CALCULATION OF THE DIRECT POTENTIAL IN ELECTRON-HELIUM SCATTERING USING NON-ORTHOGONAL LAGUERRE L^2 BASIS

Toto Winata and Agus Kartono*

Laboratory for Physics of Electronic Material, Physics Department,
Faculty of Mathematical and Natural Sciences,
Institut Teknologi Bandung, Jalan Ganesa 10, Bandung 40132, Indonesia.
email : twinata@bdg.centrin.net.id , toto@fi.itb.ac.id
*Physics Department, Faculty of Mathematical and Natural Sciences, Institut Pertanian Bogor,
Jalan Raya Pajajaran, Bogor 16143, Indonesia.
email : agukar@dosen.fisika.net

In this paper first we consider a helium atom in *LS* coupling configuration. We use a product of a radial function, a spherical harmonic and a spin function as a single-electron orbital function, which are used to build the two-electron basis. The radial function of the single-particle functions are of the non-orthogonal Laguerre basis [1]

$$\phi_m(r) = (\lambda r)^{l+1} \exp(-\lambda r/2) L_m^{2l+1}(\lambda r), \quad (1)$$

where the $L_m^{2l+1}(\lambda r)$ are the associated Laguerre polynomials, and m ranges from 1 to the basis size N. The two-electron functions is then written in terms of the product of these orbitals for coordinates r_1 and r_2. Here the configuration interaction coefficients $C_n^{(12)}$ satisfy the symmetry property

$$C_n^{(12)} = (-1)^{l_1+l_2-l-s} C_n^{(21)}, \quad (2)$$

to ensure antisymmetry of the two-electron system states.

The target states are obtained by diagonalizing the target Hamiltonian in an non-orthogonal Laguerre basis. The Hamiltonian formalism follows the frozen-core approximation where one of the electrons is in a fixed orbital while the second electron is described by a set of independent basis, thus permitting it to span the discrete and continuum excitations, in which all configurations have one of the electrons occupying the lowest orbital (see for example references 2, 3 and 4). Using the frozen-core approximation, we are able to produce the helium energies measured experimentally by Moore [5].

Finally, we present the calculation of the direct potential involved in electron-helium scattering by the close-coupling method. Our aim is to study and examine the convergence rates of the direct potential element by applying the non-orthogonal Laguerre with increasing basis size for electron-helium scattering.

References

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