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WAKE SHIFTS IN ELECTRON STATES ON SWIFT IONS PASSING THROUGH SOLIDS *

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Experiment indicates that two-electron states on swift ions passing through a solid can undergo measurable energy shifts due to interactions with the solid. A Green function formulation is used to derive an expression for the self-energy of the ion–electron system. Calculations made with this theory show reasonable agreement with measurements of Bell and co-workers.

1. Introduction

Bell et al. [1] have observed a decrease in the energy of photons emitted in transitions between well-defined electronic configurations on swift, helium-like sulfur ions penetrating thin Al foils. Subsequently resonant excitation of one-electron states on channeled, high atomic number ions has been studied by Datz et al. [2]. In both of these experimental studies the wake of electron density fluctuations trailing the ion [3] affects electronic states bound to the ion. Theoretical analysis of the latter experiments has been carried out, accounting in detail for the effect of the lattice structure in giving rise to resonant excitations, as well as for wake effects [4]. In the present paper we analyze the experiments of Bell et al. in a self-energy formulation.

2. Theory

In terms of destruction operators $C_{\boldsymbol{\kappa}n}$ for a state in which an ion bearing N bound electrons has center-of-mass momentum $\boldsymbol{\kappa}$ and is in a state of internal motion specified by the multi-component quantum index n, the energy of the ion may be written

$$H_0 = \sum_{\boldsymbol{\kappa}} \sum_{n} E_{\boldsymbol{\kappa}n} C^{+}_{\boldsymbol{\kappa}n} C_{\boldsymbol{\kappa}n} , \tag{1}$$

where $E_{\boldsymbol{\kappa}} = \kappa^2/2(M+N) + \omega_n$ and ω_n is the energy of internal motion. Atomic units are used throughout and M is the ion mass. Similarly, the energy of the valence electron ensemble is

$$H_{\mathrm{M}} = \sum_{\boldsymbol{k}} \epsilon_k a^{+}_{\boldsymbol{k}} a_{\boldsymbol{k}} , \tag{2}$$

where $a_{\boldsymbol{k}}$ is a destruction operator for an electron in a plane-wave state with momentum $\boldsymbol{k}$ and $\epsilon_k = \frac{1}{2}k^2$.

The energy of interaction between the ion and the solid may be written

$$H_{\mathrm{I}} = \frac{1}{\Omega} \sum_{n} \sum_{n'} \sum_{\boldsymbol{\kappa}} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{p}} v_q [\rho_{n'n}(\boldsymbol{q}) - Z\delta^{n'}_{n}] \, C^{+}_{\boldsymbol{\kappa}-\boldsymbol{q}n'} C_{\boldsymbol{\kappa}n} a^{+}_{\boldsymbol{p}+\boldsymbol{q}} a_{\boldsymbol{p}} , \tag{3}$$

where Ω is the normalization volume, $v_q = 4\pi/q^2$ is the Coulomb interaction in momentum representation, $\rho_{n'n}(q) = \langle n' | \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_j} | n \rangle$ is the matrix element of the density operator and Z is the charge of the ion. The Dyson equation for $G_{\boldsymbol{\kappa}n,\omega}$, the exact Green function of the interacting system, may be solved formally as

$$G_{\boldsymbol{\kappa}n\omega} = \left[\omega - \left(E_{\boldsymbol{\kappa}n} + \sum_{\boldsymbol{\kappa}n\omega} \right) \right]^{-1} , \tag{4}$$

where $\Sigma_{\boldsymbol{\kappa}n\omega}$ is the self-energy of the system. The latter may be represented by an infinite sum of proper self-energy diagrams in which interactions with the medium can occur in all possible ways. A manageable approximation to $\Sigma_{\boldsymbol{\kappa}n\omega}$ may be obtained in the pair approximation. One obtains

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$$\sum_{\mathbf{K}n\omega} = \sum_{n} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} |\rho_{n'n}(\boldsymbol{q}) - Z\delta_n^{n'}|^2$$

$$\times v_q(\epsilon^{-1}_{\boldsymbol{q},\boldsymbol{q}\cdot\boldsymbol{v}+\omega_n-\omega_{n'}} - 1)^{-1} , \quad (5)$$

where $\epsilon_{q,\omega}$ is the dielectric response function of the solid. Of the four terms in eq. (5) only two should be retained; the one representing the effect of the ion's wake on the bound electronic system and the one representing the effect of the wake of the electron cloud on the electronic system itself.

In dealing with degenerate states, a given state vector may be written as a sum over configurations, viz., $|n\rangle = \Sigma_i A_i |i\rangle$, where the A_i are to be determined. The energy of the coupled ion–medium system is found from the poles of the Green function [eq. (4)]. Solving this in the usual approximation yields the matrix equation

$$\sum_j \left[(\omega - E_{\mathbf{K}n}) A_j \delta_i^j + \sigma_{ij} A_j - \sum_{lm} \tau_{ijlm} A_j A_l A_m \right] = 0 , \quad (6)$$

where

$$\sigma_{ij} = Z \int \frac{\mathrm{d}^3 q}{(2\pi)^3} v_q(\epsilon^{-1}_{\boldsymbol{q},\boldsymbol{q}\cdot\boldsymbol{v}} - 1) \langle i | \rho_{\boldsymbol{q}} | j \rangle$$

$$= \langle i | \phi_{\mathrm{w}} | j \rangle \quad (7)$$

is the matrix element of ϕ_{w}, the wake potential of the ion evaluated at the position of each electron. Here $\rho_{\boldsymbol{q}} = \Sigma_{k=1}^{N} \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}_k}$ is the density operator and τ_{ijlm} represents the self-wake of the electron cloud.

Solving for the eigenvalues of eq. (6) yields the energies of the perturbed degenerate states. The nonlinear terms involving τ_{ijlm} are expected to be negligible when $Z \gg 1$. We employ the plasmon-pole approximation for $\epsilon_{q,\omega}$ here.

3. Comparison with experiment

To compare with the experiments of Bell et al. who measured the wake-shift in the $^1P_1 - ^1S_0$ transition of the two electron configuration on swift sulfur ions, we use variationally determined product wave functions of the form

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | {}^1\mathrm{P}_1 \rangle_0 = \frac{1}{\sqrt{2}} \{ \langle \boldsymbol{r}_1 | 1\mathrm{s} \rangle \langle \boldsymbol{r}_2 | 2\mathrm{p}_0 \rangle + \langle \boldsymbol{r}_1 | 2\mathrm{p}_0 \rangle \langle \boldsymbol{r}_2 | 1\mathrm{s} \rangle \} \, \xi_{\mathrm{spin}} ,$$

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | {}^1\mathrm{P}_1 \rangle_1 = \frac{1}{\sqrt{2}} \{ \langle \boldsymbol{r}_1 | 1\mathrm{s} \rangle \langle \boldsymbol{r}_2 | 2\mathrm{p}_1 \rangle + \langle \boldsymbol{r}_1 | 2\mathrm{p}_1 \rangle \langle \boldsymbol{r}_2 | 1\mathrm{s} \rangle \} \, \xi_{\mathrm{spin}} ,$$

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2 | {}^1\mathrm{S}_0 \rangle = \langle \boldsymbol{r}_1 | 1\mathrm{s} \rangle \langle \boldsymbol{r}_2 | 1\mathrm{s} \rangle \, \xi_{\mathrm{spin}} ,$$

where ξ_{spin} is the antisymmetric spin state vector for two electrons and $\langle \boldsymbol{r} | 1\mathrm{s} \rangle$, $\langle \boldsymbol{r} | 2\mathrm{p}_0 \rangle$ and $\langle \boldsymbol{r} | 2\mathrm{p}_1 \rangle$ are taken to be hydrogenic states with effective charge, Z_{eff}, determined variationally. The results are [5] $Z_{\mathrm{eff}}^{1\mathrm{s}} = 16$ and $Z_{\mathrm{eff}}^{2\mathrm{p}} = 15$ for the $^1P_1$ states and $Z_{\mathrm{eff}} = 15.69$ for the $^1S_0$ state.

In this approximation we find that the wake energy shift of the $^1S_0$ state is $\Delta E(^1\mathrm{S}_0) = 2\langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle$ where $Z_{\mathrm{eff}} = 15.69$. The shifts in the transition energies are then

$$\delta E_{P_0} \equiv \Delta E_{P_0}(^1\mathrm{P}_1) - \Delta E(^1\mathrm{S}_0)$$
$$= \langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle_{Z_{\mathrm{eff}}=16} + \langle 2\mathrm{p}_0 | \phi_{\mathrm{w}} | 2\mathrm{p}_0 \rangle_{Z_{\mathrm{eff}}=15}$$
$$- 2\langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle_{Z_{\mathrm{eff}}=15.69} ;$$

$$\delta E_{P_1} \equiv \Delta E_{P_1}(^1\mathrm{P}_1) - \Delta E(^1\mathrm{S}_0)$$
$$= \langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle_{Z_{\mathrm{eff}}=16} + \langle 2\mathrm{p}_1 | \phi_{\mathrm{w}} | 2\mathrm{p}_1 \rangle_{Z_{\mathrm{eff}}=15}$$
$$- 2\langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle_{Z_{\mathrm{eff}}=15.69} .$$

For the case of He-like sulfur ions moving in Al at $v = 10.69$, we find $\delta E_{P_0} = -0.849$ eV, $\delta E_{P_1} = -1.137$ eV which we average to $\delta E = -1.041$ eV. This result agrees well with the results of Bell et al. who found $\delta E = -(1 \pm 0.2)$ eV.

4. Conclusion

The present self-energy theory of energy shift includes a description of the wake potential in momentum representation. It describes collective and single-particle effects and gives reasonable agreement with experiment.

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Note added in proof. The numerical result for δE is quite sensitive to the effective Z used in computing ϕ_{w}. For example, if one takes both $\langle 1\mathrm{s} | \phi_{\mathrm{w}} | 1\mathrm{s} \rangle$ and $\langle 2\mathrm{p}_{0,1} | \phi_{\mathrm{w}} | 2\mathrm{p}_{0,1} \rangle$ proportional to $Z - 2 = 14$ one finds $\delta E \simeq -0.1$ eV. These choices are probably more realistic than those employed in obtaining the value of δE give above. Additional energy shift originating from the averaged static potential of the solid at the ion position has not been taken into account here and may explain the discrepancy between experiment and the smaller δE value. Further work along these lines is planned.

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