Variational solution of the Schrödinger equation in an inhomogeneous central field as applied to emission problems.

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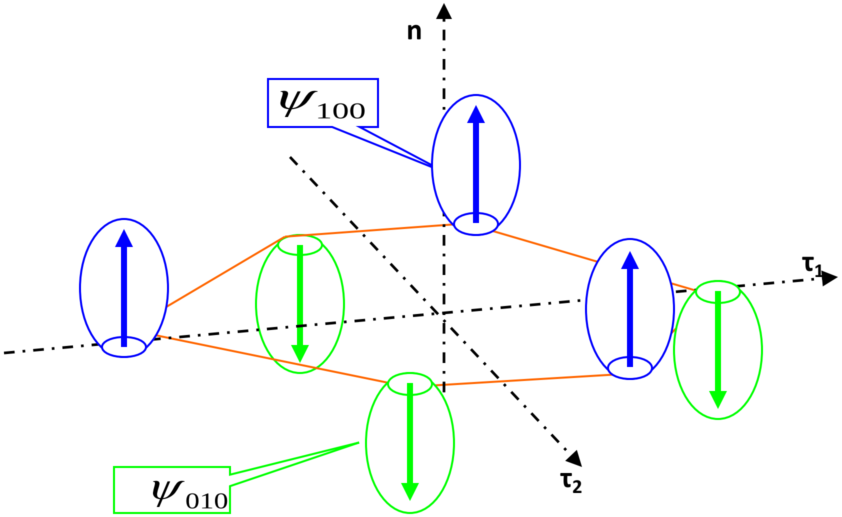
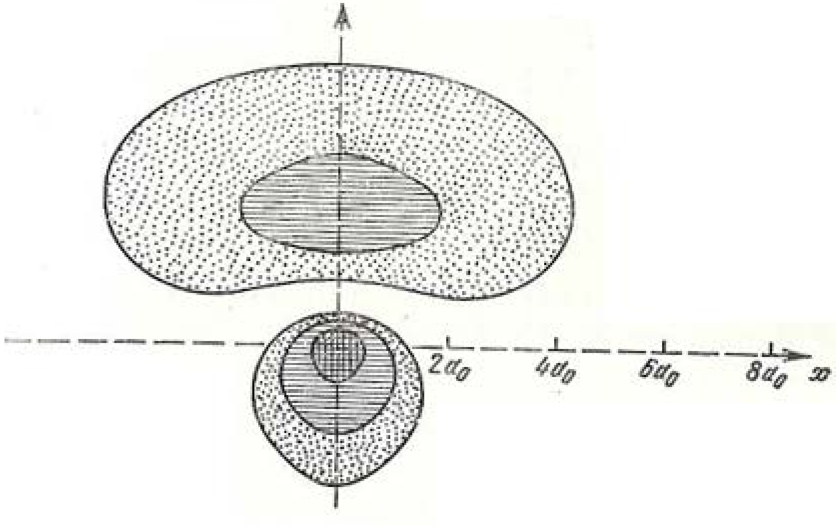




Functional for determining the effective charge for the model ion potential

$$J_1(q) = < R_s^*(x) U_i(r) R_s > \quad x = \frac{2q}{n} r$$

Hydrogen-like atom model :

$$U(\mathrm{r}) = \frac{q_{eff}}{r}$$

The operator of potential energy in a homogeneous field [W. Brandt, M. Kitagawa, Phys. Rev. B,1982,v.25,p. 5631-5637]

$$U(\mathrm{r}) = \frac{Z}{r} - \frac{Z-1}{r}\left[1 - \exp\left(-\frac{r}{\lambda}\right)\right] = \frac{1}{r} + \frac{Z-1}{r}\exp\left(-\frac{r}{\lambda}\right)$$

The functional for determining the effective charge q for a homogeneous field

$$J(q) = -\frac{q^2}{2n^2} + \int_0^\infty R_{ns}^2(r,q)V(r)r^2 dr + \frac{q^2}{n^2}$$

Variational method
[Nikiforov, Novikov, Uvarov]

$$\varepsilon_0 = \min \int \psi^* \hat{H} \psi d\xi$$

$$J(\alpha, \beta, \dots) = \int \psi^*(\xi, \alpha, \beta, \dots)\ \hat{H}\ \psi(\xi, \alpha, \beta, \dots)\ d\xi.$$

$$\frac{\partial J}{\partial \alpha} = 0, \quad \frac{\partial J}{\partial \beta} = 0, \quad \dots\ ,$$

The Brandt-Kitagawa potential is inhomogeneous in radius

$$\frac{\partial}{\partial r}U_i(r) = -\frac{U_i(r)}{r} - \frac{Z-1}{\lambda_i}\exp\left(-\frac{r}{\lambda_i}\right) \neq \chi\frac{U_i(r)}{r}$$

For the inhomogeneous field of the ion, it is necessary to take into account the full energy of the electron by using Virial theorem

$$J_2(q) = < R_s^*(x)\left[\frac{r}{2}\frac{\partial}{\partial r}U_i(r) + U_i(r)\right]R_s > \quad x = \frac{2q}{n}r$$

Objective: finding an effective uniform Coulomb field of the form

$$U(r) = -\frac{q}{r} + A \qquad \text{with ground-state energy} \qquad E_s = \frac{q^2}{2n^2}$$

Let's minimize error between full energy, found with Brandt-Kitagawa potential and homogeneous one

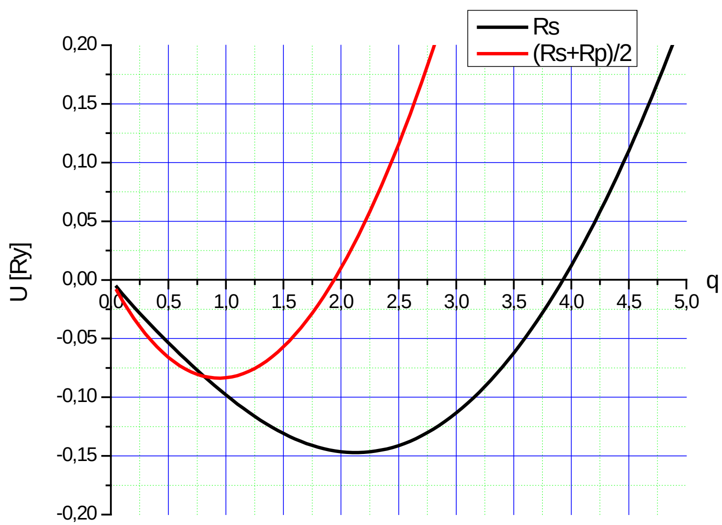
$$\frac{\partial}{\partial q}\left\{ < R_s(r)\left[\frac{r}{2}\frac{\partial}{\partial r}U_i(r) + U_i(r)\right]R_s(r) > - \frac{q^2}{2n^2}\right\} = 0$$

After solution of variation problem we can find external screening potential

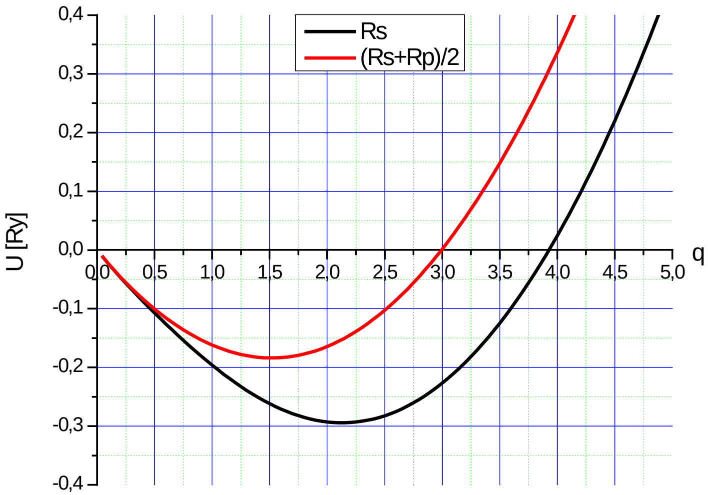
$$A = < R_s(r)\left[U_i(r) - \frac{q}{r}\right]R_s(r) >$$

Comparison of solutions of the variational problem

Average potential energy



Average full energy

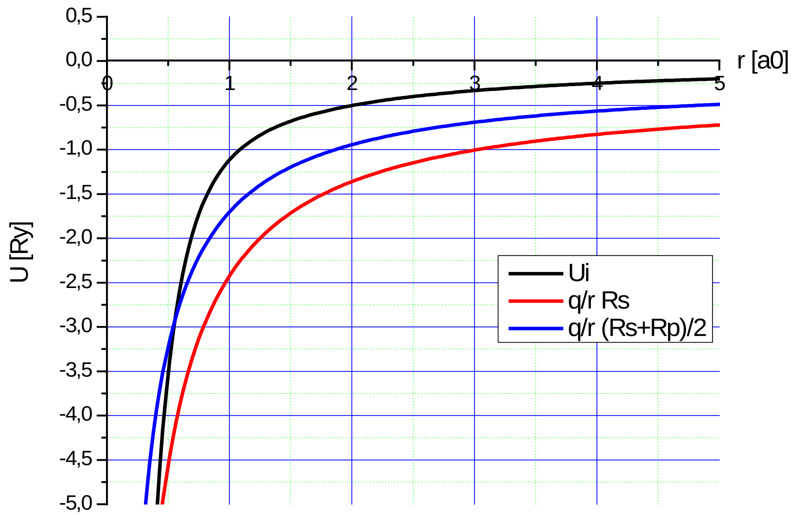


	Rs	(Rs+Rpcosθ)/2
q	2.130985	0.9417036
A	-0.1471367	-8.3710894E-02

	Rs	(Rs+Rpcosθ)/2
q	2.130985	1.519652
A	-0.2942734	-0.1839328

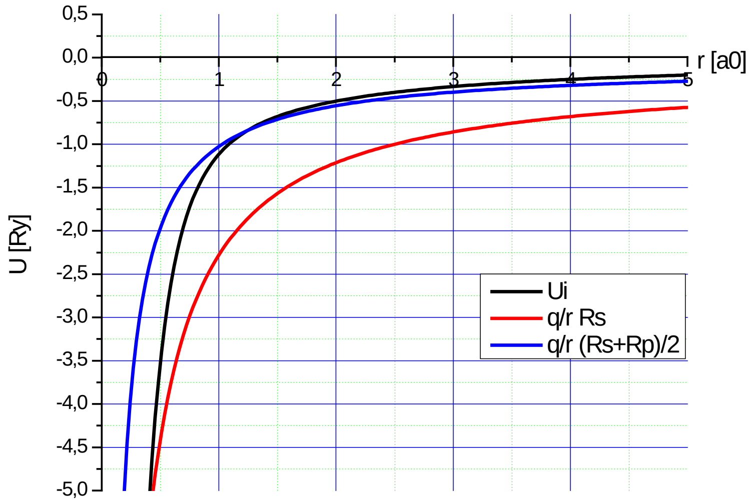
Comparison of the initial and effective fields

Average potential energy



Rs
(Rs+Rpcosθ)/2
q 2.130985 0.9417036
A -0.1471367 -8.3710894E-02

Average full energy



Rs
(Rs+Rpcosθ)/2
q 2.130985 1.519652
A -0.2942734 -0.1839328

Conclusion:

Accounting of heterogeneity allows you to specify a solution variational problem in a model of a hydrogen atom

These studies will help to build a more accurate adaptive model of the atom in the lattice, which takes into account the field of environment and external sources

The model of the hydrogen-like atom can be used to solve various problems using multiprocessor systems

Thank you for attention!