Transition Probabilities for ^{1}H in Strong Magnetic Fields

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Aim:

Computation of the dipole matrix elements

$$\boxed{\int \Psi^*(E_m)\mathbf{r}\Psi(E_n)d\mathbf{r} = \mathbf{p}}$$

General framework

Step 1. Computation of the eigenvalue(s) E **alone**, without eigenfuntions (see Balla and Benkő 1996).

Step 2. Set

$$\int_0^{z_\mathrm{c}} \int\int \Psi^*(E_m)\mathbf{r}\Psi(E_n)dxdydz = \mathbf{c}_m^{\mathrm{lT}}(z_\mathrm{c})K_{mn}^{\mathrm{l}}(z_\mathrm{c})\mathbf{c}_n^{\mathrm{l}}(z_\mathrm{c})$$

$$\int_{z_\mathrm{c}}^{\infty} \int\int \Psi^*(E_m)\mathbf{r}\Psi(E_n)dxdydz = -\,\mathbf{c}_m^{\mathrm{rT}}(z_\mathrm{c})K_{mn}^{\mathrm{r}}(z_\mathrm{c})\mathbf{c}_n^{\mathrm{r}}(z_\mathrm{c})$$

$$0 < z_\mathrm{c} < \infty$$

and compute the values of the auxiliary funtions on the right hand side. The functions are defined as:

$$\frac{dK^p_{mn}}{dz} - K^p_{mn}(Y^{p\mathrm{T}}_m Y^p_m)^{-1} Y^{p\mathrm{T}}_m \mathcal{P}_m Y^p_m -$$

$$Y^{p\mathrm{T}}_n \mathcal{P}^{\mathrm{T}}_n Y^p_n (Y^{p\mathrm{T}}_n Y^p_n)^{-1} K^p_{mn} - Y^{p\mathrm{T}}_n \mathcal{S}_2 Y^p_m = 0.$$

Here the superscripts $p = \mathrm{l}$ (left) or r (right) refer to the directions of the integrations, respectively, T denotes the transpose of a matrix. K^p_{mn} are subject to initial values

$$K^{\mathrm{l}}_{mn}(0) = 0, \qquad K^{\mathrm{r}}_{mn}(\infty) = 0.$$

That is, we get $\mathbf{p}$ by the solution of initial value problems for ODEs. The matrices $\mathcal{P}(E, z)$ and $\mathcal{S}_2(z)$ depend on the concrete pseudo-basis functions. With $q = \mathrm{l}i$, $i = \mathrm{o}(=\mathrm{odd})$, $\mathrm{e}(=\mathrm{even})$ or $q = \mathrm{r}$ $Y^q(z)$–s are the solutions of the initial value problems

$$\frac{dY^q}{dz} + \left[I_{2N} - Y^q(Y^{q\mathrm{T}}Y^q)^{-1}Y^{q\mathrm{T}}\right]\mathcal{P}Y^q = 0$$

with initial values $Y^{\mathrm{l}i}(0)$ and $Y^{\mathrm{r}}(\infty)$ and for both E_m and E_n, respectively. Next, again for both eigenvalues, let

$$\frac{dH^q}{dz} - H^q(Y^{q\mathrm{T}}Y^q)^{-1}Y^{q\mathrm{T}}\mathcal{P}Y^q -$$

$$Y^{q\mathrm{T}}\mathcal{P}^{\mathrm{T}}Y^q(Y^{q\mathrm{T}}Y^q)^{-1}H^q - Y^{q\mathrm{T}}\mathcal{J}Y^q = 0$$

$$H^{\mathrm{l}i}(0) = 0, \quad H^{\mathrm{r}}(\infty) = 0, \qquad \mathcal{J} = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}.$$

Then
$$(\mathbf{c}^{\mathrm{l}}(z_{\mathrm{c}}), \mathbf{c}^{\mathrm{r}}(z_{\mathrm{c}})) = g \cdot (V_1, V_2),$$
$$g = (V_1^{\mathrm{T}} H^{\mathrm{l}i}(z_{\mathrm{c}}) V_1 - V_2^{\mathrm{T}} H^{\mathrm{r}}(z_{\mathrm{c}}) V_2)^{-\frac{1}{2}}$$
where V_1, V_2 are solutions of
$$(Y^{\mathrm{lT}}(z_{\mathrm{c}}) Y^{\mathrm{r}}(z_{\mathrm{c}}) Y^{\mathrm{rT}}(z_{\mathrm{c}}) Y^{\mathrm{l}}(z_{\mathrm{c}}) - I) V_1 = 0,$$
$$V_2 = Y^{\mathrm{rT}}(z_{\mathrm{c}}) Y^{\mathrm{l}}(z_{\mathrm{c}}) V_1,$$
since E is an eigenvalue (computed in Step 1.),
$$det(Y^{\mathrm{l}i}(E) \mid - Y^{\mathrm{r}}(E)) = 0$$
holds.

Diamagnetic Coulomb problem

The time-independent Schrödinger equation of a hydrogen-like ion of nuclear charge Z and infinite nuclear mass is

$$\hat{H}\Psi = E\Psi,$$

Using cylindrical coordinates and atomic units $m_e = \hbar = e = 1$, $\omega = e|\mathbf{H}|/(2m_e c)$ in a homogeneous magnetic field ($\mathbf{H}$ is parallel to the axis z), the Hamiltonian takes the form

$$\hat{H}(\varrho, z) = -\frac{1}{2}\Delta + \frac{\omega n_3}{2} + \frac{\omega^2 \varrho^2}{8} - \frac{Z}{\sqrt{\varrho^2 + z^2}},$$

where $n_3 \in \mathbf{Z}$ is the magnetic quantum number, while

$$\Psi(z, \varrho, \varphi) = (2\pi)^{-1/2} \exp(\mathrm{i} n_3 \varphi) \psi(z, \varrho).$$

Thus, the eigenvalue problem is reduced to

$$\Big[\frac{\partial^2}{\partial \varrho^2} + \frac{1}{\varrho}\frac{\partial}{\partial \varrho} + \frac{\partial^2}{\partial z^2} - \frac{{n_3}^2}{\varrho^2} + \frac{2Z}{\sqrt{\varrho^2 + z^2}} - \omega^2 \varrho^2 + 2E^*\Big]\psi = 0,$$

$$0 < \varrho < \infty, \quad -\infty < z < \infty, \quad E^* = E - \omega n_3.$$

The representation

$$\psi(z, \varrho) = \sum_{n=0}^{\infty} f_n(z) \Phi_n(z, \varrho)$$

due to Liu and Starace (1987) leads to a problem depending on parameter z:

$$\Big[\frac{\partial^2}{\partial \varrho^2} + \frac{1}{\varrho}\frac{\partial}{\partial \varrho} - \frac{{n_3}^2}{\varrho^2} + \frac{2Z}{\sqrt{\varrho^2 + z^2}} - \omega^2 \varrho^2 + \mu(z)\Big]\Phi(z, \varrho) = 0,$$

$$0 < \varrho < \infty, \quad \Phi(z, \varrho) \text{ bounded w.r. to } \varrho \text{ for all } z.$$

The Liu–Starace pseudo-basis $\{\Phi_n(z,\varrho)\}_{n=0}^{\infty}$ is orthonormalized by

$$\big(\Phi_{n'}(z,\varrho),\Phi_n(z,\varrho)\big)=\int_0^{\infty}\Phi_{n'}(z,\varrho)\Phi_n(z,\varrho)\varrho d\varrho=\delta_{n'n},$$

for all z. In this case, $\{f_n(z)\}_{n=0}^{\infty}$ satisfies

$$\frac{d^2 f_n}{dz^2}+\Big[2E^*-\mu_n(z)\Big]f_n+\sum_{n'=0}^{\infty}\Big[A_{nn'}f_{n'}+B_{nn'}\frac{d\,f_{n'}}{dz}\Big]=0,$$
$$-\infty<z<\infty,\ n=0,1,\ldots,$$

where

$$A_{nn'}(z)=\Big(\Phi_n,\frac{\partial^2\Phi_{n'}}{\partial z^2}\Big),\quad B_{nn'}(z)=2\Big(\Phi_n,\frac{\partial\Phi_{n'}}{\partial z}\Big)$$

and, due to orthonormalization, $B_{nn}=0$ and $B_{nn'}=-B_{n'n}$.

For fixed N, $N=1,2,\ldots$, we investigate the eigenvalue problem

$$\frac{d^2F^N}{dz^2}+\mathcal{B}(z)\frac{dF^N}{dz}+[\mathcal{A}(z)-\mathcal{M}(z)]F^N=-2E^{*N}F^N,$$
$$-\infty<z<\infty,\quad F^N \text{ bounded};$$

$$[\mathcal{A}(z)]_{ij}=A_{i-1,j-1},\quad [\mathcal{B}(z)]_{ij}=B_{i-1,j-1},$$
$$[\mathcal{M}(z)]_{ij}=\begin{cases}0 & \text{if } i\neq j,\\ \mu_{i-1}(z) & \text{if } i=j.\end{cases}$$

The boundary conditions are

$$\text{either}\quad F^N(0)=0\quad\text{(for odd solutions) or}$$

$$F^{N\prime}(0) = 0 \quad \text{(for even solutions)}$$

and

$$F^N(z) \ \text{ bounded when } \ z \to \infty.$$

For the approximation of latter, we may use the boundary condition

$$F^{N\prime}(z_\infty) = \alpha_\infty F^N(z_\infty), \quad [\alpha_\infty]_{ij} = \begin{cases} 0 & i \neq j, \\ \mathcal{M}(\infty) - 2E^* I & i = j, \end{cases}$$

z_∞ is large.

The eigenvalue problem is formulated as a first order one

$$G' + \mathcal{P}(z, E^*) G = 0, \quad z_1 \le z \le z_\infty,$$

where

$$G = \begin{pmatrix} F^N \\ F^{N\prime} \end{pmatrix}, \quad \mathcal{P}(z, E^*) = \begin{pmatrix} 0_N & -I_N \\ \mathcal{A} - \mathcal{M} + 2E^* I_N & \mathcal{B} \end{pmatrix},$$

The solution is represented as

$$G(z) = Y^q(z) \mathbf{c}^q(z)$$

on intervals $[z_1, z_\mathrm{c})$, $(z_\mathrm{c}, z_\infty]$, respectively with $Y^q(z) \in \mathbf{R}^{2N \times N}$ $\mathbf{c}^q(z) \in \mathbf{R}^N$ and satisfy $z_1 = z_0$, $0 < z_0 \ll 1$ when $n_3 = 0$, otherwise $z_1 = 0$, z_∞ is large. q as above,

$$Y_1^{\mathrm{lo}} = \begin{pmatrix} 0_N \\ I_N \end{pmatrix}, \quad Y_1^{\mathrm{le}} = \begin{pmatrix} I_N \\ 0_N \end{pmatrix},$$

while the (normalized) right boundary condition is,

$$Y_\infty^{\mathrm{r}} = \begin{pmatrix} (\alpha_\infty^{\mathrm{T}} \alpha_\infty + I_N)^{-1/2} \\ \alpha_\infty (\alpha_\infty^{\mathrm{T}} \alpha_\infty + I_N)^{-1/2} \end{pmatrix}.$$