta$ , where  $C_0$  is a fit constant and  $\Xi(Z, \xi_e)$  and  $\eta$  are functions of quantities that depend on the microphysics. We use recent light and charge yield data for LAr [11, 18–20] and LXe [21] to test the model. To obtain  $C_0$ ,

we used LXe because more data are available. In this way, we get  $(\xi/N_i)_{\text{LXe}} = (0.061 \pm 0.008)/F_0^{0.106}$  and  $(\xi/N_i)_{\text{LAr}} = (1.48 \pm 0.016)/F_0^{0.591}$ . From these, we calculate the charge and light efficiencies for both LAr and LXe (see figure 3). At nuclear recoil energies above 80 keV, due to the energy dependence of the exciton-ion ratio, our model predicts a reduction in charge production, which is confirmed by measurements in LAr and LXe. In figure 4, we show the comparison our calculation with existent measurements. The lower field dependence of LXe can be understood by the low value of  $\xi_e$  value, resulting in a less screen plasma box than lighter elements.



**Figure 3.** (top left) Charge yield computed in this work for LAr compare to measurements and NEST curve, (top right) Charge yield computed in this work for LXe compare to measurements and NEST curve. (bottom left) Light yield computed in this work for LAr compare to measurements and NEST curve and (bottom right) Light yield computed in this work for LXe compare to measurements and NEST curve.



**Figure 4.** (left) Ratio  $4\xi/N_i$  for LAr compare to data and, fit result, (right) the same but for LXe.

## 6 Conclusions

We present a theoretical model of the nuclear recoil response in noble liquids that adequately explains photon and charge production in LXe and LAr, which is relevant for the next generation of low-threshold neutrino and dark matter experiments. The model was developed from the second-order solution of the Lindhard integro-differential equation, which includes both electronic straggling and electronic and nuclear stopping power. Using the Bates-Griffin mechanism, we incorporate inelastic electronic emission and show that  $W_i^e < W_i^R$ , where  $W_i^e$  and  $W_i^R$  are the electron-atom and atom-atom ionization energies, respectively. Inelastic emission becomes more important for elements with higher atomic numbers; in particular,  $W_i = 19.9$  eV for LXe and  $W_i = 34.3$  eV for LAr. The interpretation of the scaling parameter  $\xi_e$ , introduced in the context of the Thomas-Fermi approximation, is examined in detail. It is assumed that this parameter affects the recombination process in the Thomas-Imel box model, and the box size is estimated based on  $\xi_e$  and the interatomic potentials. The agreement between the model predictions and the data is reasonable, considering that only one fitting parameter is required for both LAr and LXe.

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