ELSEPA–Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules (version 2020)

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The present version 2020 of the ELSEPA code differs from the previous version in its internal structure. The calculation of phase shifts is now performed by the generic subroutines of the RADIAL package [4]; a more flexible optical-model potential for scattering in solids is included [3]; and stricter criteria for convergence of the partial-wave series are applied. The calculations performed by the code still follow the description in the original article [1]. The input files have the same formats as those of the previous version, now including an additional option in the selection of the potential model. The present Note describes only the new potential model for scattering in solids. The notation adopted here is the same as in the original article [1].

1 Optical-model potential

The ELSEPA code calculates elastic collisions of electrons and positrons having kinetic energy E with atoms and randomly oriented molecules. The projectile particles have mass m_e and charge $Z_0 e$, with $Z_0 = -1$ and $+1$ for electrons and positrons, respectively. The scattering potential is the sum of the electrostatic interaction energy with the target atom, $V_{st}(r)$, the electron exchange potential, $V_{ex}(r)$ (for positrons $V_{ex} = 0$), the correlation-polarization potential, $V_{cp}(r)$, and the inelastic absorption potential $-iW_{abs}(r)$,

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cp}(r) - iW_{abs}(r). \quad (1)$$

The absorption potential is calculated as

$$W_{\rm abs}(r) = A_{\rm abs}\frac{\hbar}{2}\sqrt{\frac{2(E_{\rm L}+m_{\rm e}c^2)^2}{m_{\rm e}c^2\,(E_{\rm L}+2m_{\rm e}c^2)}\,\frac{2E_{\rm L}}{m_{\rm e}}}\,\rho_{\rm e}(r)\,\sigma_{\rm feg}(E_{\rm L},\rho_{\rm e},\Delta), \tag{2}$$

where $\rho_{\rm e}(r)$ is the atomic electron density at r and $A_{\rm abs}$ is an empirical dimensionless parameter of the order of unity. $E_{\rm L}$ is the local kinetic energy of the projectile, which in the original *elsepa* subroutine is obtained as

$$E_{\rm L} = \begin{cases} E - V_{\rm st}(r) - V_{\rm ex}(r) & \text{for electrons,} \\ \max\{E - V_{\rm st}(r), 0\} & \text{for positrons.} \end{cases} \tag{3a}$$

The quantity $\sigma_{\rm feg}(E_{\rm L},\rho_{\rm e},\Delta)$ is the total cross section (per target electron) for collisions of the projectile electron or positron moving with energy $E_{\rm L}$ in a degenerate electron gas of density $\rho_{\rm e}$, restricted to collisions involving energy transfers larger than the "gap energy" Δ, which corresponds to the lowest excitation energy of the target atom or material (see [1]). ELSEPA allows considering an absorption potential only for projectiles with $E \leq 1$ MeV; for higher energies, $W_{\rm abs}$ is set to zero to prevent the occurrence of numerical instabilities.

The cross section $\sigma_{\rm feg}$ is calculated from the non-relativistic Born approximation, with the generalized oscillator strength derived from Lindhard's dielectric function of the electron gas (local-density approximation, LDA), with electron exchange effects accounted for by means of Ochkur's approximation. In the original ELSEPA code, as well as in the calculations of Salvat [2] for atoms, $\sigma_{\rm feg}$ was set equal to the cross section for binary collisions with the electrons in the gas, which accounts for only electron-hole excitations (LDA-I model). This approximation gives differential cross sections in close agreement with experimental elastic scattering data when the value of the $A_{\rm abs}$ constant is about 2. Bote *et al.* [3] argued that in the case of collisions in solids it is not justified to ignore collective plasmon-like excitations, and they calculated $\sigma_{\rm feg}$ from the full Lindhard dielectric function, *i.e.*, by also including plasmon-like excitations (LDA-II model). With $A_{\rm abs}$ values of the order of unity, the LDA-II model gives absorption cross sections that are in good agreement with measured inelastic mean free paths of electrons in elementary solids, see Ref. [3]. It is worth pointing out that in the LDA-II model, the local kinetic energy is estimated as

$$E_{\rm L} = E - Z_0 E_{\rm F}, \tag{3b}$$

where

$$E_{\rm F} = \frac{\hbar^2}{2m_{\rm e}}\left(3\pi^2\rho_{\rm e}\right)^{2/3}, \tag{4}$$

is the Fermi energy of the local electron gas. In this new version of ELSEPA, the user is offered the option of selecting either the LDA-I model or the LDA-II model of the absorption potential.

Bote *et al.* [3] also proposed the following modified muffin-tin model for scattering in elementary solids. The electron density of an atom in the solid is approximated as

$$\rho_{\mathrm{e}}(r) = \rho_{\mathrm{at}}(r) + \rho_{\mathrm{at}}(2R_{\mathrm{mt}} - r) + \rho_0\,, \tag{5}$$

where $\rho_{\mathrm{at}}(r)$ is the electronic density of the free atom, R_{mt} is the radius of the muffin-tin sphere, and ρ_0 is a constant, which is fixed by requiring that the muffin-tin sphere contains the Z electrons of the atom

$$\int_0^{R_{\mathrm{mt}}} \rho_{\mathrm{e}}(r)\, 4\pi r^2 \mathrm{d}r = Z. \tag{6}$$

The muffin-tin radius is set by the user, or defined internally as half the inter-atomic distance. Notice that the volume of the muffin-tin sphere, $4\pi R_{\mathrm{mt}}^3/3$ must not exceed that of the Wigner-Seitz cell, which equals the reciprocal of the atomic density $\mathcal{N}$ (= number of atoms per unit volume). The scattering potential is calculated from Eq. (1) for radii from zero to R_{mt}, with a modified correlation potential (see Ref. [3]). Outside the muffin-tin sphere, the potential is assigned a constant value,

$$V(r) = V(R_{\mathrm{mt}}) = -\Delta E - \mathrm{i}\Gamma \qquad \text{for } r \geq R_{\mathrm{mt}}, \tag{7}$$

which represents the background potential of the projectile within the solid. The (complex) Dirac phase shifts δ_κ are calculated by solving the radial Dirac equations with the "core" potential

$$V_1(r) = V(r) + \Delta E + \mathrm{i}\Gamma, \tag{8}$$

which vanishes for $r > R_{\mathrm{mt}}$, and the direct and spin-flip scattering amplitudes are computed by summing their respective partial-wave series,

$$\begin{aligned} f(\theta) \;=\; \frac{1}{2\mathrm{i}k} \sum_{\ell=0}^{\infty} \Big\{ &(\ell+1) \Big[\exp\left(2\mathrm{i}\delta_{\kappa=-\ell-1}\right) - 1 \Big] \\ &+ \ell \Big[\exp\left(2\mathrm{i}\delta_{\kappa=\ell}\right) - 1 \Big] \Big\} P_\ell(\cos\theta) \end{aligned} \tag{9}$$

and

$$g(\theta) = \frac{1}{2\mathrm{i}k} \sum_{\ell=0}^{\infty} \Big[\exp\left(2\mathrm{i}\delta_{\kappa=\ell}\right) - \exp\left(2\mathrm{i}\delta_{\kappa=-\ell-1}\right) \Big] P_\ell^1(\cos\theta). \tag{10}$$

The differential cross section (DCS) for spin-unpolarized projectiles is calculated as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \Big| f(\theta) \Big|^2 + \Big| g(\theta) \Big|^2, \tag{11}$$

and the total elastic cross section is obtained by integration of the DCS,

$$\sigma = 2\pi \int_0^{\pi} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \sin\theta \, \mathrm{d}\theta. \tag{12}$$

The grand total cross section, for elastic scattering *plus* inelastic absorption in the core potential $V_1(r)$, is calculated by invoking the optical theorem,

$$\sigma_{\rm T} = \sigma + \sigma_{\rm abs,core} = \frac{4\pi}{k}\,{\rm Im} f(\theta). \tag{13}$$

The background potential component $-{\rm i}\Gamma$ inside the Wigner-Seitz cell, also contributes to the absorption cross section by an amount [3]

$$\sigma_{\rm abs,bk} = \frac{2\Gamma}{\hbar}\,(\mathcal{N}v)^{-1}\,, \tag{14}$$

where $\mathcal{N}$ is the number of atoms per unit volume, and v is the relativistic velocity of the projectile. The atomic cross section for inelastic absorption is

$$\sigma_{\rm abs} = \sigma_{\rm abs,core} + \sigma_{\rm abs,bk}. \tag{15}$$

When using the LDA-II absorption potential with an adjusted value of the constant $A_{\rm abs}$, the quantity

$$\lambda_{\rm abs} = (\mathcal{N}\sigma_{\rm abs})^{-1} \tag{16}$$

closely approximates the inelastic mean free paths derived from measurements or calculated from suitable theoretical approximations for projectiles with kinetic energies up to about 1 MeV [3].

In the case of scattering by free atoms, the LDA-II model with $A_{\rm abs} \sim 0.75$ yields DCSs that are in good agreement with experimental measurements [3]. They practically coincide with the DCSs obtained from the LDA-I model with $A_{\rm abs} \sim 2$.

This optical-model potential has been implemented in the ELSEPA subroutine. The input file of the program ELSCATA has been extended by permitting the user to optionally select the LDA-I and LDA-II absorption potential models, which account for electron-hole excitations only and for the full excitation spectrum of the local electron gas, respectively. As indicated above, the main changes in the programs are the use of the RADIAL subroutine package [4] for the solution of the radial Dirac equations, and the adoption of stricter convergence criteria in the summation of the partial-wave series, Eqs. (9) and (10). These changes only affect the internal structure of the programs; they do not modify the code operation. As a matter of fact, the input files of the original code can be run with the new version. Notice, however, that the list of input parameters to the `ELSEPA` subroutine differs from the original code in that now it includes the atomic density `VMOL` $= \mathcal{N}$. The calculation results are consistent with those of the original code (within the estimated numerical uncertainties), except naturally for the few cases where convergence problems were identified by users, which now converge correctly.

References

[1] F. Salvat, A. Jablonski, C. J. Powell, ELSEPA–Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules, Comput. Phys. Commun. 165 (2005) 157–190.

[2] F. Salvat, Optical-model potential for electron and positron elastic scattering by atoms, Phys. Rev. A 68 (2003) 012708.

[3] D. Bote, F. Salvat, A. Jablonski, C. J. Powell, The effect of inelastic absorption on the elastic scattering of electrons and positrons in amorphous solids, J. Electron. Spectrosc. Rel. Phenom. 175 (2009) 41–54.

[4] F. Salvat, J. M. Fernández-Varea, RADIAL: a Fortran subroutine package for the solution of the radial Schrdinger and Dirac wave equations, Comput. Phys. Commun. 240 (2019) 165–177.