Symbols for the Scattering Equations

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1 Wavefunction

emw: $\psi_\gamma(\tau, \vec{r}, \sigma; R_\alpha)$; full wavefunction of electron + molecule

ew: Φ; target electronic wavefunction

ewa: $\Phi_{(n\Lambda)_\gamma}(\bar{1}; R_\alpha)$

ewaa: $\Phi_\gamma(\bar{1}; R_\alpha)$

ewah: $\Phi_\gamma(2, 3; R)$

ewahs: $\Phi_\gamma(\vec{r}_2, \vec{r}_3; R)$

ewb: $\Phi_{(n\Lambda)_\gamma}(\overline{N+1}; R_\alpha)$

ewc: $\Phi_\gamma(\overline{N+1}; R_\alpha)$

ewd: ${\Phi_\gamma}^*(\overline{N+1}; R_\alpha)$

ewn: $\Phi_{(n\Lambda)_\gamma}$

ewh: ${\Phi_\gamma}^*(1, 2; R)$

ewhs: ${\Phi_\gamma}^*(\vec{r}_1, \vec{r}_2; R)$

ewt: $\Phi_{(n\Lambda)_\gamma}(\tau; R_\alpha)$

mw: $\mathbf{X}$; molecular wavefunction

mwg: $\mathbf{X}_{\gamma'}(1, 2, \cdots, N; R_\alpha)$

mwga: $\mathbf{X}_{\gamma'}(1, 2, \cdots, i-1, i+1, \cdots, N+1; R_\alpha)$

mwgb: $\mathbf{X}_{\gamma'}(\bar{i}; R_\alpha)$; convenient denotation of mwga

mwgg: $\mathbf{X}_{\gamma''}(\overline{N+1}; R_\alpha)$

mwgn: $\mathbf{X}_{\gamma'}(\overline{N+1}; R_\alpha)$

ow: ϕ; orbital wavefunction

owa: ϕ_α

scf: $\bar{F}^{\gamma}_{\gamma'}(i)$; scattering function including the spin dependence

scfa: $\bar{F}^{\gamma}_{\gamma'}(1)$

scfaa: $\bar{F}^{\gamma}_{\gamma''}(1)$

scfael: $\bar{F}^{(\gamma)}(1)$

scfb: $\bar{F}^{\gamma}_{\gamma'}(2)$

scfc: $\bar{F}^{\gamma}_{\gamma'}(3)$

scfj: $\bar{F}^{\gamma}_{\gamma'}(j)$

scfn: $\bar{F}^{\gamma}_{\gamma'}(N+1)$

sof: $F^{(\gamma)}_{\gamma'}(\vec{r}_i)$; spatial scattering function

sofn: $F^{(\gamma)}_{\gamma'}(\vec{r}_{N+1})$

sofnel: $F^{(\gamma)}(\vec{r}_{N+1})$

sow: $\bar{\phi}$; spin-orbital target wavefunction

sowa: $\bar{\phi}_\alpha$

sowb: $\bar{\phi}_\beta$

sowp: $\bar{\phi}_\pi$

srf: $\mathcal{Y}^{(\gamma)}_{\gamma'}(r)$; radial scattering function

srfn: $\mathcal{Y}^{(\gamma)}_{\ell' m'}(r_{N+1})$

srfna: $\mathcal{Y}^{(\gamma)}_{\ell' m'}(r_1)$

srfnb: $\mathcal{Y}^{(\gamma)}_{\ell'' m'}(r_{N+1})$

srfnc: $\mathcal{Y}^{(\gamma)}_{\ell'' m'}(r_1)$

srfnd: $\mathcal{Y}^{(m')}_{\ell''}(r_1)$

srfh: $\mathcal{Y}^{(m')}_{\ell' \ell_0}(r_3)$; radial scattering function of e-H_2

sshf: $\mathrm{Y}^{m_{\gamma'}}_{\ell_{\gamma'}}(\hat{r})$; angular scattering function

sshfn: $\mathrm{Y}^{m'}_{\ell'}(\hat{r}_{N+1})$

sshfna: $\mathrm{Y}^{m'}_{\ell'}(\hat{r}_1)$

sshfnb: $\mathrm{Y}_{\ell''}^{m'\,*}(\hat{r}_{N+1})$

sshfnc: $\mathrm{Y}_{\ell'}^{m'\,*}(\hat{r}_{N+1})$

sshfnd: $\mathrm{Y}_{\ell''}^{m'}(\hat{r}_1)$

sshfnh: $\mathrm{Y}_{\ell'}^{m'\,*}(\hat{r}_3)$

sw: χ; orbital spin wavefunction

swa: $\chi_{m_s}^{\alpha}(\sigma_i)$; spin wavefunction of the bound electron

swg: $\chi_{m_s}^{\gamma}(\sigma_i)$; spin wavefunction of the scattering electron

swga: $\chi_{m_s}^{\gamma'}(\sigma_{N+1})$

swgb: $\chi_{m_s}^{\gamma}(\sigma_{N+1})$

swgc: $\chi_{m_s}^{\gamma}(\sigma_1)$

swgd: $\chi_{m_s}^{\gamma\,*}(\sigma_{N+1})$

swgg: $\chi_{m_s}^{\gamma''}(\sigma_{N+1})$

swgh: $\chi_{m_s}^{\gamma\,*}(\sigma_3)$

tsw: $\bar{\delta}$; total spin wavefunction

tswh: $\bar{\delta}(\sigma_1\sigma_2)$

vw: χ; vibrational wavefunction

2 Operator

dgg: $\delta_{\gamma'\gamma''}$; Delta operator

Escr: $\mathcal{E}$;

Ham: $\hat{\mathcal{H}}$; Hamiltonian

Hscr: $\mathcal{H}$;

LC: ϵ; Levi-Civita density

lap: ∇^2; Laplace operator

Kex: $\mathrm{K}^{(m')}(\ell'\ell''|r_1 r_{N+1})$; Exchange kernel

Kexh: $\mathrm{K}^{(m')}(\ell'\ell''|r_1 r_3)$; Exchange kernel of H_2

T: $\mathbf{T}$; kinetic

Th: $\hat{\mathbf{T}}$

The: $\hat{\mathbf{T}}_e$

Ther: $\hat{\mathbf{T}}_e(\vec{r})$; kinetic operator of the scattering electron

Vint: V_{int}; potential operator between the scattering and bound electrons

vl: v_λ; single-center expansion coefficients of potential

vls: v_λ^{st}

vln: v_λ^{nuc}

vle: v_λ^{el}

vst: $\mathrm{V}^{st}_{\gamma'\gamma''}$; static potential

vstee: $\mathrm{V}^{el,st}_{\gamma''\gamma'}$

vsteea: $\mathrm{V}^{st,el}_{\gamma'\gamma''}$

vsten: $\mathrm{V}^{nuc,st}_{\gamma''\gamma'}$

vstena: $\mathrm{V}^{st,nuc}_{\gamma'\gamma''}$

vstr: $\mathrm{V}^{st}_{\gamma'\gamma''}(\vec{r}_{N+1})$

vsteer: $\mathrm{V}^{el,st}_{\gamma''\gamma'}(\vec{r}_{N+1})$

vstlm: $\mathrm{V}^{(m')}_{\ell'\ell''}$

vstrel: $\mathrm{V}_{st}(\vec{r}_{N+1})$

3 Coordinates

abp: $\alpha\beta\cdots\pi$

abpi: $\alpha_i\beta_i\cdots\pi_i$

nl: $n\Lambda$

nlg: $(n\Lambda)_\gamma$

nlv: $n\Lambda v$

nlvg: $(n\Lambda v)_\gamma$

Ra: R_α; nuclear coordinates collectively

ran: $r_{\alpha,N+1}$; distance between the scattering electron and the nuclear

rjn: $r_{j,N+1}$; distance between the scattering and the bound electrons

rln: $r_{1,N+1}$

rlh: $r_{1,3}$

vR: $\vec{R}$; spatial nuclear coordinates

vRa: $\vec{R}_\alpha$

vRb: $\vec{R}_\beta$

ver: $\vec{r}$; spatial scattering electron coordinates

vri: $\vec{r}_i$; spatial target electron coordiantes

vrj: $\vec{r}_j$

Za: Z_α; nuclear charge

Zb: Z_β