

On the additivity of scattering phases in collisions of electrons on endohedrals

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Synopsis It is demonstrated that an inner atom, either Ne or Ar, qualitatively affects the electron scattering phases upon an endohedral, in spite of the fact that the fullerene consists of 60 carbon atoms, while the atom stuffed inside is only one. Calculations are performed in the one-electron Hartree-Fock (HF) and random phase approximation with exchange (RPAE) for the inner atom while the fullerenes shell is substituted by static potential without and with the polarization potential. The total endohedral scattering phase is a sum of atomic, Ne or Ar, and fullerenes C_{60} phases, contrary to the intuitive assumption that the total phases on C_{60} and $Ne@C_{60}$ or $Ar@C_{60}$ has to be the same.

1. We suggest after performing calculation of a concrete example that the total partial wave l phase $\delta_l^{A@C_N}$ of an electron scattered upon endohedral $A@C_N$ is with good accuracy equal to the sum of scattering phases δ_l^A and $\delta_l^{C_N}$ of electrons upon atom A that is stuffed inside the fullerene C_N .

We generalize this result to any target that consists of loosely bound atoms. It is counter-intuitive, since it is reasonable to assume, at least in the case of the considered target $A@C_N$ that the scattering is absolutely dominated by the very “big atom” so that the contribution of atom A can be neglected.

2. If the target consists of electrons and nuclei and exchange between incoming and target electrons is taken into account, one has for the place $\delta_l(0) = (n_l + q_l)\pi$, where q_l (n_l) is the number of bound electron states in the target itself (in $e + \text{target}$). Therefore, the behavior of phases as functions of E is qualitatively different in cases when we treat the target in Hartree or HF approximation. In these two cases the phases deviate from each other (in numbers of π) although the strength of the potential is almost the same.

3. The atom A was treated in HF and RPAE, while the fullerene was represented by square well potential $W_c(r)$ and polarization potential $V_c^{pol}(r) = -\alpha_c / [2(r^2 + b^2)^2]$. The choice of potential parameters and some details of calculations are presented in [1].

4. Figure 1 illustrates the *property of additivity*, namely the fact that the following equation is valid with quite high accuracy

$$\delta_l^{A@C_{60}}(E) = \delta_l^A(E) + \delta_l^{C_{60}}(E). \quad (1)$$

Inclusion of $V_c^{pol}(r)$ modifies the phases, adding a number of bound states in $(e + C_{60})$.

If the electronic structure of the target, namely exchange between the incoming and target electrons will be taken into account, the phases will increase, acquiring an addition (in units of π) to the phase, equal to the number of bound in the target electrons with the given angular momentum l .

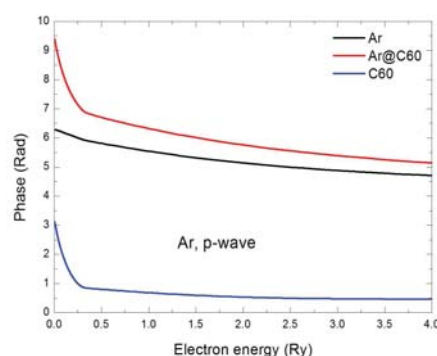


Figure 1. Elastic scattering p -phase of electrons upon atom Ar, fullerene C_{60} , and endohedral $Ar@C_{60}$.

5. Correlations between atomic electrons are essential, modifying the low-energy cross-section. The atomic cross-section at $E \rightarrow 0$ is much less than the cross-section upon C_{60} , but fullerene adds prominent structure. Phase additivity (1) does not lead to corresponding additivity in the cross-sections. The modification of the cross-section due to presence even of a single additional atom can affect not only elastic scattering but some other connected to it properties and characteristics of electron-target collisions.

References

- [1] M. Ya. Amusia and L. V. Chernysheva 2015 *JETP Letters* **101**

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