Dual Kinetic Balance Method in Finite Basis Set Expansions for Dirac Equation with Axial Symmetry

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The solution of the time-dependent Dirac equation is necessary to study the interaction of highly charged ions with laser fields. The use of a finite basis set to solve the Dirac equation leads generally to the appearance of so-called spurious states. It is rather difficult to separate the physical and the spurious solutions. Besides that, the latter ones can make the convergence of the numerical calculations worse. Moreover, the removing of the spurious states from the spectral expansion of the time propagator makes it be non-unitary.

The Dual Kinetic Balance (DKB) technique allows one to get rid of the spurious states occurring in finite basis set schemes for the Dirac equation. The DKB method was developed for the radial Dirac equation in Ref. [1]. In the present work this method is generalized to be employed in the case of the three-dimensional systems with the axial symmetry. In particular, we can apply this approach to the problems of the interaction between heavy ions and strong laser field, including the calculations of the probabilities of the electron-positron pair production.

The transformation of the basis set is the central part of the DKB method. It establishes the connections between the upper and the lower spinors making the bispinors have a form of the solutions of the non-relativistic limit of the Dirac equation.

Let r, θ, and φ be the spherical coordinates. $\{B_k(r)\}_{k=1}^{N_r}$ and $\{P_l(\theta)\}_{l=1}^{N_\theta}$ are the sets of the one-component basis functions. In case of four-component two-variable basis set given by

$$W_{kl}^{(u)}(r,\theta) = B_k(r)P_l(\theta)\boldsymbol{e_u}\,,\ u = 1, \dots, 4, \qquad (1)$$

where $\boldsymbol{e_u}$ are the standard four-component basis orts, we get the spurious solutions. The DKB-transformed basis set can be represented as follows:

$$W_{kl}^{(u)}(r,\theta) = \begin{pmatrix} \mathbb{I}_2 & \frac{1}{2mc}D_{m_j}^\dagger \\ \frac{1}{2mc}D_{m_j}^\dagger & \mathbb{I}_2 \end{pmatrix} B_k(r)P_l(\theta)\boldsymbol{e_u}\,,\ u = 1, \dots, 4. \qquad (2)$$

The differential operator D_{m_j} is obtained by excluding the azimuth angle φ from the Dirac equation in the spherical coordinates for particular projection m_j of the total angular momentum j.

The calculations of the spectra of H-like ions confirm that the spurious states do not appear, provided the basis (2) is employed. To demonstrate the efficiency of the DKB method, the total ionization probability of the hydrogenlike tin ion (Z = 50) in the laser field is calculated as a function of the wavelength (see Figure 1). The present results are in a good agreement with the corresponding data in Ref. [2].

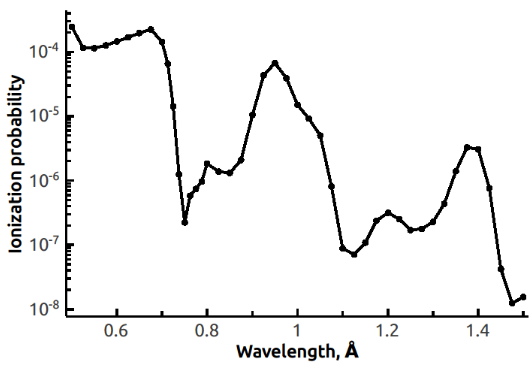

Figure 1. Ionization probability of the H-like tin ion vs. the wavelength of the laser field. The sin^2-shaped laser pulse contains 20 cycles, its peak intensity is $5 \cdot 10^{22}$ W/cm^2.

References:
[1] V. M. Shabaev *et. al.*, Phys. Rev. Lett. **93**, 130405 (2004).
[2] Yulian V. Vanne, Alejandro Saenz, Phys. Rev. A **85**, 033411 (2012).