R-Matrix with time-dependence for atoms in arbitrarily-polarized laser fields

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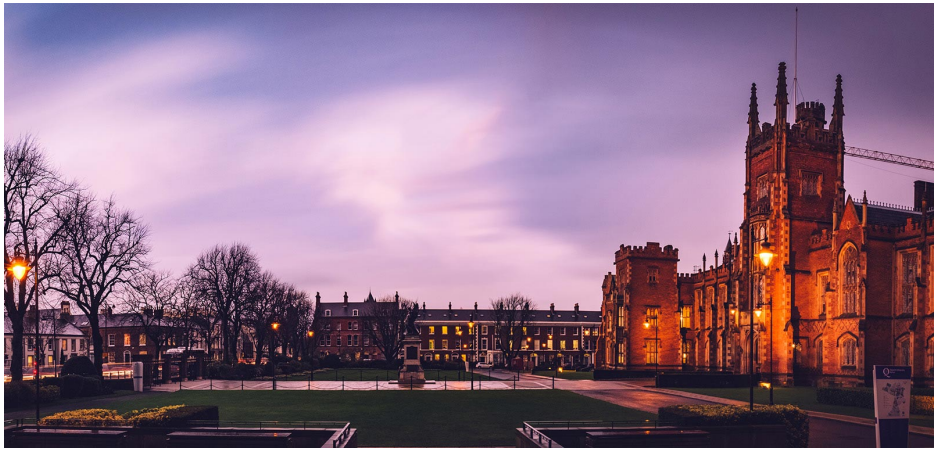

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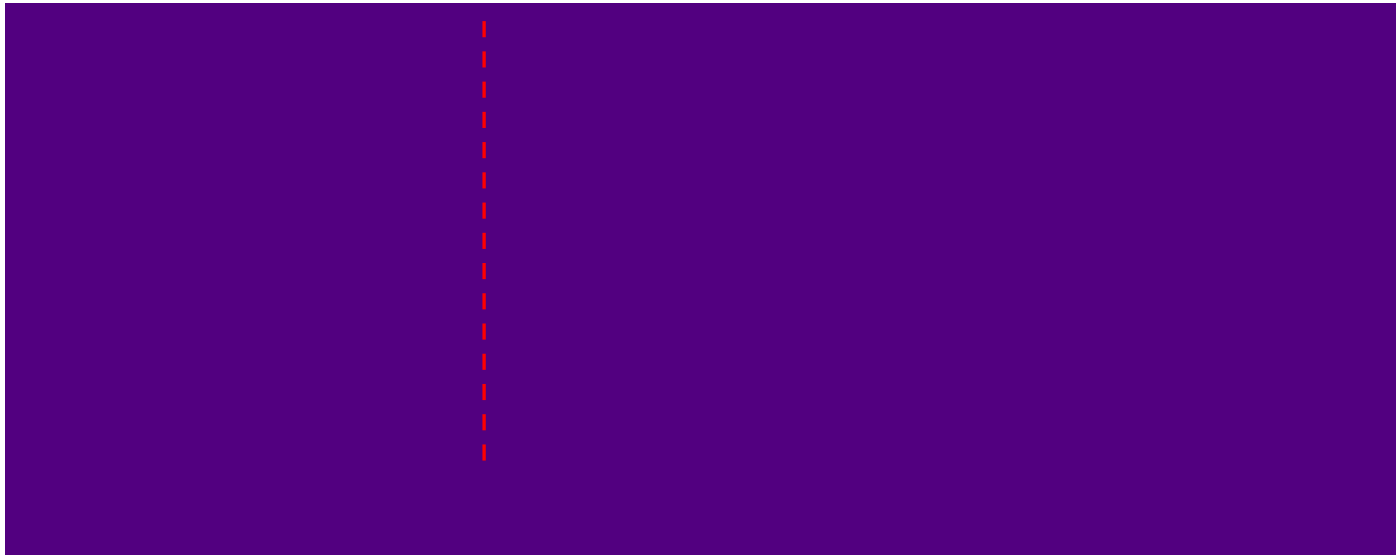
R-Matrix theory

- Division of space etc...



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Inner region

- $(N+1)$-electron wavefunction

$$\Psi(\mathbf{X}_{N+1}, t) = \sum_k C_k(t)\psi_k(\mathbf{X}_{N+1})$$

- Time-dependent coefficients given by

$$\frac{d}{dt}\mathbf{C}(t) = -i\sum_{k'}\mathbf{H}(t)\mathbf{C}(t) + i\mathbf{S}(t)$$

- For linear polarization along z-axis, dipole selection rules give $\Delta M_L = 0$, $\Delta L = \pm 1$ — dipole matrix takes the form:

$$\begin{array}{c} \begin{array}{ccccc} {}^1S^e & {}^1P^o & {}^1D^e & {}^1F^o & {}^1G^e \end{array} \\ \begin{pmatrix} & \mathrm{D} & & & \\ \mathrm{U} & & \mathrm{D} & & \\ & \mathrm{U} & & \mathrm{D} & \\ & & \mathrm{U} & & \mathrm{D} \\ & & & \mathrm{U} & \end{pmatrix} \end{array} \begin{array}{l} {}^1S^e \\ {}^1P^o \\ {}^1D^e \\ {}^1F^o \\ {}^1G^e \end{array}$$

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Dipole matrix structure ($L = 0, 1, 2$)

- For arbitrary polarization, $\Delta M_L = 0, \pm 1$, $\Delta L = 0, \pm 1$.

$^1S^e$	$^1P^e_{-1}$	$^1P^e_0$	$^1P^e_1$	$^1P^o_{-1}$	$^1P^o_0$	$^1P^o_1$	$^1D^e_{-2}$	$^1D^e_{-1}$	$^1D^e_0$	$^1D^e_1$	$^1D^e_2$	$^1D^o_{-2}$	$^1D^o_{-1}$	$^1D^o_0$	$^1D^o_1$	$^1D^o_2$	
				D	D	D											$^1S^e$
				S	S							D	D	D			$^1P^e_{-1}$
				S		S							D	D	D		$^1P^e_0$
					S	S								D	D	D	$^1P^e_1$
U	S	S					D	D	D								$^1P^o_{-1}$
U	S		S					D	D	D							$^1P^o_0$
U		S	S						D	D	D						$^1P^o_1$
				U								S	S				$^1D^e_{-2}$
				U	U							S	S	S			$^1D^e_{-1}$
				U	U	U							S		S		$^1D^e_0$
					U	U								S	S	S	$^1D^e_1$
						U									S	S	$^1D^e_2$
	U						S	S									$^1D^o_{-2}$
	U	U					S	S	S								$^1D^o_{-1}$
	U	U	U					S		S							$^1D^o_0$
		U	U						S	S	S						$^1D^o_1$
			U							S	S						$^1D^o_2$

Challenges

- Symmetry blocks spread over large number of cores — at least one core per symmetry block.
- For z-axis polarization, number of $LS\Pi$ symmetry blocks is

$$N_{LS\Pi} = 2\left(L_{\max} + 1\right).$$

- For arbitrary polarization, number of $LM_LS\Pi$ symmetry blocks is

$$N_{LM_LS\Pi} = 2\left(L_{\max} + 1\right)^2.$$

- For strong-field problems, $L_{\max} \gg 10$ is typical.
- Large increase in number of cores allocated to inner region alone.

Outer region

- $(N+1)$-electron wavefunction

$$\Psi(\mathbf{X}_{N+1},t)=\sum_p \overline{\Phi}_p(\mathbf{X}_N,\hat{r}_{N+1},\sigma_{N+1})\frac{1}{r}f_p(r,t)$$

- Solve coupled-channels radial TDSE for outgoing electron:

$$i\frac{\partial}{\partial t}f_p(r,t)=\sum_{p'}\left\langle\overline{\Phi}_p|H|\overline{\Phi}_{p'}\right\rangle f_{p'}(r,t).$$

$$p=(\underbrace{\alpha_i L_i M_{L_i} S_i \Pi_i}_{ion}\ \underbrace{l_i m_{l_i} s_i \pi_i}_{electron}\ \underbrace{L M_L S \Pi}_{ion+electron}\ )$$

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