Bethe Logarithm Calculations

V.I. Korobov

BLTP, Joint Institute for Nuclear Research 141980, Dubna, Russia

In this contribution we would like to present a modified version of Schwartz's method [1] for the Bethe logarithm calculations. That means that we are using the standard velocity gauge formalism. Still full diagonalization is performed for a matrix of intermediate states with optimization, which provides the best value for an integral of $J(k)$ on the interval of $k \in [0;\Lambda]$. Here Λ is a cut-off parameter separating low and high energy photons.

Extrapolation procedure is improved by direct calculation of the coefficient C_3 in the asymptotic expansion

$$J(k) = \frac{1}{k}\left\langle J^2 \right\rangle - \frac{2\pi}{k^2}\sum_{i>j} z_i z_j \left[\frac{z_i}{m_i} - \frac{z_j}{m_j}\right]^2 \langle\delta(\boldsymbol{r}_{ij})\rangle$$

$$-\frac{4\pi}{k^3}\sum_{i>j} z_i^2 z_j^2 \left[\frac{z_i}{m_i} - \frac{z_j}{m_j}\right]^2 \left(\sqrt{2m_{ij}k} + z_i z_j m_{ij}\ln k + C_3\right)\langle\delta(\boldsymbol{r}_{ij})\rangle + \cdots$$

which may be expressed in term of expectation values of some singular operators, such as a distribution $\langle 1/r^4 \rangle$.

The results obtained in this way for the helium ground state

$$\beta_{\mathrm{He}} = 4.37016022306(2)$$

and for the ground state of H_2^+ molecular ion

$$\beta_{\mathrm{H}_2^+} = 3.012230334(1)$$

are the best by now. We show that one of the limitations in getting better precision is the initial state accuracy, and convergence over the basis size of the initial state has to be studied as well.

The major aim of this study is to use the ideas of this approach to improve the accuracy of calculations for the relativistic Bethe logarithms in case of the two-center problem.

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[1] C. Schwartz, Phys. Rev. 123 1700 (1961).