PROCEEDINGS OF SCIENCE

Recent study and results for ionization efficiency theory in pure materials

Y. Sarkis[a,*] **and Alexis Aguilar-Arevalo and Juan Carlos D'Olivo**[a]

[a] *Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, 04510 CDMX, Mexico*

E-mail: youssef@ciencias.unam.mx, dolivo@nucleares.unam.mx

Low-energy nuclear recoils induced by elastic neutrino nuclear coherent scattering with nuclei in pure materials have become an important topic of research, in particle physics. We present a detailed model to compute the ionization efficiency for nuclear recoils in silicon (quenching factor) based on original integral equation, which is capable of describing recent measurements at low-energy. We take as case example a silicon based reactor antineutrino experiment and compare the effect of this quenching factor in the calculation of the CEνNS rate with that of other curves that have been previously used. We are going to discuss the universal applicability of this model to other materials, such as noble liquid TPCs, which in recent years have become relevant for neutrino low energy CENS searches. Finally, a general discussion of the different effects that directly account for the conversion of nuclear recoil energy (eV_{nr}) into electron equivalent energy (eV_{ee}) in ionization detectors.

XVIII International Conference on Topics in Astroparticle and Underground Physics (TAUP)
August 28, 2023 to September 1, 2023
University of Vienna, Vienna, Austria

*Speaker

PoS(TAUP2023)225

1. Introduction

Coherent elastic neutrino-nucleus scattering (CEνNS) is a Standard Model prediction [1] that was observed by the COHERENT collaboration using the neutrinos produced by the Neutron Spallation source at Oak Ridge National Laboratory first, using CsI[Na] ionizaton detectors [2] and later, in an independent way, with a liquid argon (LAr) detector [3]. Signals from CEνNS-induced nuclear recoils have eluded promising reactor neutrino experiments based in semiconductor ionization detectors like CONNIE [4] and CONUS [5], because of high backgrounds near the threshold (50-100 eV), and the fact that a large fraction of the deposited energy does not find its way to ionization electrons due to quenching effects. Similarly, dark matter (DM) interactions in direct detection experiments are expected to produce low nuclear recoil energy depositions ($< 1\text{keV}_{\text{nr}}$) in ionization detectors [6]. In general, for ionization experiments specialized in rare events detections, it is crucial to know the nuclear recoil ionization efficiency in order to properly reconstruct the energy of such events.

The visible energy signal in a pure ionization detector is directly related to the energy used to liberate free electrons. Considering the situation where a neutral particle produces an initial nuclear recoil that kicks-off an atom from its site in the detector sensitive material, we define the ionization efficiency (quenching factor) as the ratio of the electronic energy E_{ee} to the total recoil energy E_R. Lindhard *et al.*[7] proposed to divide the recoil energy in two parts, the energy given to electrons E_{ee} and the energy that goes to nuclear collisions E_n, and derived a general integral equation for studying this partitioning. His famous formula [1] for ionization efficiency that formally takes into account only effects of nuclear collisions and electronic excitation at energies above $\approx$ 50 keV, describes the data in this regime, e.g, for Ge and Si [8].

In recent CEνNS and direct DM searches the energy threshold is below the interval where Lindhard's formula is valid, and a reformulation of the theory is needed. At first, the most important addition to Lindhard theory to describe low energy measurements is to include the effect of atomic binding energy [8]. In this work, we expand the study to understand ionization efficiency at low energies [9], incorporating a variable binding energy model and a semi-classical model for electronic stopping valid for light elements.

2. Integro-Differential Equation For Pure Element (crystal) Ionization Detectors

As in Lindhard's theory [7], we assume that E_R, the total energy deposited in the material by the incoming particle, can be written as the sum of the total energy given to electrons E_{ee} and the total energy given to atomic motion E_n, so that $E_R = E_{ee} + E_n$. We can divide E_{ee} (E_n) in to electrons (nucleus) kinetic energy E^0_{ee} (E^0_n) plus the electron (nuclei) binding energy U_e (U_n), that is: $E_{ee} = E_{ee0} + U_e$ and $E_n = E^0_n + U_n$. By defining the total binding energy $U = U_e + U_n$ we can deduce the relation $E_R = E + U$ where E is the kinetic energy of the moving atom. For binary collisions, it is convenient to use the Ziegler scaling length $Z = Z_1^{0.23} + Z_2^{0.23}$ [10], where Z_1 and Z_2 are the atomic numbers of the incident ion and the target atom, respectively, $a = 0.8853 a_0/Z$, and the Bohr radius

[1] $f_n = kg(\varepsilon)/(1 + kg(\varepsilon))$, $g(\varepsilon) = \varepsilon + 3\varepsilon^{0.15} + 6\varepsilon^{0.7}$, with $\varepsilon = 11.5E/\text{keV}$ and $k = 0.133Z^{2/3}/A^{1/2}$

a_0, to define $\varepsilon = QE$, $\eta = QE_{ee}$, $\nu = QE_n$ and $u = QU$ with $Q = a/2e^2Z_1Z_2 = 16.2616/ZZ_1Z_2$ keV^{-1}. We also assume that the energies averaged over many cascades initiated by a moving atom with kinetic energy ε, satisfy $\varepsilon_R = \bar{\eta}(\varepsilon) + \bar{\nu}(\varepsilon)$. The ionization efficiency for nuclear recoils $\varepsilon_R = \varepsilon + u$, is given by

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

From the general integral equation for $\bar{\nu}$ [7] we can derive an integro-differential equation using the following approximations [9]: 1) electrons not contribute to atomic motion, 2) E^0_{ee} and E^0_n are small compared to E and 3) nuclear and electronic interactions are separable. It is also necessary to define the electronic stopping power $\tilde{S_e} = N_e^{-1}(dE/dR)_e = \int d\sigma_e(\Sigma_i T_{ei})$, where N_e is the electron number density and R is the distance traveled by the projectile, and the electronic straggling $\Omega^2 = \langle(\Delta E - \langle\Delta E\rangle)^2\rangle$. In terms of the reduced quantities ε and $\rho = \pi a^2 N_e R$, we can write $S_e(\varepsilon, P, \Lambda, V(x)) = d\varepsilon/d\rho$ and $W(\varepsilon, P, \Lambda, V(x)) = d\omega^2/d\rho$, with $\omega^2 = (Q\Omega)^2$ [2]. Here, P is the average impact parameter, Λ the inter-atomic separation and $V(x)$ the inter-atomic potential for two atoms in the media [10, 11] . These terms appear in the approximations required to expand the Lindhard integral equation up to second order [9]. According to the above considerations, we derive the following integro-differential equation that incorporate straggling:

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

where $u(\varepsilon)$ is the binding energy and $t = \varepsilon^2 \sin^2(\theta/2)$, with θ the scattering angle in the center of mass frame. Here, $f(t^{1/2})$ is related to the nuclear differential cross section in the Lindhard-Scharff-Schiott (LSS) [12] approximation: $d\sigma_n = \pi a^2 dt f(t^{1/2})/2t^{3/2}$ [7]. Eq. (2) can be solved with an appropriate parametrization for $\bar{\nu}$, by applying a shooting method, for details [8, 9]. what is described here implies that the ionization efficiency f_n is a problem of many variables that depends at least, on nuclear stopping, electronic straggling, electronic stopping power, average impact parameter of the collisions, interatomic distance and the interaction between two atoms. Most of these variables are not considered in Lindhad's formula or in a data fit.

2.1 Binding Energy

When atomic collisions are active in the medium a fraction of the energy transferred to ions is used to excite atomic inner degrees of freedom (U_e) and to remove atoms from their sites in the lattice (U_n). To model U_e we assume the semi-classical approach of Thomas-Fermi theory, where the effective electron atomic binding is a continuous function of distance from nuclei. By means of the semi-classical model, U_e may be given in terms of the minimum approach distance x_0 in the binary collision, defined by the equation $E = V(x_0)$, since we are neglecting any electron tunneling or resonance effects beyond this distance. Thus,

$$U_e(E, \xi_e) = U_0 \int_{x_0}^{\infty} dy\, \phi^{5/2}(y, \xi_e)/y^{1/2}, \tag{3}$$

[2]Here we assume the approximation that electronic and nuclear straggling are equal

where ϕ is the screening function of the interatomic potential $V(x)$, $U_0 = (12.02/\xi_e^{2/3})Z_1^\dagger Z$ eV, with $Z^\dagger$ denoting the effective number of electrons in the atom and ξ_e the scaling length, both defined in [9]. The binding energy U_n can be associated with the energy required to remove the atom from its site in the lattice, U_F, creating a Frenkel-pair (FP) [13]. This energy is independent of the incoming atom energy and is specified for each media, e.g. in Si $U_F = 23.6^{+15.2}_{-12.1}$ eV. We want to remark that at higher energies U_n is dominated by electron binding energy U_e, that in this limit is of the order ≈ 500 eV and when atom incoming energy is of the order of U_F the situation is reversed $U_e \ll U_n$.

2.2 Electronic Stopping power

For ions moving freely in a pure crystal medium, collisions with outer atomic electrons activate multiple inner electronic transitions or excitations, witch contribute to electron momentum transfer that defines electronic stopping. For ion energies above $\approx (10)Z_1^{7/3}$ eV and lower than $\approx (10^5)Z_1^{2/3}$ eV the electronic stopping power can be modeled as a function proportional to velocity[14]. For lower energies, the effects of Coulomb repulsion [15] between ions reduce the effective electron density and excited levels available for electrons, dimming the electronic stopping power which is not longer proportional to the velocity. For high energies Bohr stripping effect[16] and Z-oscillations in ions [17] generate a modulation of electronic stopping power that provides better description of the available data for Si, see Fig. 1. These effects are described by the general expression $\tilde{S_e} = \xi_e 8\pi N e^2 a_0 \frac{Z_1^\dagger Z_2^\dagger}{Z^3} \left(\frac{v}{v_0}\right) \tau(E, \frac{Z_1}{Z_2})$, where v_0 and a_0 are the Bohr velocity and Bohr radius, respectively τ is a correction factor at low velocities, $Z_{1,2}^\dagger$ are the effective number of electrons, and N is the atomic bulk density. The τ function depends on the minimal approach distance, the inter-atomic potential, and the energy [9], while $Z_{1,2}^\dagger$ depends on electron Fermi energy [9]. In this work, we use three different models for S_e: Tilinin [18], based on kinetic theory and semi-classical analysis momentum transfer cross section, Kishinevsky [19], which considers non uniform velocity at collision, and Arista [20], with uses the dielectric function. The result obtained by solving Eq. (2) and applying Eq. (1) for Si is shown in Fig. 1. Let us notice that these approach is valid for low atomic number media ($Z \leq 20$), since semi-classical picture breaks down at nuclear recoil energies above ≈ 100 eV for heavier targets, underestimating f_n at low energies. Thus, a formal quantum approach has to be used for this case.

3. Liquid Argon and Xenon

Here we present a preliminary analysis to compute the total quanta, excitations and ionizations, for noble liquid time-projection chambers (TPC) detectors, based on a constant binding energy model and the Lindhard stopping power ($S_e = k\varepsilon^{1/2}$) [8, 21]. The main signals (quanta) produced in this detectors are photons n_γ and electrons n_e, where these are generated by ionizations N_i and excitations N_{ex} coming from the recoil atoms in the medium, where usually it is assumed that each atomic ionization gives one electron and each excitation produce a single photon, $N_i + N_{ex} = n_e + n_\gamma$, unless it recombines [22] . In noble liquids ionization detectors some ionizations are quenched by intermediate states of the atoms, producing a recombination that convert some fraction r of ionizations to photons, this can be modeled as $n_\gamma = N_{ex} + rN_i$, from this we can derive for electrons, $n_e = (1-r)N_i$. Furthermore for electrons and photons we also consider the following assumptions:

total energy given to electrons is $\bar{\eta} = f_n \varepsilon_R$, the ratio among excitations and ionizations, $\beta = N_{ex}/N_i$ doesn't depend on the recoil energy, and recombination is given by Thomas-Imel box model [23]. Accordingly, $N = N_{ex} + N_i = n_e + n_\gamma = N_i(1+\beta)$, and $\bar{\eta} = w_i N_i$, where $w_i = QW_i$ is the mean energy to produce an ionization in the medium e.g. LAr, $W_i = 23.6 \pm 0.4$ eV [24]. Then by Thomas-Imel box model the recombination fraction of ions is $r = 1 - \frac{1}{\xi}\ln(1+\xi)$, where $\xi = C_0 N_i$ and C_0 is a constant obtained from data. Results of this study can be seen in Ref. [21], where the values of β, C_0, k, U, and W_i were obtained from a chi-square fit to available measurements up to nuclear recoil energies of 100 keV. Quite good results are obtained for both, LAr and LXe, in particular for energies below 10 keV. A discrepancy at higher energy is associated with the fact that Bohr stripping effects were not taken in to account. For light yield we incorporate the quenching Penning effect by means of the model described in [25] that required an extra free parameter η'.

4. Conclusions

We present a study of the ionization efficiency based on the Lindhard integral equation for pure ionization media. The modeling of the electronic stopping power was improved for media with atomic number $Z \leq 20$ considering Coulomb repulsion effects, electronic straggling, and Bohr stripping criteria. Se also define the physical parameters needed to compute ionization efficiency, in order to call the attention of the community for future works. In the case of silicon there is a good agreement with measurements from nuclear recoils from 3 MeV to 500 eV. Lower energies measurements [26] could indicate that quantum corrections for electronic stopping power and straggling may be needed. In plots of figure 3 from [21], is shown the light and charge yield as a function of f_n, where in the low energy regime our model predict lower values of f_n than the Lindhard model (see plots of f_n, light and charge as a function of recoil energy [21]). This was already observed in Xe for $E_R < 1$ keV and expected for Ar, where future studies and measurements are needed.

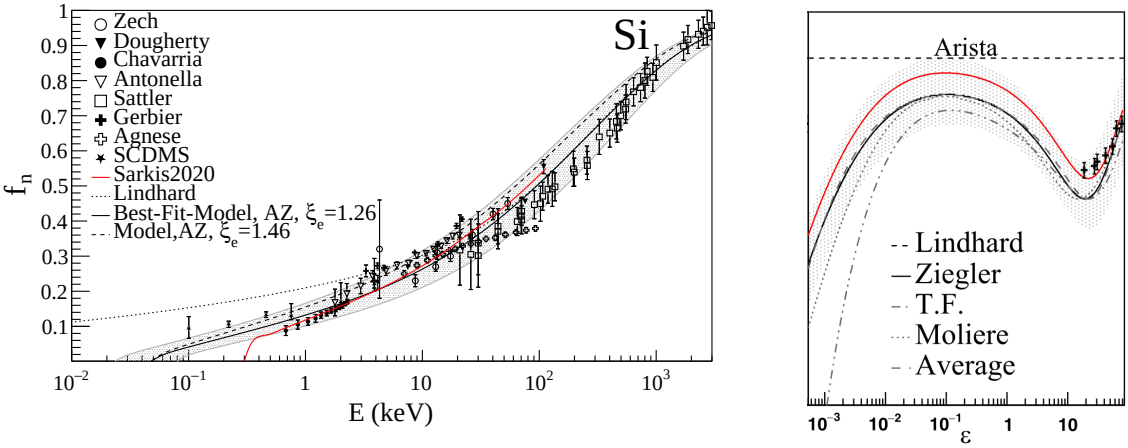

Figure 1: (left) Ionization efficiency for Si according to Eq. (2) and data from [9] and [26], (right) electronic stopping power (Arista) and measurements from [9], the red curve is the electronic stopping that best fits f_n data. Analytical expressions for the central curve and the bands are shown in supplemental material.

5. Acknowledgments

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

References

[1] Daniel Z. Freedman. Coherent effects of a weak neutral current. *Phys. Rev. D*, 9:1389–1392, Mar 1974. doi: 10.1103/PhysRevD.9.1389. URL https://link.aps.org/doi/10.1103/PhysRevD.9.1389.

[2] D Akimov and others COHERENT Collaboration. Observation of coherent elastic neutrino-nucleus scattering. *Science*, 357(6356):1123–1126, September 2017.

[3] D. Akimov et al. First measurement of coherent elastic neutrino-nucleus scattering on argon. *Phys. Rev. Lett.*, 126:012002, Jan 2021. doi: 10.1103/PhysRevLett.126.012002. URL https://link.aps.org/doi/10.1103/PhysRevLett.126.012002.

[4] Alexis Aguilar-Arevalo et al. Search for coherent elastic neutrino-nucleus scattering at a nuclear reactor with CONNIE 2019 data. *JHEP*, 05:017, 2022. doi: 10.1007/JHEP05(2022)017.

[5] H. Bonet, A. Bonhomme, C. Buck, K. Fülber, J. Hakenmüller, G. Heusser, T. Hugle, M. Lindner, W. Maneschg, T. Rink, H. Strecker, and R. Wink. Constraints on elastic neutrino nucleus scattering in the fully coherent regime from the conus experiment. *Phys. Rev. Lett.*, 126:041804, Jan 2021. doi: 10.1103/PhysRevLett.126.041804. URL https://link.aps.org/doi/10.1103/PhysRevLett.126.041804.

[6] Mark W. Goodman and Edward Witten. Detectability of certain dark-matter candidates. *Phys. Rev. D*, 31:3059–3063, Jun 1985. doi: 10.1103/PhysRevD.31.3059. URL https://link.aps.org/doi/10.1103/PhysRevD.31.3059.

[7] J. Lindhard, V. Nielsen, M. Scharff, and P.V. Thomsen. Integral equations governing radiation effects. *Kong.Dan.Vid.Sel.Mat.Fys.Med.*, 33(10):10, 1963.

[8] Y. Sarkis, Alexis Aguilar-Arevalo, and Juan Carlos D'Olivo. Study of the ionization efficiency for nuclear recoils in pure crystals. *Phys. Rev. D*, 101:102001, May 2020. doi: 10.1103/PhysRevD.101.102001. URL https://link.aps.org/doi/10.1103/PhysRevD.101.102001.

[9] Y. Sarkis, A. Aguilar-Arevalo, and J. C. D'Olivo. Ionization efficiency for nuclear recoils in silicon from about 50 ev to 3 mev. *Phys. Rev. A*, 107:062811, Jun 2023. doi: 10.1103/PhysRevA.107.062811. URL https://link.aps.org/doi/10.1103/PhysRevA.107.062811.

[10] F. Ziegler, J.P. Biersack, and U. Littmark. The Stopping and Range of Ions in Solids. *Pergamon Press New York*, 1985.

[11] W. D. Wilson, L. G. Haggmark, and J. P. Biersack. Calculations of nuclear stopping, ranges, and straggling in the low-energy region. *Phys. Rev. B*, 15:2458–2468, Mar 1977. doi: 10.1103/PhysRevB.15.2458. URL https://link.aps.org/doi/10.1103/PhysRevB.15.2458.

[12] J Lindhard, M Scharff, and H E Schioett. Range concepts and heavy ion ranges (notes on atomic collisions, ii). *Kgl. Danske Videnskab. Selskab. Mat. Fys. Medd.*, Vol: 33: No. 14, 1 1963. URL https://www.osti.gov/biblio/4153115.

[13] J. Frenkel. Über die wärmebewegung in festen und flüssigen körpern. *Zeitschrift für Physik*, 35(8):652–669, Aug 1926. ISSN 0044-3328. doi: 10.1007/BF01379812. URL https://doi.org/10.1007/BF01379812.

[14] J. Lindhard and M. Scharff. Energy dissipation by ions in the kev region. *Phys. Rev.*, 124: 128–130, Oct 1961. doi: 10.1103/PhysRev.124.128. URL https://link.aps.org/doi/10.1103/PhysRev.124.128.

[15] Dieter Semrad. Coulomb effect and threshold effect in electronic stopping power for slow protons. *Phys. Rev. A*, 33:1646–1652, Mar 1986. doi: 10.1103/PhysRevA.33.1646. URL https://link.aps.org/doi/10.1103/PhysRevA.33.1646.

[16] Juana L. Gervasoni and Salvador Cruz-Jiménez. Bohr's adiabatic criterion and effective charge of heavy ions. *Radiation Physics and Chemistry*, 48(4):433–436, 1996. ISSN 0969-806X. doi: https://doi.org/10.1016/0969-806X(96)00001-1. URL https://www.sciencedirect.com/science/article/pii/0969806X96000011.

[17] M. Peñalba, A. Arnau, and P.M. Echenique. Z1 oscillations in slow channeled ion stopping power. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, 67(1):66–68, 1992. ISSN 0168-583X. doi: https://doi.org/10.1016/0168-583X(92)95773-K. URL https://www.sciencedirect.com/science/article/pii/0168583X9295773K.

[18] I. S. Tilinin. Elastic scattering of electrons and positrons by complex atoms at medium energies. *Zh. Eksp. Teor. Fiz.*, 94:96–103, Aug 1988. URL file:///tmp/mozilla_youssef0/e_067_08_1570-1.pdf.

[19] L.M Kishinevsky. *Izv. Akad. Nauk SSSR*, 26:1410, 1962.

[20] José M. Fernández-Varea and Néstor R. Arista. Analytical formula for the stopping power of low-energy ions in a free-electron gas. *Radiation Physics and Chemistry*, 96:88–91, 2014. ISSN 0969-806X. doi: https://doi.org/10.1016/j.radphyschem.2013.08.015. URL https://www.sciencedirect.com/science/article/pii/S0969806X13005008.

[21] Y. Sarkis, Aguilar-Arevalo, and J.C. D'Olivo. Lindhard integral equation with binding energy applied to light and charge yields of nuclear recoils in noble liquid detectors. *Journal of Instrumentation*, 18(03):C03006, mar 2023. doi: 10.1088/1748-0221/18/03/C03006. URL https://dx.doi.org/10.1088/1748-0221/18/03/C03006.

[22] Peter Sorensen and Carl Eric Dahl. Nuclear recoil energy scale in liquid xenon with application to the direct detection of dark matter. *Phys. Rev. D*, 83:063501, Mar 2011. doi: 10.1103/PhysRevD.83.063501. URL https://link.aps.org/doi/10.1103/PhysRevD.83.063501.

[23] J. Thomas and D. A. Imel. Recombination of electron-ion pairs in liquid argon and liquid xenon. *Phys. Rev. A*, 36:614–616, Jul 1987. doi: 10.1103/PhysRevA.36.614. URL https://link.aps.org/doi/10.1103/PhysRevA.36.614.

[24] T. Takahashi, S. Konno, T. Hamada, M. Miyajima, S. Kubota, A. Nakamoto, A. Hitachi, E. Shibamura, and T. Doke. Average energy expended per ion pair in liquid xenon. *Phys. Rev. A*, 12:1771–1775, Nov 1975. doi: 10.1103/PhysRevA.12.1771. URL https://link.aps.org/doi/10.1103/PhysRevA.12.1771.

[25] E. Aprile, M. Anthony, Q. Lin, Z. Greene, P. de Perio, F. Gao, J. Howlett, G. Plante, Y. Zhang, and T. Zhu. Simultaneous measurement of the light and charge response of liquid xenon to low-energy nuclear recoils at multiple electric fields. *Phys. Rev. D*, 98:112003, Dec 2018. doi: 10.1103/PhysRevD.98.112003. URL https://link.aps.org/doi/10.1103/PhysRevD.98.112003.

[26] Albakry et al. First measurement of the nuclear-recoil ionization yield in silicon at 100 ev. *Phys. Rev. Lett.*, 131:091801, Aug 2023. doi: 10.1103/PhysRevLett.131.091801. URL https://link.aps.org/doi/10.1103/PhysRevLett.131.091801.

PoS(TAUP2023)225