

Improved Ionization Potential Depression and Polarization Shift Models in Dense Plasmas

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For plasmas encountered in high energy density physics (HEDP) experiments, the effects of high densities must be taken into account. In these situations, the interaction of radiator ions and the surrounding background electrons and ions causes lowered continuum, or ionization potential depression (IPD), plasma polarization line shifts, and Stark broadening. In this memo, we give a detailed accounting of physical theories and numerical approaches to address these effects.¹

1 Ionization Potential Depression

Most plasma spectroscopic simulation tools employ some variant of empirical models for IPD. Ecker-Kröll [1], Ion-sphere [2] and Stewart-Pyatt [3] are some of the more widely used ones. The value of IPD in Eker-Kröll and Ion-sphere models are given by,

$$\Delta E = C \frac{e^2}{a}, \quad (1)$$

where C is a numerical constant of order unity, e is the electron charge, and a is a measure of mean inter particle distance. The Ion-sphere model assumes a is the ion-sphere radius defined by,

$$a_{is} = \left(\frac{3}{4\pi n_i} \right)^{1/3}, \quad (2)$$

where n_i is the ion density, and the Eker-Kröll model assumes

$$a_{ek} = \left(\frac{3}{4\pi(n_i + n_e)} \right)^{1/3}, \quad (3)$$

where the density entering the equation is the sum of all ions and electrons.

The Ion-sphere and Eker-Kröll models as defined above are generally applicable in the high density regime where the Debye screening length is much smaller than a . At plasma conditions where the Debye screening length becomes comparable or larger than a , the Stewart-Pyatt model provides an interpolation formula that smoothly bridges the Ion-sphere and

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Debye screening limits. For HEDP plasma conditions, the Stewart-Pyatt model resembles the Ion-sphere model.

Ion-sphere and Eker-Kröll obviously produce very different IPD values. There are currently active debates on which one is more accurate, and different experimental benchmarks have produced conflicting results. *PrismSPECT* provides both model options. In addition to those, a model introduced by More [4] can also be used, which is numerically similar to Stewart-Pyatt for most common plasma conditions.

In addition to the model choices of IPD, how the continuum lowering model is implemented in the solution of the ionization distribution also has a major impact on the final results. Some models employ a hard cutoff such that energy levels over the lowered continuum are assumed to be destroyed, while others use an occupation probability formalism to gradually reduce the statistical weights of atomic levels across the depressed ionization threshold. *PrismSPECT* employs this method by default, and implements the occupation probability of Hummer-Mihalas [5] combined with the IPD formula of More.

The solution of the ionization distribution used to determine the IPD and occupation probabilities in *PrismSPECT* assumes LTE conditions even if the simulation itself is non-LTE. This choice is made to avoid unnecessary numerical complexity and instability. It is justifiable since IPD models are based on LTE to begin with. Ensuring self-consistency of IPDs, occupation probabilities, and ionization distribution is not numerically trivial. We developed an iterative procedure such that a solution can be found efficiently. Starting with an initial guess of ionization distribution (usually LTE populations with zero IPD), a set of IPD and occupation probabilities of all atomic levels can be determined, which results in a new set of level populations and ionization fractions. In practice, we found that a straightforward iteration of this procedure is numerically unstable. To increase the stability and efficiency of the solution, we inserted an intermediate step of solving the implicit equation for the mean charge in each iteration. The key to this method is that IPDs and occupation probabilities mainly depend on the mean charge, with very weak dependence on the shape of the ionization distribution. The solution of ionization distribution in each iteration can be symbolically represented as

$$\bar{z}_o = S(\bar{z}_i, \phi_z), \quad (4)$$

where $\bar{z}_i$ and $\bar{z}_o$ are the mean charge of the plasma before and after the iteration, ϕ_z represents the shape of the ionization distribution. ϕ_z from the output of the iteration is in principle different from that of the input. However, due to the weak dependence of IPDs and occupation probabilities on ϕ_z , we ignore this difference and solve the above implicit equation to enforce $\bar{z}_i = \bar{z}_o$. For a given ϕ_z , it is sometimes possible to have multiple solutions of $\bar{z}$. Our strategy is to search for the highest $\bar{z}$ solution. Numerically, we compute the curve $\bar{z}_o = S(\bar{z}_i)$ on the $\bar{z}_i - \bar{z}_o$ plane for a range of all possible $\bar{z}_i$, and search for the intersection of this curve and the straight line $\bar{z}_o = \bar{z}_i$ that results in the highest $\bar{z}$. With this intermediate step, the iterative procedure only needs to converge on the shape ϕ_z , which is much more stable and efficient numerically. Figure 1 illustrates this implicit intermediate step for an Ar plasma at ion density of $3 \times 10^{24} \text{ cm}^{-3}$ and at two different temperatures, 35 and 350 eV. At the higher temperature, the effect of continuum lowering is rather smooth, and there is only one intersection for $\bar{z}$. At the lower temperature of 35 eV, continuum lowering causes the stepwise changes of $\bar{z}_o$ in response to increases in $\bar{z}_i$, and there are multiple intersections

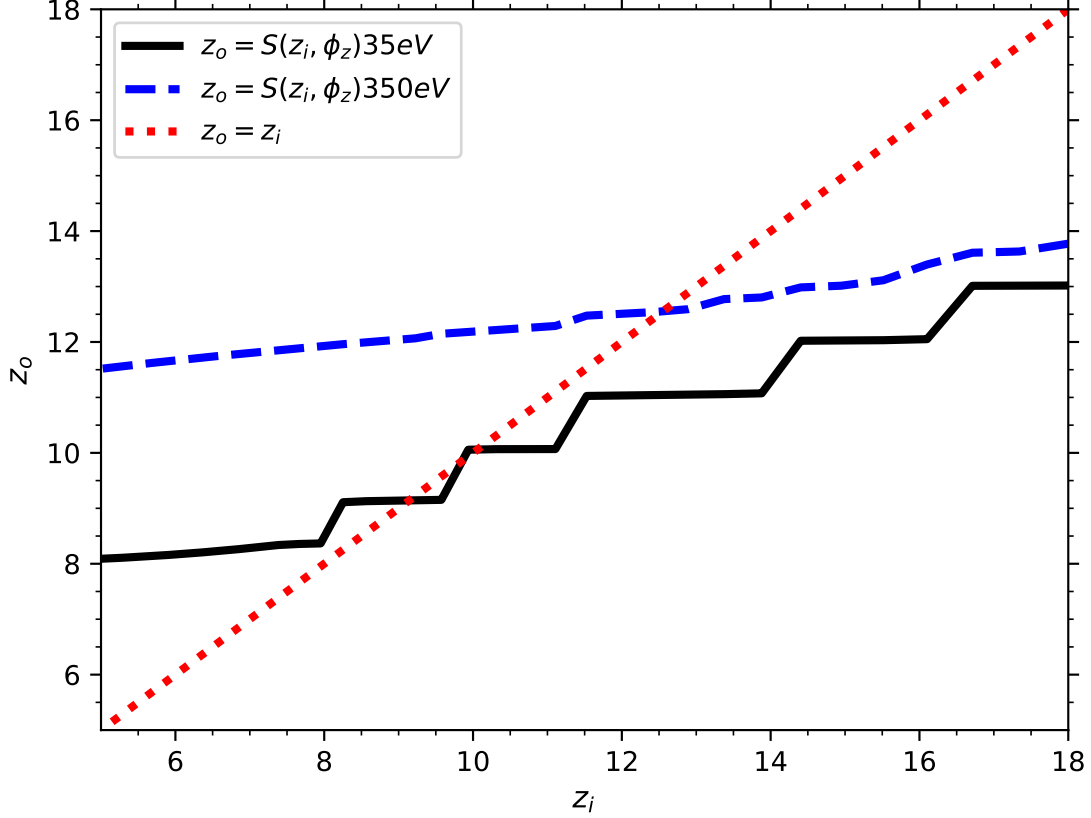


Figure 1: An example of the implicit intermediate step to determine the self-consistent $\bar{z}$ for a given charge state distribution shape. The $\bar{z}_o = S(\bar{z}_i, \phi_z)$ curves are calculated for an Ar plasma at ion density of $3 \times 10^{24} \text{ cm}^{-3}$ and two different temperatures, 35 and 350 eV.

with the $\bar{z}_o = \bar{z}_i$ line, in which case we choose the solution with the highest $\bar{z}$.

2 Plasma Polarization Shifts

The IPD models discussed in the previous section depend only on the ionization stage. Transition energies within a single ion remain the same regardless of plasma conditions. The Stewart-Pyatt IPD formula is in fact an approximation to the original plasma screening theory where the different influence of screening on different atomic orbitals is ingored. We have developed a more detailed atomic model using FAC by solving the radial Dirac equations under the influence of Stewart-Pyatt screening potential. The implementation details in FAC was described in [6]. We have carried out systematic calculations and tabulated shifts in radial orbital energies on a large grid of electron densities and temperatures. *PrismSPECT* has been updated to interpolate on the tabulated data to obtain energy level dependent effects of dense plasma environment. This simultaneously determines the ionization potential

depressions and polarization shifts of transition energies. The IPD table can be invoked as a new model option independent of transition energy shifts in *PrismSPECT*.

Recently, several forms of plasma screening potentials have been implemented in FAC [6], including Debye-Hückel and ion sphere potentials, which are valid in two opposite regimes of plasma conditions, as well as a more sophisticated screening potential due to [3], which smoothly interpolates those two regimes, and is expected to work in a wider range of plasma temperature and density parameters.

The screening potential due to the free electrons and ions is defined as a perturbation,

$$V(r) = V_0(r) + V_f(r), \quad (5)$$

where $V_0(r)$ is the potential of an isolated ion, while $V_f(r)$ accounts for the screening of free electrons and ions in the plasma. The simplest form for $V_f(r)$ is the Debye-Hückel potential. After subtracting $V_0(r)$, we obtain $V_f(r)$ as

$$V_f(r) = V_0(r) \left(e^{-\frac{r}{R_d}} - 1 \right), \quad (6)$$

where R_d is the Debye screening lengths due to both electrons and ions, whose exact definition will be given later. Note that instead of taking into account the screening of the inter-electronic Coulomb interactions and the nuclear potential separately, we are using the screening of the total mean potential generated by the nucleus and the bound electrons. This is valid when the Debye length is much larger than the size of the ionic system, which is generally where Debye screening model can be justified, i.e. in the limit of low density and high temperature. Under this assumption, we can simplify Equation 6 by approximating $V_0(r) = -\frac{z}{r}$, where $z = Z - N_b + 1$ is the residual charge of the ion, and Z is the nucleus charge, N_b is the number of bound electrons.

In the opposite limit of high density and low temperature, the ion-sphere model is often employed [7],

$$V_f(r) = 4\pi \left[\frac{1}{r} \int_0^r r' + \int_r^{R_s} \right] r' \rho_f(r') dr', \quad (7)$$

where $\rho_f(r)$ is the radial distribution of the free electrons in the ion sphere of radius $R_s = [3(Z - N_b)/4\pi n_e]^{1/3}$. The local free electron densities are assumed to follow the Fermi-Dirac distribution as

$$\rho_f(r) = \frac{1}{\pi^2} \int_{\kappa_0}^{\infty} \frac{\kappa d\kappa}{e^{[\sqrt{\kappa^2 c^2 + c^4 - c^2 + V(r) - \mu}]/kT} + 1}, \quad (8)$$

where c is the speed of light, $\kappa_0 = \sqrt{-2V(r)c^2 + V(r)^2}$, and $V(r)$ is the total potential experienced by the free electron. The chemical potential μ is implicitly defined through the charge neutrality condition inside the sphere,

$$4\pi \int_0^{R_s} r^2 \rho_f(r) dr = Z - N_b. \quad (9)$$

Note that in this model, only the screening by electrons is taken into account. When the temperature is high enough, this screening potential reduces to that of a uniformly distributed electron sphere,

$$V_f(r) = \frac{Z - N_b}{2R_s} \left[3 - \left(\frac{r}{R_s} \right)^2 \right]. \quad (10)$$

The ion-sphere and Debye-Hückel screening models are valid under different physical conditions. The ion-sphere model is valid where $R_d \ll R_s$, while the Debye-Hückel model applies when $R_d \gg R_s$. In the intermediate regime where $R_d \sim R_s$, both models fail. The screening potential proposed by the Stewart-Pyatt model naturally interpolates the two limits, and is considered to be more accurate [3]. The potential induced by the free electrons is defined by a second order differential equation based on the Thomas-Fermi model. The equations are often expressed in dimensionless form in terms of $v(x) = V_f(r)/kT$, $y(x) = V(r)/kT$, and $x = r/R_d$, where the total Debye length is defined by

$$\frac{1}{R_d^2} = \frac{4\pi e^2}{kT} (z^* + 1)n_e, \quad (11)$$

where n_e is the electron density far away from the ion, and $z^* = \bar{z}^2/\bar{z}$ is the ratio of the second and first moments of the ionic charge of a multi-component plasma.

$y(x)$ is the solution of

$$\frac{1}{x} \frac{d^2}{dx^2} (xy) = \frac{1}{z^* + 1} \left[\frac{F(y - \alpha)}{F(-\alpha)} - e^{-z^*y} \right], \quad (12)$$

where

$$F(y) = \int_0^\infty \frac{t^{1/2} dt}{e^{t-y} + 1}, \quad (13)$$

and the constant α is related to the electron density, n_e , far from the ion,

$$n_e = \frac{2(2\pi mkT)^{3/2}}{h^3} \frac{2}{\sqrt{\pi}} F(-\alpha) \quad (14)$$

$y(x)$ satisfies the boundary conditions $y(\infty) = 0$, and $xy = Ze^2/(R_d kT)$ at the origin.

$v(x)$ is the solution of

$$\frac{1}{x} \frac{d^2}{dx^2} (xv) = \frac{1}{z^* + 1} \left[\frac{F(y - \alpha, y)}{F(-\alpha)} - e^{-z^*y} \right], \quad (15)$$

where

$$F(y - \alpha, y) = \int_y^\infty \frac{t^{1/2} dt}{e^{t+\alpha-y} + 1}. \quad (16)$$

The boundary conditions for this second order differential equation is $dv/dx = 0$ at the origin, and $v(\infty) = 0$.

The three forms of screening potentials discussed above have been implemented in FAC.

An example of computed IPD dependence on temperature, density, and atomic orbitals are shown in Figure 2 and Figure 3. An example of K_α polarization shifts are shown in Figure 4, which are the differences between the IPDs of 1s and 2p orbitals.

The spectroscopic signature of the polarization shift is demonstrated in Figure 5 for He-like and H-like Kr transitions and associated satellites at the electron temperature of 5 keV and density of $3 \times 10^{25} \text{ cm}^{-3}$. The redshift induced by dense plasma effect is readily observed.

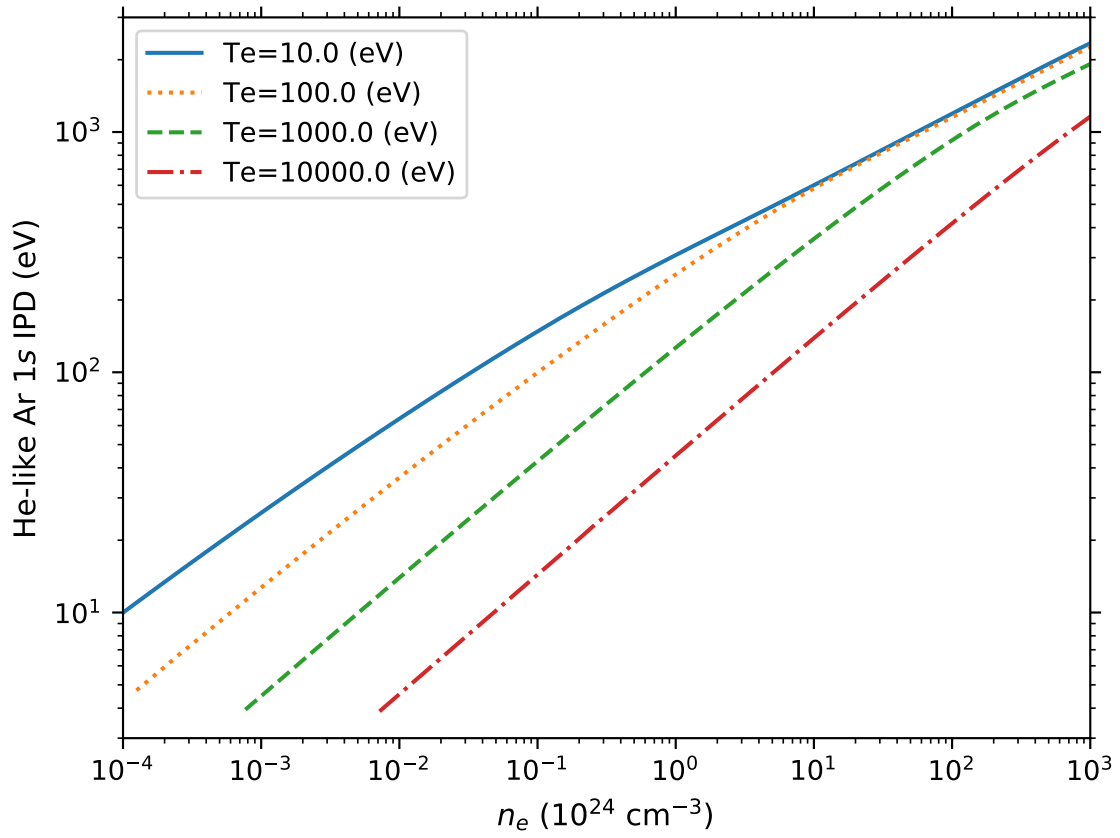


Figure 2: Ionization potential depression (IPD) of He-like Ar 1s orbital at four representative temperatures

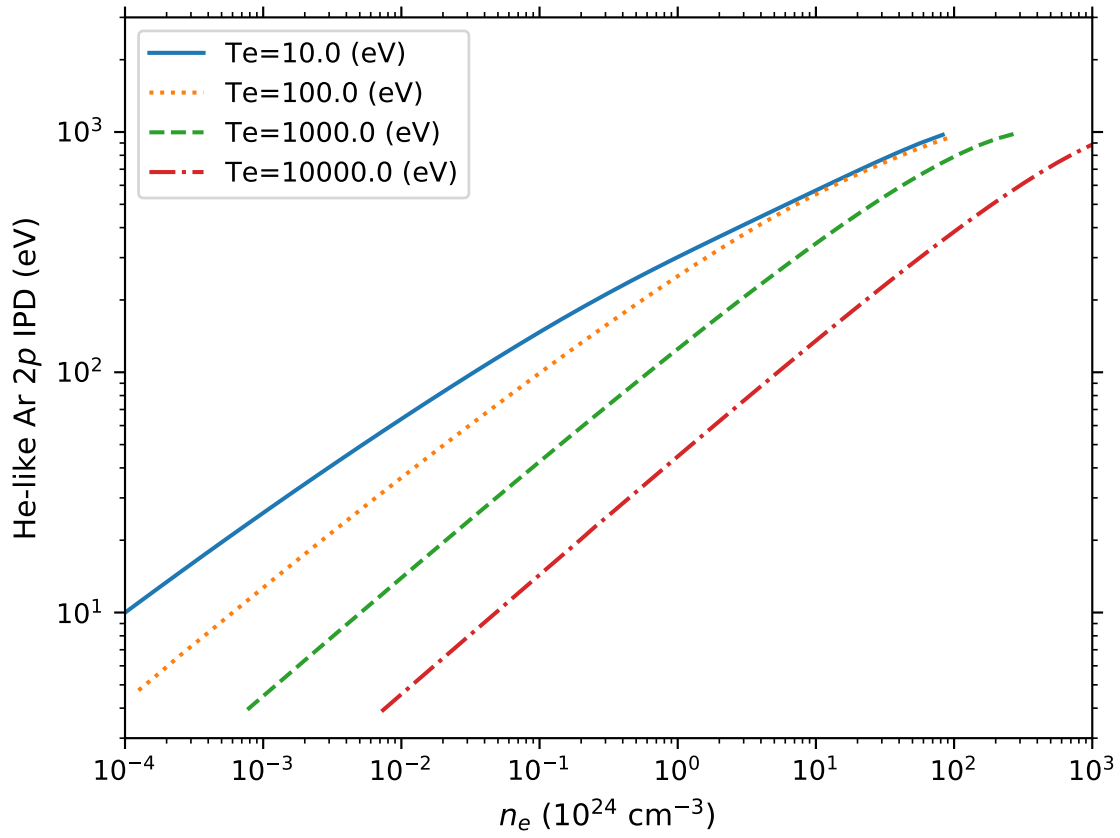


Figure 3: Ionization potential depression (IPD) of He-like Ar $2p$ orbital at four representative temperatures

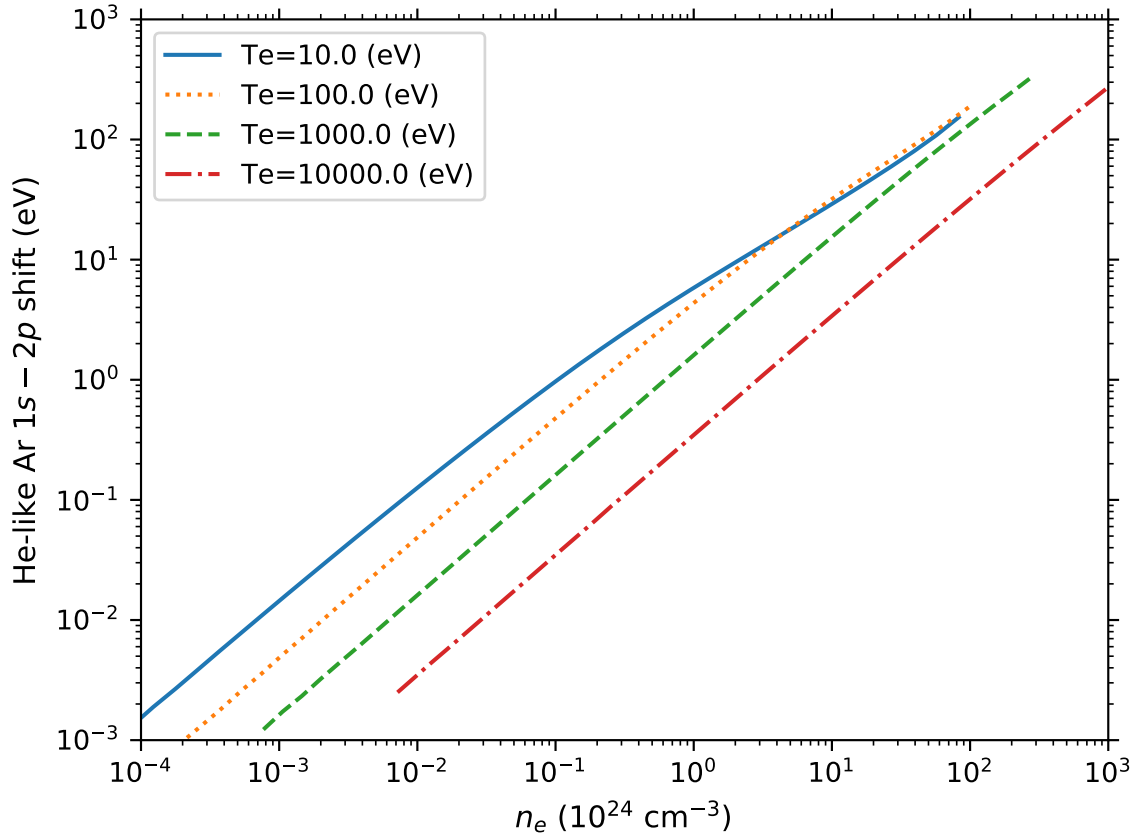


Figure 4: Plasma polarization shift of He_α transition of He-like Ar at four representative temperatures.

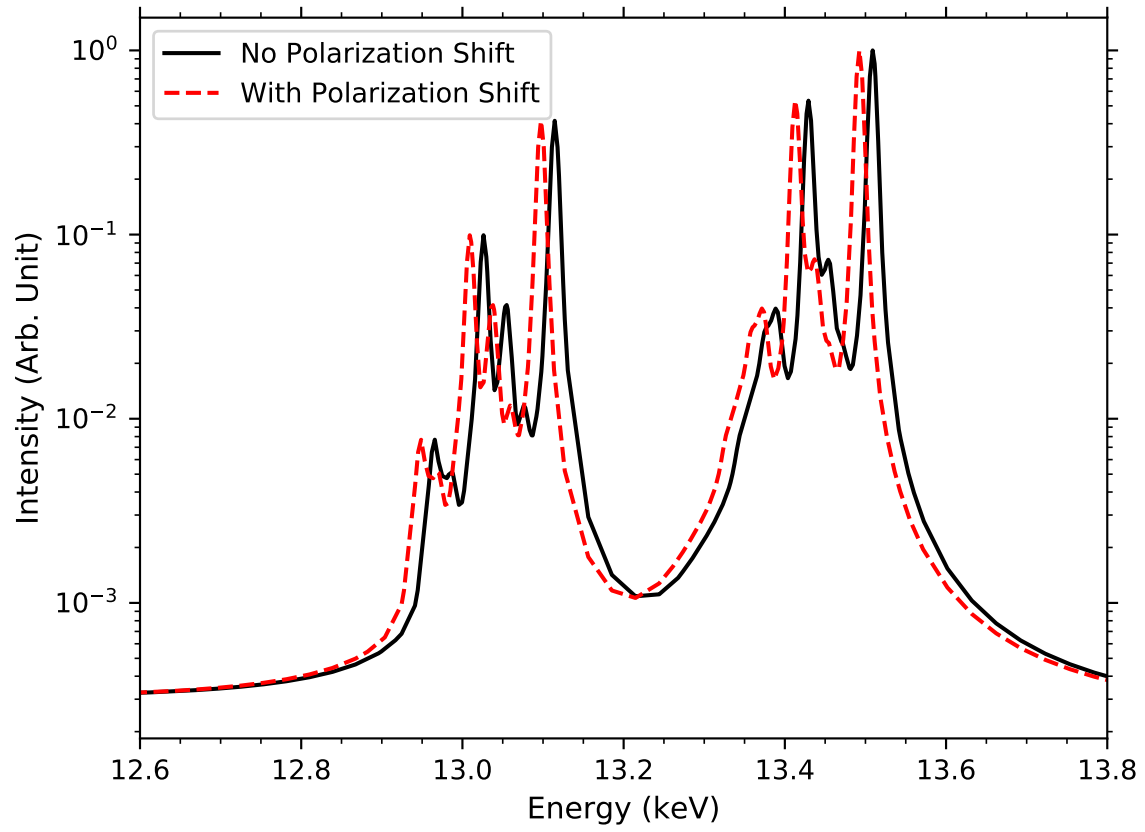


Figure 5: Spectroscopic signature of polarization shift for He-like and H-like Kr transitions.

Appendix 1: BIBLIOGRAPHY & REFERENCES CITED

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