# THE PROBLEM OF THREE BODIES INTERACTING ACCORDING TO THE COULOMB LAW

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Some results are presented of a matrix-elements calculations based on the wave functions of the two-center problem, a knowledge of which permits one to approach the solution of many quantum-mechanics problems in a new way. The possibility of applying the results obtained to a description of processes involving three particles interacting according to the Coulomb law are discussed. The binding energy of the $e^+e^-e^+$ system is calculated as an example.

THE previously obtained [2] general solution of the two-center problem [1] makes possible a new approach to the solution of many problems which arise in the study of processes involving three particles interacting in accordance with Coulomb's law. In particular, it becomes possible to make practical use in such problems of the Born-Oppenheimer method [3] and also of the "method of perturbed stationary states" - using the terminology of Mott and Massey [4] [1)]. The latter is particularly important, since no method having a generality comparable to the Born method for fast-particle collisions has yet been developed in the theory of low-energy scattering of atoms.

The Hamiltonian of a system of three particles interacting in accordance with Coulomb's law is

$$\mathcal{H} = -\frac{\hbar^2}{2M_1}\Delta_{\mathbf{R}_1} - \frac{\hbar^2}{2M_2}\Delta_{\mathbf{R}_2} - \frac{\hbar^2}{2M_3}\Delta_{\mathbf{R}_3} - \frac{Z_1Z_3}{|\mathbf{R}_3-\mathbf{R}_1|} - \frac{Z_2Z_3}{|\mathbf{R}_3-\mathbf{R}_2|} + \frac{Z_1Z_2}{|\mathbf{R}_2-\mathbf{R}_1|}. \quad (1)$$

(The Hamiltonian has been written out for an interaction between one negative and two positive particles. For convenience we shall henceforth refer to the negative particle with charge $Z_3$ as an electron, and to the positive particles with charges $Z_1$ and $Z_2$ as nuclei.)

Separating the motion of the center of mass in Jacobi coordinates [5]

$$\mathfrak{R} = \frac{M_1\mathbf{R}_1 + M_2\mathbf{R}_2 + M_3\mathbf{R}_3}{M_1+M_2+M_3},$$

$$\mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1, \quad \mathbf{r} = \mathbf{R}_3 - \frac{M_1\mathbf{R}_1 + M_2\mathbf{R}_2}{M_1+M_2}, \quad (2)$$

introducing the notation

$$\frac{1}{m} = \frac{1}{M_3} + \frac{1}{M_1+M_2}, \quad \frac{1}{M} = \frac{1}{M_1} + \frac{1}{M_2} \quad \mu = M_1+M_2+M_3,$$

$$R = |\mathbf{R}_2-\mathbf{R}_1|, \quad r_1 = |\mathbf{R}_3-\mathbf{R}_1|, \quad r_2 = |\mathbf{R}_3-\mathbf{R}_2|, \quad (3)$$

and choosing measurement units in which h = m = $Z_2$ = 1, we get

$$\mathcal{H} = -\frac{1}{2\mu}\Delta_{\mathfrak{R}} + H,$$

$$H = -\frac{1}{2M}\Delta_{\mathbf{R}} + \frac{Z_1Z_2}{R} + H_0,$$

$$H_0 = -\frac{1}{2}\Delta_{\mathbf{r}} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}. \quad (4)$$

According to Born and Oppenheimer [3,4], we seek the solution of the Schrödinger equation

$$H\psi(\mathbf{R},\mathbf{r}) = \varepsilon\psi(\mathbf{R},\mathbf{r}) \quad (5)$$

in the form of an expansion

$$\psi(\mathbf{R},\mathbf{r}) = \sum_n \chi_n(\mathbf{R})\varphi_n(R;\mathbf{r}), \quad (6)$$

where $\varphi_n(R;\mathbf{r})$ are the eigenfunctions of the operator $H_0$ at a fixed value of R, and $n \equiv \{Nlm\}$ is the total set of quantum numbers for the solution of the Schrödinger equation of the two-center problem [1,2]:

$$H_0\varphi_n(R;\mathbf{r}) = E_n(R)\varphi_n(R;\mathbf{r}). \quad (7)$$

Substituting the expansion (6) in the Schrödinger equation (5), we reduce the latter to a system of equations in the following form:

[1)] In their book [4] they wrote: ". . .This method of calculating the scattering amplitudes leads to much more correct results than the earlier methods. . . However, owing to the considerable difficulty in obtaining exact perturbed functions, this method has had limited application so far. We discuss it here since we hope that it may turn out to be quite fruitful in the future."

$$-\frac{1}{2M}\Delta_R\chi_m(\mathbf{R})+\frac{1}{M}Q_{mn}(R)\nabla_R\chi_n(\mathbf{R})+\frac{1}{2M}K_{mn}(R)\times\chi_n(\mathbf{R})+\left[E_m(R)+\frac{Z_1Z_2}{R}\right]\chi_m(\mathbf{R})=\varepsilon_m\chi_m(\mathbf{R}). \quad (8)$$

Expanding the wave function $\chi_n(R)$ of the nuclear motion in terms of partial waves

$$\chi_n(\mathbf{R})=\sum_{l,m}\chi_{nkL\Lambda}(R)Y_{L\Lambda}(\theta,\Phi) \quad (9)$$

and introducing the notation $\chi_j(R)=\chi_{nkL\Lambda}(R)$, we can reduce the problem to the solution of the system of ordinary differential equations

$$-\frac{1}{R^2}\frac{d}{dR}\left(R^2\frac{d\chi_i}{dR}\right)+2Q_{ij}(R)\frac{d\chi_j}{dR}+K_{ij}(R)\chi_j+\frac{L(L+1)}{R^2}\chi_i=2M(\varepsilon_i-W_i(R))\chi_i. \quad (10)$$

In most cases of interest, the wave function $\chi_j$ of the nuclear motion does not depend on the azimuthal angle $\Phi$. Then

$$W_j(R)=W_n(R)=E_n(R)+\frac{Z_1Z_2}{R},$$

$$Q_{ij}(R)=\frac{\mathbf{R}}{R}\int d\mathbf{r}\varphi_i(\mathbf{r};R)(-\nabla_R)\varphi_j(\mathbf{r};R),$$

$$K_{ij}(R)=\int d\mathbf{r}\varphi_i(\mathbf{r};R)(-\Delta_R)\varphi_j(\mathbf{r};R), \quad (11)$$

where $i=\{N'l'm'k'L'\Lambda'\}$ and $j=\{Nlmk L\Lambda\}$. With this, as can be readily seen, in the case of a discrete spectrum ($\epsilon_i<0$) the energy of the system $\epsilon_i$ and the wave functions $\chi_i(R)$ depend on six quantum numbers, three ($Nlm$) due to the electron motion and three ($kL\Lambda$) due to the nuclear motion. For $k=L=\Lambda=0$, obviously, we have $n=i$.

We have previously described [2] an algorithm for the calculation of the wave functions $\varphi_n(R;\mathbf{r})$ and the terms $W_n(R)$ of the two-center problem, and also of the matrix elements $Q_{ij}(R)$ and $K_{ij}(R)$ in terms of these functions. Figure 1 shows the diagonal matrix elements $K_{ii}$ for the $\sigma$-terms of the system $Z_1eZ_2$ with $Z_1=Z_2=1$; as $R\to 0$ they behave like $l(l+1)/R^2$, and as $R\to\infty$ they tend to the limit $1/4n^2$, where n is the principal parabolic quantum number of the term. (For the $\sigma$-terms of the system $Z_1=Z_2=1$ we have $n=N-\mathrm{Ent}(l/2)$, where Ent(x) denotes the integer part of x [1].)

Figures 2 and 3 give an idea of the diagonal and off-diagonal matrix elements, respectively of the system $Z_1eZ_2$ with $Z_1=1$ and $Z_2=2$:

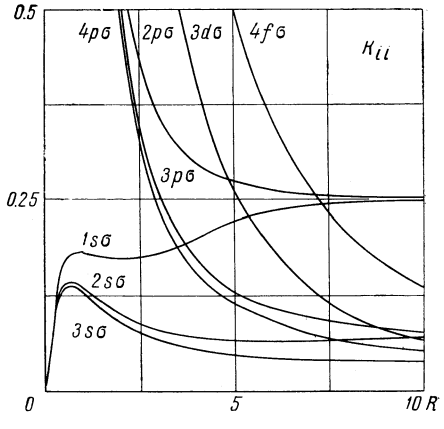


FIG. 1. Diagonal matrix elements $K_{ii}$ with respect to the wave functions $\varphi_i(R;\mathbf{r})$ of the $\sigma$-terms of the system $Z_1=Z_2=1$, $M_1=M$. $K_{ii}\approx l(l+1)/R^2$ is $R\to 0$; $K_{ii}\approx 1/4n^2$ as $R\to\infty$.

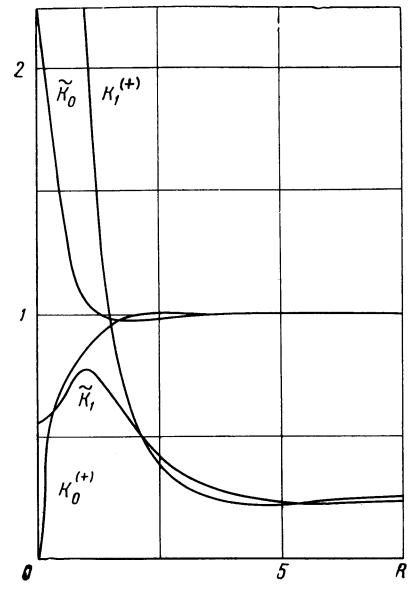


FIG. 2. Diagonal matrix elements for the $Z_1eZ_2$ system at $Z_1=1$ and $Z_2=2$. The indices 0 and 1 denote respectively the terms $1s\sigma$ and $2p\sigma$.

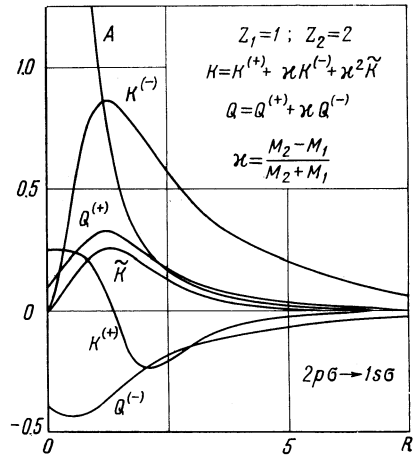


FIG. 3. Non-diagonal matrix elements $K_{ij}$ of the $Z_1eZ_2$ at $Z_1=1$ and $Z_2=2$, which describe the transitions $2p\sigma\to 1s\sigma$ in the $Z_1eZ_2$ system. The indices of the matrix elements have been omitted (for example, K stands for $K_{10}$, see Fig. 2).

$$K_{ij} = K_{ij}^{(+)} + \varkappa K_{ij}^{(-)} + \varkappa^2 \tilde{K}_{ij},$$
$$Q_{ij} = Q_{ij}^{(+)} + \varkappa Q_{ij}^{(-)}, \qquad (12)$$
$$\varkappa = (M_2 - M_1)/(M_2 + M_1),$$

where $M_1$ and $M_2$ are the masses of the nuclei with charges $Z_1$ and $Z_2$. These matrix elements describe the transitions $2p\sigma \to 1s\sigma$ and make it possible to describe, for example, collisions of $\alpha$ particles with hydrogen atoms.

## POSSIBLE APPLICATIONS

Let us point out a few problems which can now be solved, once the mathematical difficulties connected with the integration of the system (10) are overcome.

1. Problems concerning asymmetrical charge exchange of the type

$$A^+ + B \to B^+ + A, \qquad (13)$$

for the solution of which no satisfactory unified method has yet been proposed [6]. These include, in particular, the so-called transfer problem of mesoatomic physics:

$$p\mu^- + Z \to Z\mu^- + p, \qquad (14)$$

which now can be solved numerically, at least in the approximation of two interacting levels $E_m$ and $E_n$. Processes of this type accompany all experiments on weak interactions of $\mu^-$ mesons in matter, and were thoroughly investigated experimentally [7] and theoretically [8]. In the theoretical calculation of the transfer constants for the reaction (14), it was assumed that the greatest contribution to the cross section for the transfer of a $\mu^-$ meson from hydrogen to carbon and oxygen is made by the term intersections at relatively small distances between nuclei ($R \sim 10$). It follows from the earlier papers [2], however, that there are no such intersections and therefore the calculation must be repeated with allowance for the results of those papers.

2. Included in the same group are problems involving the calculation of the cross sections of mesic-molecule production during collisions:

$$p\mu^- + Z \to Z\mu^- p, \qquad (15)$$

and also the description of catalysis of nuclear reactions by $\mu^-$ mesons [5]:

$$p\mu^- + Z \to p\mu^- Z \to (Z+1) + \mu^-. \qquad (16)$$

3. So far only individual attempts [6,9] have been made to describe radiative charge-exchange processes of the type

$$p\mu^- + Z \to Z\mu^- + p + \gamma. \qquad (17)$$

Within the framework of the method of perturbed stationary states, the probability of such a process is determined by averaging, over the nuclear motion, the probabilities $A_{ij}(R)$ of the radiative transition at a fixed value of R [10]:

$$A_{ij}(R) = {}^4/_3\, \alpha^3 \omega_0 m \omega_{ij}^3 |\mathbf{r}_{ij}|^2. \qquad (18)$$

Here $\alpha$ is the fine-structure constant, $m = 207$, $\omega_0 = 4.1 \times 10^{16}$ sec$^{-1}$, $\omega_{ij} = E_i - E_j$, and $\mathbf{r}_{ij} = \int d\tau \varphi_i \mathbf{r} \varphi_j$ is the matrix element of the dipole transition between the states $E_i$ and $E_j$ of the $p\mu^- Z$ system at a fixed value of R.

The results of the earlier papers [2] make it possible to calculate the integral (18), and consequently also to calculate the process (17).

4. The quantity $A_{ij}(R)$ determines the probability of the radiative transitions in mesic molecules. Its calculation is now possible, and of interest, in connection with work on the absorption of slow $\pi^-$ meson in hydrogen-containing substances [11], and also for an explanation of the results of the latest investigations [12] of the structure of the mesic x-ray series in chemical compounds.

5. The method of perturbed stationary states can be used also to describe collisions between protons or positrons with hydrogen atoms:

$$p + H \to H^* + e,$$
$$e^+ + H \to H^* + e^+, \qquad (19)$$
$$e^+ + H \to e^+ e^- + p$$

etc., for the calculation of which other methods were used in the past.

6. In particular, this group of problems includes the calculation of the lifetime of the $\pi^-$ meson in hydrogen [13], knowledge of which is necessary in the problems of meson physics.

7. It was observed in our earlier paper [2] that highly excited states of molecular ions of the type $Z_1 e Z_2$ exist. Solving numerically the equation

$$-\frac{1}{2M}\frac{1}{R^2}\frac{d}{dR}\left(R^2 \frac{d\chi_i}{dR}\right) + \left[W_i(R) + \frac{1}{2M} K_{ii}(R)\right]\chi_i = \varepsilon_i \chi_i, \qquad (20)$$

we obtain the energies $\epsilon_i$ of these states.

## BINDING ENERGY OF THE $e^+e^-e^+$ SYSTEM

Let us use the obtained results to calculate the binding energy J of the $e^+e^-e^+$ system (or of the equivalent $e^-e^+e^-$ system. Solving Eq. (20) in the Morse-potential approximation [14], we get

$$V(R) = W_0(R) + \frac{1}{2M} K_{00}(R)$$
$$= A + De^{-2a(R-R_0)} - 2De^{-a(R-R_0)},$$

$$J = D - \frac{\omega_0}{2}\left(1 - \frac{\omega_0}{8D}\right) = D\left(1 - \frac{\omega_0}{4D}\right)^2;$$
$$\omega_0 = \sqrt{\frac{k}{M}}, \quad k = 2a^2D = V''(R_0). \tag{21}$$

When $M_1 = M_2 = M_3$ it follows from (3) that $m = 2M_1/3$, and in these units $M = 3/4$. Using the results of the calculations for $W_0(R)$ and $K_{00}(R)$, we obtain also

$$D = V(\infty) - V(R_0) = 0.154.$$
$$A = V(\infty) = -0.333, \quad a = 0.624.$$
$$R_0 = 2. \quad k = 0.12. \quad \omega_0 = 0.40. \tag{22}$$

Finally, J = 0.012 a.u. = 0.33 eV. A variational calculation gives in this case [15] J = 0.326 eV. The agreement is unexpectedly good, in view of the simplicity of the employed method, and this is one more argument in favor of the correctness of such a choice of the zeroth approximation when solving problems of this type.

Without allowance for the adiabatic corrections $K_{00}/2M$, the parameters of the Morse potential [14] are

$$D = 0.1026. \quad a = 0.6678.$$

In this case, for $M = 3/4$, we obtain $\omega_0 = 0.35$ and J = 0.0015 a.u. = 0.041 eV, which is much worse (see Fig. 4).

It is of interest to trace the dependence of the binding energy J of a three-particle system on the masses $M_i$ of the particles making up the system: J = 2.79 eV for the molecular hydrogen ion $H_2^+$ [16], J = 0.734 eV for the negative hydrogen ion $H^-$ [17], and J = 0.326 eV for the $e^+e^-e^+$ system. We note that although formally the described method is not applicable to the $H^-$ system (in this case m = 2 and $M = 1/4$), it gives nonetheless the correct order of magnitude of the binding energy J = 0.98 eV.

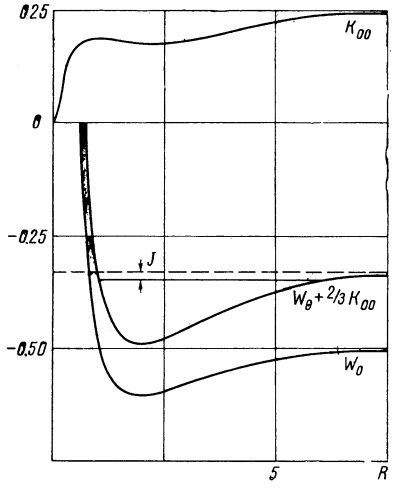


FIG. 4. Effective potentials of the $e^+e^-e^+$ system, without ($W_0$) and with ($W_0 + 2K_{00}/3$) allowance for the adiabatic corrections $K_{00}$ for the positron motion. J—binding energy of the $e^+e^-e^+$ system.

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