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During annihilation of the positron with an electron, two gamma rays are emitted. Information contained in these rays can be used to study the electronic environment around the annihilation site. This information is unique to each atom, and can be used, in particular, to identify annihilation sites in molecules [1].

The gamma rays carry away the energy of the two particles, $E \approx 2mc^2$, and their total momentum, $\mathbf{P}$, is equal to the momentum of the electron-positron pair. The distribution of these momenta leads to the following spectrum of energies E_γ of the gamma quanta,

$$w(\epsilon) = \frac{4\pi}{c} \sum_n \int_{2|\epsilon|/c}^{\infty} |A_n(\mathbf{P})|^2 \frac{PdP}{(2\pi)^3}, \quad (1)$$

where $\epsilon = E_\gamma - mc^2$, and $A_n(\mathbf{P})$ is the amplitude of annihilation for the electron orbital n . Using many-body theory, this amplitude can be represented as the following set of diagrams:

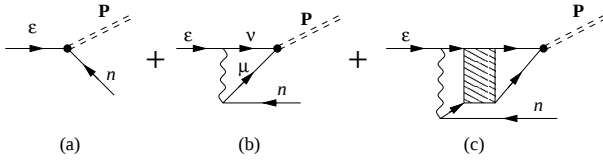


Fig. 1. ϵ is the incident positron, n is the hole, ν and μ are intermediate positron and electron states, wavy lines represent Coulomb interactions, and double dashed lines describe γ -quanta.

The shaded block in diagram (c) of Fig. 1 is the sum of the electron-positron ladder diagram series, known as the electron-positron vertex function. It is found from the linear equation [2]

$$e^+ \text{---} \text{---} e^- = \text{---} + \text{---} \text{---}$$

In the lowest order, the amplitude is given by

$$A_{\nu\epsilon}(\mathbf{P}) = \int e^{i\mathbf{P}\cdot\mathbf{r}} \psi_n(\mathbf{r}) \varphi_\epsilon(\mathbf{r}) d\mathbf{r} \equiv \langle 2\gamma\mathbf{P} | \delta | n\epsilon \rangle \quad (2)$$

where $\psi_n(\mathbf{r})$ is the wavefunction of the bound electron and $\varphi_\epsilon(\mathbf{r})$ is the wavefunction of the

positron. To obtain accurate results, we need to ensure convergence of correlation corrections (e.g., Fig. 1 (b)) with respect to the maximal angular momentum of the electron and positron intermediate states included in the calculation. In our calculations, we calculated the spectra $w(\epsilon)^{[l_{\max}]}$ for values up to $l_{\max} = 8$ and extrapolated the result according to [3],

$$w(\epsilon) = w(\epsilon)^{[l_{\max}]} + \frac{C}{l_{\max} + 1/2}, \quad (3)$$

where C is a constant.

In Fig. 2 the spectra obtained by using the 0th and 1st-order diagrams [4], (a) and (b) in Fig. 1, are compared with experimental data [1, 5].

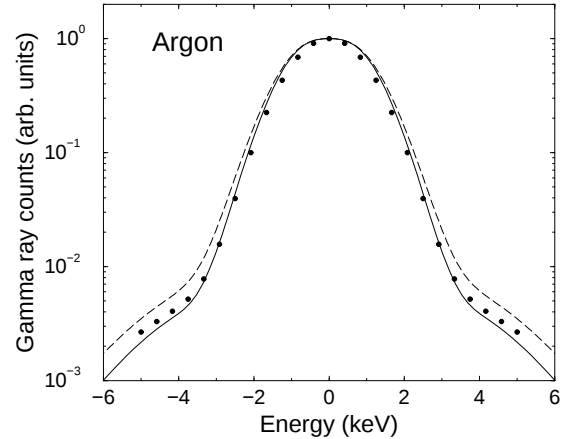


Fig. 3. Annihilation spectra for Ar normalised to unity at $\epsilon = 0$: dashed curve, 0th-order diagram, Fig. 1 (a); solid curve, 0th and 1st-order diagrams, Fig. 1 (a), (b); solid circles, experiment [1, 5].

References

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