Multiphoton Double Ionization of Molecules

Roger Y. Bello

I. THEORETICAL FRAMEWORK

A. *J*, *K* integrals

$$J_n(\mathbf{r_1}) = \int \frac{|\phi_n(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_2 \tag{1}$$

$$\phi_n(\mathbf{r}) = \sum_i \sum_{lm} c^n_{ilm} \chi_i(r) B^m_l(\Omega) \tag{2}$$

$$J^{l_1 m_1 l_2 m_2}_{ij} = \langle B^{m_1}_{l_1}(\Omega_1)\chi_i(r_1) | J_n(\mathbf{r_1}) | B^{m_2}_{l_2}(\Omega_1)\chi_j(r_1)\rangle \tag{3}$$

$$\begin{aligned} J^{l_1 m_1 l_2 m_2}_{ij} = &\sum_{l'm'} \sum_{l''m''} \sum_{k'} \sum_{k''} c^n_{k'l'm'} c^n_{k''l''m''} \int\int \chi_{k'}(r_2)\chi_{k''}(r_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \chi_i(r_1)\chi_j(r_1) \\ &\times B^{m_1}_{l_1}(\Omega_1) B^{m_2}_{l_2}(\Omega_1) B^{m'}_{l'}(\Omega_2) B^{m''}_{l''}(\Omega_2) d\mathbf{r}_1 d\mathbf{r}_2 \end{aligned} \tag{4}$$

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = 4\pi \sum_{lm} \frac{(-1)^m}{2l+1} \frac{r^l_<}{r^{l+1}_>} Y^m_l(\Omega_1) Y^m_l(\Omega_2) \tag{5}$$

$$CJ^{lm}_{l_1 m_1 l_2 m_2} = \int B^{m_1}_{l_1}(\Omega) B^{m_2}_{l_2}(\Omega) Y^m_l(\Omega) d\Omega \tag{6}$$

$$\begin{aligned} J^{l_1 m_1 l_2 m_2}_{ij} = &\sum_{lm} \sum_{l'm'} \sum_{l''m''} \sum_{k'} \sum_{k''} c^n_{k'l'm'} c^n_{k''l''m''} \int\int 4\pi \frac{(-1)^m}{2l+1} \chi_{k'}(r_2)\chi_{k''}(r_2) \frac{r^l_<}{r^{l+1}_>} \chi_i(r_1)\chi_j(r_1) \\ &\times CJ^{lm}_{l_1 m_1 l_2 m_2} CJ^{lm}_{l'm'l''m''} dr_1 dr_2 \end{aligned} \tag{7}$$

$$J^{l_1 m_1 l_2 m_2}_{ij} = \sum_{lm} \sum_{l'm'} \sum_{l''m''} \sum_{k'} \sum_{k''} c^n_{k'l'm'} c^n_{k''l''m''} 4\pi \frac{(-1)^m}{2l+1} T^l_{ij} \delta_{ij} \delta_{k'k''} CJ^{lm}_{l_1 m_1 l_2 m_2} CJ^{lm}_{l'm'l''m''} \tag{8}$$

$$J^{l_1 m_1 l_2 m_2}_{ij} = \sum_{lm} \sum_{l'm'} \sum_{l''m''} \sum_{k'} c^n_{k'l'm'} c^n_{k'l''m''} 4\pi \frac{(-1)^m}{2l+1} T^l_{ij} \delta_{ij} CJ^{lm}_{l_1 m_1 l_2 m_2} CJ^{lm}_{l'm'l''m''} \tag{9}$$

$$K_n(\mathbf{r_1})\chi(\mathbf{r}_1) = \phi_n(\mathbf{r}_1) \int \frac{\phi_n(\mathbf{r}_2)^* \chi(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_2 \tag{10}$$

$$K^{l_1 m_1 l_2 m_2}_{ij} = \langle B^{m_1}_{l_1}(\Omega_1)\chi_i(r_1) | K_n(\mathbf{r_1}) | B^{m_2}_{l_2}(\Omega_1)\chi_j(r_1)\rangle \tag{11}$$

$$\begin{aligned} K^{l_1 m_1 l_2 m_2}_{ij} = &\sum_{l'm'} \sum_{l''m''} \sum_{k'} \sum_{k''} c^n_{k'l'm'} c^n_{k''l''m''} \int\int \chi_{k'}(r_1)\chi_{k''}(r_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \chi_i(r_1)\chi_j(r_2) \\ &\times B^{m_1}_{l_1}(\Omega_1) B^{m_2}_{l_2}(\Omega_2) B^{m'}_{l'}(\Omega_1) B^{m''}_{l''}(\Omega_2) d\mathbf{r}_1 d\mathbf{r}_2 \end{aligned} \tag{12}$$

$$K_{ij}^{l_1m_1l_2m_2} = \sum_{lm}\sum_{l'm'}\sum_{l''m''}\sum_{k'}\sum_{k''} c^n_{k'l'm'}c^n_{k''l''m''}\int\int 4\pi\frac{(-1)^m}{2l+1}\chi_{k'}(r_1)\chi_{k''}(r_2)\frac{r_<^l}{r_>^{l+1}}\chi_i(r_1)\chi_j(r_2) \times CJ^{lm}_{l_1m_1l'm'}CJ^{lm}_{l_2m_2l''m''}dr_1dr_2 \tag{13}$$

$$K_{ij}^{l_1m_1l_2m_2} = \sum_{lm}\sum_{l'm'}\sum_{l''m''}\sum_{k'}\sum_{k''} c^n_{k'l'm'}c^n_{k''l''m''}4\pi\frac{(-1)^m}{2l+1}T^l_{ij}\delta_{ik'}\delta_{jk''}CJ^{lm}_{l_1m_1l'm'}CJ^{lm}_{l_2m_2l''m''} \tag{14}$$

$$K_{ij}^{l_1m_1l_2m_2} = \sum_{lm}\sum_{l'm'}\sum_{l''m''} c^n_{il'm'}c^n_{jl''m''}4\pi\frac{(-1)^m}{2l+1}T^l_{ij}CJ^{lm}_{l_1m_1l'm'}CJ^{lm}_{l_2m_2l''m''} \tag{15}$$