A METHOD FOR THE PROJECTION OF ANGULAR MOMENTUM

N. Mankoč-Borštnik
Faculty of Natural Sciences and Technology and
J.Stefan Institute, University of Ljubljana,

M.V. Mihailović
J.Stefan Institute, University of Ljubljana

A method is presented for the exact projection of wave functions on states with definite angular momentum. Wave functions can be linear combination of generally non orthogonal Slater determinants. Instead of the usually used rotation operator

$$\hat{D}_R(\Omega) = e^{-i\alpha \hat{J}_z} e^{-i\vartheta \hat{J}_y} e^{-i\gamma \hat{J}_z} , \qquad (1)$$

we use the following operator

$$\hat{\Delta}_R(\Omega) = e^{-i\alpha \hat{J}_z} e^{-\vartheta \hat{J}_+} e^{\tilde{\vartheta} \hat{J}_-} e^{-i\gamma \hat{J}_z} \qquad (2)$$

Its expectation value between Slater determinants is expanded as a set of linearly independent functions

$$e^{-i\alpha M_1} e^{-i\gamma M_2} \tilde{\vartheta}^{M_3} \qquad (3)$$

When Slater determinants can be expressed in terms of functions with angular momentum $J \leq J_{max}$ $(<\infty)$ the set (3) is finite. Also the expectation value of the product of the operator (2) with any scalar or tensor operator leads to a finite set of linearly independent functions $e^{-i\alpha M1} e^{-i\gamma M2} \tilde{\vartheta}^{M3}$.

Expectation values of scalar or tensor operators between states of definite angular momentum can be obtained by solving finite systems of linear equations.

In the case when the basic functions have axial symmetry the operator (2) reduces to the operator $\hat{\Delta}'_R(\vartheta) = e^{-\vartheta J_+} e^{\tilde{\vartheta} J_-}$ and instead of the functions $e^{-i\alpha M_1} e^{-i\gamma M_2} \tilde{\vartheta}^{M_3}$ only the polynomials $\tilde{\vartheta}^{M}$ appear in the expansion set.

The method can be used in the microscopic methods like the configuration mixing method or the generator coordinate method. From the solution of the system of linear equations the expectation value of the unit operator, the hamiltonian of the system and tensors operators between states of definite angular momentum can be calculated. Then the secular equation can be solved to find the energy levels and transition probabilities.

References: N. Mankoč-Borštnik, M.V. Mihailović, to be published in 2 nd of August in Computational Physics