Quasicrossings of the energy terms in the two-Coulomb-centre problem

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Outline

- Relevance for the adiabatic theory of atom collisions and the unclearness of the available energy splitting formulas
- The wave functions of Z_1eZ_2 system
- Energy splitting: comparison of results
- Conclusions

The adiabatic approximation in atomic collision theory

In adiabatic approximation ($v_n \ll v_e$), solution of the Schrödinger equation

$$\hat{H}(\vec{R})\Psi(\vec{r},t) = i\frac{\partial\Psi}{\partial t} \tag{1}$$

is usually represented in the form

$$\Psi(\vec{r},t) = \sum_p g_p(t)\psi_p(\vec{r},R)\exp\left(-i\int^t E_p\left(R(vt')\right)dt'\right), \tag{2}$$

leading to Born-Fock equations [1] for $g_p(t)$

$$\frac{dg_p(t)}{d\tau} = {\sum_{p'}}' \left\langle \psi_p(\tau) \middle| \frac{d}{d\tau} \middle| \psi_{p'}(\tau) \right\rangle \exp\left(\frac{i}{v}\int^{\tau} \Delta E_{p\,p'}(\tau')\,d\tau'\right) g_{p'}(\tau'),$$

$$\tau = v\,t, \qquad \Delta E_{p\,p'}(\tau') = E_p(\tau) - E_{p'}(\tau),$$

The inelastic transition cross section then

$$\sigma_{pq} = 2\pi\int_0^{\infty} \lim_{t\to\infty}|g_p(t)|^2 d\rho. \tag{3}$$

[1] M. Born and V. A. Fock, Zeitschrift für Physik a Hadrons and Nuclei 51.3-4 (1928), pp. 165180.

The unclearness of the ΔE formulas

For the zeroth-order in R^{-1} approximation, different formulas for ΔE in the case of different $(Z_1 \neq Z_2)$ and equal $(Z_1 = Z_2)$ charges are available, obtained using different methods. In the simpler case of equal charges, using the Landau-Herring method, Chibisov & Janev [2] have obtained

$$\Delta E \sim R^{2n_1+2n_2+m+1} e^{-\gamma R}. \tag{4}$$

Komarov & Slavyanov [3], using the comparison equation method, have found another expression

$$\Delta E \sim R^{2n_2+m+1} e^{-\gamma R}. \tag{5}$$

[2] M. Chibisov and R. Janev, Phys. Rep. **166** (1988), pp. 1–87.
[3] I.V. Komarov and S.Yu. Slavyanov, J. Phys. B **1** (1968), pp. 1066–72

The unclearness of the ΔE formulas. Different charges

For the case of different charges ($Z_1 \neq Z_2$), one can find three formulas obtained in terms of comparison equation. They can be represented by

$$\Delta E = T\delta(n_2, n_2', m, R), \tag{6}$$

where $\delta \sim R^{n_2+n_2'+m+1}e^{-\gamma R}$ is the so-called quantum number "splitting". Komarov & Slavyanov [3], Power [4] and Ponomarev [5] proposed to determine T by different formulas

$$T_{KS} = 2\frac{(Z_2 - Z_1)^2}{(n_2' - n_2)^3}, \qquad T_{Pow} = \frac{\partial E_1}{\partial n_2} + \frac{\partial E_2}{\partial n_2'} \tag{7}$$

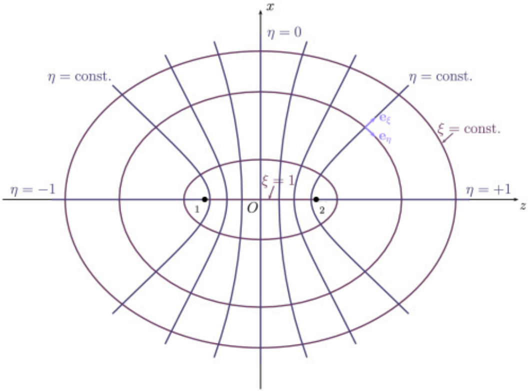
$$T_{Pon} = \frac{\partial E_1/\partial n_2}{\sqrt{1 + \frac{\partial \beta}{\partial E_1}\frac{\partial E_1}{\partial n_2}}} + \frac{\partial E_2/\partial n_2'}{\sqrt{1 - \frac{\partial \beta}{\partial E_2}\frac{\partial E_2}{\partial n_2'}}}, \qquad \beta = \frac{Z_2 - Z_1}{\gamma} \tag{8}$$

[3] I.V. Komarov and S.Yu. Slavyanov, J. Phys. B **1** (1968), pp. 1066–72
[4] J.D. Power, Phil. Trans. Roy. Soc. London. Ser. A **274** (1973), p. 663
[5] L.I. Ponomarev, Sov. Phys.–JETP **28** (1969), pp. 971–5

Important coordinate system for this problem

The prolate spheroidal coordinate system:

$$\xi = \frac{r_1 + r_2}{R}, \quad \eta = \frac{r_1 - r_2}{R}, \quad \phi = \arctan\frac{y}{x}, \tag{9}$$
$$\xi \in [1;\infty), \qquad \eta \in [-1;1], \qquad \phi \in [0;2\pi)$$



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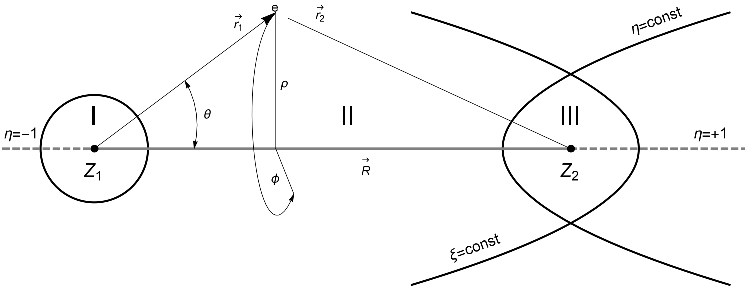

Solution of the two-Coulomb-centre problem

The wave function after the separation of variables has the form

$$\Psi\left(\vec{r}, R\right) = \frac{U\left(\xi, R\right)}{\sqrt{\xi^2 - 1}} \frac{V\left(\eta, R\right)}{\sqrt{1-\eta^2}} \frac{e^{\pm im\phi}}{\sqrt{2\pi}} = \frac{\psi\left(\xi, \eta, R\right)}{\sqrt{(\xi^2-1)(1-\eta^2)}} \frac{e^{\pm im\phi}}{\sqrt{2\pi}}. \quad (10)$$

Next, the shifted variables has been used:

$$\mu = \frac{R}{2}\left(\xi - 1\right), \quad \mu \in [0, \infty), \quad \nu = \frac{R}{2}\left(1 + \eta\right), \quad \nu \in [0, R]. \quad (11)$$

For $\mu \ll R$ (near the internuclear axis) and $\nu \ll R$ (near the left atomic core) the perturbation theory was used:

$$\psi^{pert}(\mu, \nu) = C(R)\, U^{pert}(\mu)\, V^{pert}(\nu),$$

$$U^{pert} = f^{(0)}_{n_1}(\mu) + \sum_{p=1}^{3} \sum_{k=-p}^{p} c^{(p)}_{n_1+k}(R^{-p}) f^{(0)}_{n_1+k}(\mu),$$

$$V^{pert} = f^{(0)}_{n_2}(\nu) + \sum_{p=1}^{3} \sum_{k=-p}^{p} c^{(p)}_{n_2+k}(R^{-p}) f^{(0)}_{n_2+k}(\nu),$$

$$f^{(0)}_{n_i}(x) = \left(\frac{(n_i+m)!}{n_i!(m!)^2(2n_i+m+1)}\right)^{1/2} (2\gamma x)^{(m+1)/2} e^{-\gamma x} F(-n_i,\ m+1,\ 2\gamma x).$$

Solution of the two-Coulomb-centre problem

In the internuclear region for the quasiangular part of the wave function a WKB approximation has been used ($\hbar = 1$):

$$V^{quas} = \frac{C_0}{\sqrt{q}} \exp\left[-\int_{\nu_2}^{\nu} q d\nu' + S_1 + S_2\right] \tag{12}$$

where the quasiclassical corrections S_1 and S_2 are determined by the formulae

$$S_1 = -\frac{\tilde{Z}_1}{4\gamma^3\nu^2}\left(1 + \frac{17\tilde{Z}_1}{6\gamma^2\nu}\right) + \frac{\tilde{Z}_2}{4\gamma^3(R-\nu)^2}\left(1 + \frac{17\tilde{Z}_2}{6\gamma^2(R-\nu)}\right)$$
$$+ \frac{m^2-1}{16\gamma^3}\left(\frac{1}{\nu^3} + \frac{1}{\nu^2 R} - \frac{1}{R(R-\nu)^2} - \frac{1}{(R-\nu)^3}\right) + \frac{\tilde{Z}_1\tilde{Z}_2}{2\gamma^5 R^3}\ln\frac{\nu}{R-\nu}$$
$$+ \frac{\tilde{Z}_1\tilde{Z}_2}{4\gamma^5 R}\left(\frac{3}{(R-\nu)^2} - \frac{3}{\nu^2} + \frac{1}{R}\left[\frac{1}{R-\nu} - \frac{1}{\nu}\right]\right) + C_1, \tag{13}$$

$$S_2 = \frac{\tilde{Z}_1}{4\gamma^4\nu^3} + \frac{\tilde{Z}_2}{4\gamma^4(R-\nu)^3} + C_2. \tag{14}$$

Solution of the two-Coulomb-centre problem

The final expression for two-Coulomb-centre wave function Ψ of $Z_1 e Z_2$ system has the form

$$\Psi(\vec{r}, R) = C(R) \frac{U^{pert}(\mu, R)}{\sqrt{\xi^2 - 1}} \frac{V^{quas}(\nu, R)}{\sqrt{1 - \eta^2}} \frac{e^{\pm i m \phi}}{\sqrt{2\pi}}. \qquad (15)$$

This wave function has been used to calculate the exchange energy splitting ($A_i = 2n_i + m + 1,\ A'_i = 2n'_i + m + 1$):

$$\Delta E = \oint_S \left(\Psi_I \vec{\nabla}\Psi_{II} - \Psi_{II}\vec{\nabla}\Psi_I\right) d\vec{S} = \frac{2\gamma^2(-1)^{n_2+n'_2}(2\gamma R)^{n_2+n'_2+m+1}\mathrm{e}^{-\gamma R}}{\left[n\, n'\ n_2!\,(n_2+m)!\, n'_2!\,(n'_2+m)!\right]^{1/2}} \times$$
$$\left\{1 - \frac{1}{2\gamma R}\left[\frac{A_2^2+A_2'^2}{4} + A_2 A'_2 + \frac{1-m^2}{2}\right] - \frac{A_2+A'_2}{2\gamma R} - \frac{A_1}{2\gamma^2 R}\left(\frac{Z_1}{n} + \frac{Z_2}{n'}\right)\right.$$
$$+ \frac{[A_2^2+A_2'^2+4A_2A'_2+2(1-m^2)]^2}{128\gamma^2R^2} + \frac{A_2^3+A_2'^3+(A_2A'_2-4A_1+2m^2-6)(A_2+A'_2)}{32\gamma^2R^2}$$
$$\left. + \frac{A_1(3A_1+1-m^2)}{4\gamma^2R^2} + \frac{(A_1-1)(A_2+A'_2)^2+2A_2A'_2(A_1-2)}{8\gamma^2R^2}\right\}. \qquad (16)$$

Energy splitting: comparison of results

Table: Adiabatic energy splittings ΔE at quasicrossing points R_c in the system (p, e, Z_2); $a(-b)$ stands for $a \cdot 10^{-b}$

Z_2	$(Nlm) - (N'l'm')$	R_c	ΔE	ΔE_{Pow} [4]	ΔE_{num} [6]	ΔE_B [7]
4	$(4,3,0) - (3,2,0)$	7.76	$6.66(-2)$	$6.56(-2)$	$6.94(-2)$	–
5	$(5,4,0) - (4,3,0)$	12.92	$4.07(-3)$	$6.09(-3)$	$4.25(-3)$	$4.16(-3)$
6	$(6,5,0) - (5,4,0)$	21.4	$2.40(-5)$	$3.37(-5)$	–	$2.41(-5)$
7	$(7,6,0) - (6,5,0)$	31.9	$2.06(-8)$	$2.44(-8)$	–	$2.14(-8)$
8	$(8,7,0) - (7,6,0)$	44.3	$3.04(-12)$	$4.51(-12)$	–	$2.88(-12)$

[4] J.D. Power, Phil. Trans. Roy. Soc. London. Ser. A 274, 663 (1973).
[6] I.V. Komarov and N.F. Truskova, JINR Report No. P4-11445, (1978).
[7] A.A. Bogush and V.S. Otchik, J. Phys. A 30, 559 (1997).

Conclusions

- Using fully consisted scheme, the asymptotic wave functions for the $Z_1 e Z_2$ problem has been obtained
- The energy splitting ΔE at the psedocrossing points was calculated.
- A good agreement of our results for ΔE with the numerical results has been obtained.

Thank you for attention