Semiclassical three-charged-particle system in the framework of the Pechukas self-consistent method

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(Received 30 July 1993)

To describe the rearrangement channels for three-particle atomic reactions and for three-particle muonic processes a semiclassical formalism of the Faddeev-Hahn equations is applied. The relative motion of heavy particles is treated from the classical point of view while the motion of the lighter particle is described from the quantum-mechanical point of view. To find correct trajectories of heavy particles the self-consistent Pechukas method, based on the Feynman path-integral theory, is employed.

PACS number(s): 34.10.+x, 34.20.Cf, 34.70.+e, 36.10.Gv

I. INTRODUCTION

A quantum three-charged-particle system is of a particular interest for muon-catalyzed fusion problems [1, 2], some problems of atomic and molecular physics [3], and astrophysics [4].

The well known Faddeev equations [5] are not valid for Coulomb three-body systems due to the long-range character of the Coulombic forces. That is why various alternative approaches to this problem have been developed. In this regard some attention should be given to articles [6, 7].

According to Ref. [8] three-dimensional Faddeev equations have been solved in the configuration space for some atomic and μ-mesoatomic bound states. It should be noted that great computer resources have been used in these calculations.

In the meantime, to consider some collision problems in atomic physics a semiclassical model has been employed. The motion of atomic nuclei (their masses $M_i, i = 1, 2$) has been described by classical trajectories $\vec{R}_i(t)$, while dynamics of electrons (their masses are m, $m/M_i \ll 1$) has been treated from the quantum-mechanical point. It is necessary to point out that in this approach one deals with time-dependent quantum equations.

In the case of short-range potentials, all three channels (elastic, rearrangement, and break-up) have been described in the unified manner by the time-dependent Faddeev-type equations [9]. To solve the time-dependent Faddeev-Hahn equations a modified strong-channel method has been employed for some atomic and μ-mesoatomic collisions [10].

Note that in various semiclassical models correct trajectories of heavy particles have to be taken into account. Nevertheless, to solve most of atomic problems straight-line trajectories have been chosen. It is necessary to indicate that the problem of choosing correct trajectories is of importance for low-energy collisions when the straight-line trajectories are not correct.

Revai [11] pointed out that in order to solve a trajectory problem the self-consistent Pechukas method might be used [12]. It is based on the Feynman path-integral theory.

In this work, to examine low-energy collisions for the three-charged-particle systems, a semiclassical self-consistent approach has been used in the framework of the nonstationary Faddeev-Hahn (NFH) equations [10].

This paper is organized as follows. In the next section we describe NFH equations, a method for solving them, and a brief description of the Pechukas method. In Sec. III the results of calculations for resonance charge exchange of protons on hydrogen atoms with the correct classical proton trajectories taken into account are shown. The conclusion is given in Sec. IV.

The atomic ($e = \hbar = m_e = 1$) and μ-mesoatomic ($e = \hbar = m_\mu = 1$) units are used.

II. FADDEEV-HAHN EQUATIONS AND SELF-CONSISTENT METHOD

(1) We shall examine the rearrangement reactions

$$1 + (23) \rightarrow (13) + 2 \tag{1}$$

in the framework of a semiclassical model.

Let us write down the nonstationary Faddeev equations

$$\left(i\frac{\partial}{\partial t} - \hat{H}_0 - V_{ij}\right)|\Psi_k\rangle = V_{ij}\left(|\Psi_i\rangle + |\Psi_j\rangle\right) , \tag{2}$$

$$i \neq j \neq k = 1, 2, 3 .$$

Here, $\hat{H}_0$ is the kinetic-energy operator of particles,

$$\hat{H}_0 = \hat{T}_{\vec{r}_{ij}} + \hat{T}_{\vec{R}_k} , \tag{3}$$

where $\vec{r}_{ij}$ and $\vec{R}_k$ are the Jacobi coordinates; V_{ij} are paired potentials of particle interaction; $|\Psi_k\rangle$ are the Faddeev components.

Heavy particles are numbered by a label $j = 1, 2$. We consider pure Coulomb three-body systems where the

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charge of one of the particles is of opposite sign with respect to the others. We have a specific mass relation

$$\frac{m_\alpha}{m_j} \ll 1 , \tag{4}$$

with $\alpha = 3$ being the number of a particle with the unlike charge.

According to (4) the motion of heavy particles could be treated classically, while the motion of lighter particles is described quantum mechanically. Putting $m_1 \sim m_2 \sim \infty$, we come to $\hat{T}_{\vec{R}_1} \sim \hat{T}_{\vec{R}_2} \sim 0$ and obtain the following semiclassical equations:

$$\left(i\frac{\partial}{\partial t} - \hat{T}_{\vec{r}_{23}} - V_{23} - a_{11}\right)|\Psi_1\rangle = (V_{23} - a_{22})|\Psi_2\rangle ,$$

$$\left(i\frac{\partial}{\partial t} - \hat{T}_{\vec{r}_{13}} - V_{13} - a_{22}\right)|\Psi_2\rangle = (V_{13} - a_{11})|\Psi_1\rangle , \tag{5}$$

where

$$\hat{T}_{\vec{r}_{23}} = \hat{T}_{\vec{r}_{13}} = \frac{\hat{p}^2}{2m_3}$$

is the kinetic-energy operator of a light particle, $\hat{p}$ is the momentum operator, and m_α are masses of the particles, and arbitrary operators a_{11} and a_{22} allow the construction of equations with the preset properties [10, 13, 14].

Thus, the total Hamiltonian of the system may be written in the form

$$\hat{h} = \frac{\hat{p}^2}{2m_3} + V_{13}(|\vec{r} - \vec{R}_1^t|) + V_{23}(|\vec{r} - \vec{R}_2^t|) + U(R_{12}^t)$$
$$= \hat{H}(t) + U(R_{12}^t) , \tag{6}$$

where $\vec{r}$, $\vec{R}_i$ are the coordinates of particles, $\vec{R}_{12} = \vec{R}^t = \vec{R}_1^t - \vec{R}_2^t$. $U(R^t) = V_{12}$, the constant number in the $\vec{r}$-Hilbert space. Therefore, in Eqs. (5) we can also put $V_{12} = 0$ and $\Psi_3 = 0$.

Hence, the total wave function of a three-particle system has to be presented by two components,

$$|\Psi(t)\rangle = |\Psi_1(t)\rangle + |\Psi_2(t)\rangle . \tag{7}$$

Let us assume that $a_{11} = \hat{p}^2/(2m_2)$ and $a_{22} = \hat{p}^2/(2m_1)$. Then, in the left-hand sides of NFH Eqs. (4) we obtain proper Hamiltonians of {23} and {13} atom subsystems, i.e., instead of

$$\hat{h}_j = \frac{\hat{p}^2}{2m_3} + V_j(|\vec{r} - \vec{R}_j(t)|) , \tag{8}$$

we have

$$\hat{h}'_j = \frac{\hat{p}^2}{2\mu_j} + V_j(|\vec{r} - \vec{R}_j(t)|) , \tag{9}$$

where μ_j are the reduced masses of targets $\{\alpha j\}$

$$\mu_j = \frac{m_\alpha m_j}{m_\alpha + m_j} , \tag{10}$$

the label $j = 1$ stands for the interaction pair {23} and $j = 2$ for {13}.

To solve Eqs. (5) a modified strong-channel coupling method is applied. In a regular manner we expand the wave function components over the eigenfunction of the subsystem Hamiltonian $\hat{h}'_j$

$$|\Psi_j(t)\rangle = \left(\sum + \int\right)_n C_n^j(t)|\Phi_n^j(t)\rangle \tag{11}$$

(here summation is done over the whole discrete spectrum, and integration over the whole continuous spectrum).

Functions $|\Phi_n^j(t)\rangle$ satisfy the Schrödinger equation

$$\left(i\frac{\partial}{\partial t} - \frac{\hat{p}^2}{2\mu_j} - V_j[|\vec{r} - \vec{R}_j(t)|]\right)|\Phi_n^j(t)\rangle = 0 . \tag{12}$$

It is easy to show that for the case of $\dot{\vec{R}}_j(t) = \text{const}$ [15]

$$|\Phi_n^j(t)\rangle = \exp\{i\mu_j\dot{\vec{R}}_j(t)\vec{r} - i[E_n^j - \tfrac{1}{2}\mu_j\dot{\vec{R}}_j^2(t)]t\}$$
$$\times\varphi_n^j(|\vec{r} - \vec{R}_j(t)|) , \tag{13}$$

where functions φ_n^j are defined by the following equations

$$\left[\frac{\hat{p}^2}{2\mu_j} + V_j(\vec{x})\right]\varphi_n^j(\vec{x}) = E_n^j\varphi_n^j(\vec{x}) . \tag{14}$$

Then, the initial conditions for the wave function components are written in the following way:

$$|\Psi_1(t)\rangle \sim |\Phi_{1s}^1(t)\rangle , \quad |\Psi_2(t) \sim 0 , \quad t \to -\infty , \tag{15}$$

where $|\Phi_{1s}^1\rangle$ is the ground state of the bound particles {23}.

Substituting (11) into Eqs. (5), we can obtain for the unknown expansion coefficients $C_n^j(t)$ a set of equations

$$\frac{\partial C_n^1(t)}{\partial t} = i\left(\sum + \int\right)_m M_{nm}^{12}(|\vec{R}(t)|)\gamma_{nm}^{(12)}C_m^2(t) ,$$

$$\frac{\partial C_m^2(t)}{\partial t} = i\left(\sum + \int\right)_n M_{mn}^{21}(|\vec{R}(t)|)\gamma_{nm}^{(12)*}C_n^1(t) , \tag{16}$$

where $M_{nm}^{jk}(|\vec{R}(t)|)$ are the matrix elements of the potential $V_j(|\vec{r} - \vec{R}_j(t)|)$ and channel functions, i.e.,

$$M_{nm}^{(jk)}(R_t) = \left\langle \exp\left(i\mu_j\vec{v}\vec{r} - \frac{1}{2}i\mu_j\vec{v}^2t\right)\varphi_n^j[|\vec{r} - \vec{R}_j(t)|]\middle| V_j(|\vec{r} - \vec{R}_j(t)|)\middle|\exp\left(i\mu_k\vec{v}\vec{r} - \frac{1}{2}i\mu_k\vec{v}^2t\right)\varphi_n^k[|\vec{r} - \vec{R}_k(t)|]\right\rangle , \tag{17}$$

$$\vec{v} = \frac{\partial\vec{R}(t)}{\partial t} ,$$

and

$$\gamma_{nm}^{(jk)}(t) = e^{i(E_n^j - E_m^k)t} , \quad E_n^j = -\mu_j/(2n) . \tag{18}$$

Taking into account that $m_1 \sim m_2 \gg m_\alpha$ the operators a_{11} and a_{22} may be omitted in the right sides of Eqs. (16).

In line with (15) one can write the initial conditions for the coefficients $C_n^j(t)$

$$C_n^1(t) \sim \delta_{n1} ; \quad C_n^2(t) \sim 0 , \quad t \to -\infty. \tag{19}$$

In order to obtain capture probabilities $|C_n^2(t \sim \infty)|^2$ one should solve the Cauchy problem Eqs. (16)–(19).

For the low-energy collisions (in the center-of-mass E ~1–50 eV) the relative velocity of nuclei motion is $v \ll 1$ (in atomic units). That is why the translation factor is equal to unity.

Thus, the matrix elements $M_{nm}^{(jk)}(R_t)$ are expressed in the following way:

$$M_{nm}^{(jk)}(|\vec{R}(t)|) \approx \int d^3 r \varphi_n^j[|\vec{r} - \vec{R}_j(t)|] \times V_j(|\vec{r} - \vec{R}_j(t)|)\varphi_m^k[|\vec{r} - \vec{R}_k(t)|] , \tag{20}$$

and may be calculated in the explicit way [10].

(2) Let us now apply to a classic part of the problem. Due to quantum transitions of the light particle some amount of the energy must be absorbed by a classic motion of heavy particles. That is why the state of the classic motion must be changed. In accordance with Eqs. (16)–(19), the influence of the classic relative motion upon the light particle have been taken into account. However, taking account of the reaction in the opposite direction is completely ignored. Beyond doubt this fact is of concern for the low-energy collisions, for instance, for μ-mesoatomic processes.

In order to take account of the interplay of classic and quantum freedom degrees and to determine correct classic trajectories one should employ the Pechukas self-consistent method [12]. It is based on the Feynman path-integral theory [16].

In accordance with the self-consistent approach a reduced propagator containing exact information about the reaction $\beta \to \alpha$ may be written in the form of the continual integration

$$G_{\alpha\beta}(\vec{R}_2 t_2 | \vec{R}_1 t_1) = \int_{\vec{R}_1 t_1}^{\vec{R}_2 t_2} D[\vec{R}(t)] e^{iS_0[\vec{R}(t)]/\hbar} T_{\alpha\beta}[\vec{R}(t)] , \tag{21}$$

where $S_0[\vec{R}(t)]$ is the classic action of the heavy particle motion along $\vec{R}(t)$; $T_{\alpha\beta}[\vec{R}(t)]$ are transition amplitudes used for finding a quantum particle at t_2 in the state $|\alpha\rangle$ if at t_1 it was in the state $|\beta\rangle$. Consequently, $T_{\alpha\beta}$ is related with the model which was discussed above and determined from Eqs. (16)–(19). Of course, we use a "natural" limit for defining the amplitudes, i.e., $t \to \infty$; $D[\vec{R}(t)]$ is the measure of continual integration.

One should note that the time behavior of the amplitudes $T_{\alpha\beta}$ is determined by the Hamiltonian $\hat{h}(t)$ [12]

$$\hat{h} = -\frac{\hbar^2}{2\mu}\triangle_{\vec{r}} + V_{13}(|\vec{r} - \vec{R}_1^t|) + V_{23}(|\vec{r} - \vec{R}_2^t|) + U(R_{12}^t) . \tag{22}$$

So, in accordance with the method a basic variational principle is

$$\delta(S_0[\vec{R}(t)] + \hbar \operatorname{Im} \ln T_{\alpha\beta}[\vec{R}(t)]) = 0 . \tag{23}$$

In turn, the variation of Eq. (23) gives us a classic equation of motion in the potential field $\mathcal{V}(\vec{R}(t))$ while taking into account quantum corrections [12]

$$M\frac{\partial^2 \vec{R}(t)}{\partial t^2} + \vec{\nabla}_R \mathcal{V}(\vec{R}(t)) = 0 , \tag{24}$$

$$\mathcal{V}[\vec{R}(t)] = \operatorname{Re}\frac{\langle\alpha(t,t'')|\hat{h}(t)|\beta(t,t')\rangle}{\langle\alpha(t,t'')|\beta(t,t')\rangle} , \tag{25}$$

where $|\alpha(t,t'')\rangle$ and $|\beta(t,t')\rangle$ are two solutions of the time-dependent Schrödinger equation with different boundary conditions

$$i/\hbar\frac{\partial}{\partial t}|\alpha(t,t'')\rangle = \hat{h}(t)|\alpha(t,t'')\rangle , \quad |\alpha(t'',t'')\rangle = |\alpha\rangle, \tag{26}$$

$$i/\hbar\frac{\partial}{\partial t}|\beta(t,t')\rangle = \hat{h}(t)|\beta(t,t')\rangle , \quad |\beta(t',t')\rangle = |\beta\rangle . \tag{27}$$

Then

$$T_{\alpha\beta}[\vec{R}_t] = \langle\alpha(t,t'')|\beta(t,t')\rangle . \tag{28}$$

Bearing in mind that the potential $U(R_t)$ is a constant number in the $\vec{r}$-Hilbert space [11] we can write down

$$\mathcal{V}(R_t) = U(R_t) + \mathcal{W}_{\text{quant}}(R_t) , \tag{29}$$

$$\mathcal{W}_{\text{quant}}(R_t) = \operatorname{Re}\frac{\langle\alpha(t,t'')|\hat{H}(t)|\beta(t,t')\rangle}{T_{\alpha\beta}[\vec{R}_t]} . \tag{30}$$

Thus, the problem of interplay of the classical and quantum freedom degrees has been solved in the self-consistent manner. In practice, it may be realized by iterations.

To solve a quantal part of the problem one must solve Eqs. (16)–(19) and define $C_n^2(t \to \infty)$ for some arbitrary $R^{(0)}(t)$, for example, for a Coulomb trajectory. After that a classic-quantum potential $\mathcal{V}(\vec{R}(t))$ is obtained.

To determine a trajectory $R^{(1)}(t)$ a classical formula [17] is used,

$$t = M\int_{r_m}^{R'} \frac{RdR}{\sqrt{2MR^2[E-\mathcal{V}^{(1)}(R)-J^2]}} , \tag{31}$$

where $J=\sqrt{2ME}b$; b is an impact parameter; E is an impact energy; and M is a reduced mass of the heavy particles

$$M = \frac{M_1M_2}{M_1+M_2} . \tag{32}$$

Thus, defining R_j as a function of t_j and calculating spline

$$R^{(1)}(t) = \sum_\alpha Z_{\alpha j}(t-t_j)^\alpha , \quad t_j \le t \le t_{j+1} , \tag{33}$$

we obtain $R^{(1)}(t)$ and so on.

A cross section for the reaction is determined using Refs. [12] and [17],

$$\left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{d\sigma}{d\Omega}\right)_{\rm cl} |T_{\alpha\beta}[\vec{R}(t)]|^2 , \tag{34}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\rm cl} = \frac{b(\theta)\csc(\theta)}{|d\theta/db|},$$

where the deviation angle is

$$\theta(b) = \pi - 2\int_{r_m}^{\infty} \frac{dR}{R^2\sqrt{\frac{1}{b^2}(1-\frac{V}{E})-\frac{1}{R^2}}} , \tag{35}$$

r_m is maximum of R when the root is zero.

(3) The most interesting and challenging problem in mesic atomic scattering is the isotope exchange reaction

$$(d\mu)_{1s} + t \to (t\mu)_{1s} + d , \tag{36}$$

where d and t denote hydrogen isotope nuclei deuterium and tritium, respectively, and μ is muon.

There are a lot of publications devoted to this problem, for instance, Refs. [1], [18], or [19]. By the way, the NFH Eqs. (5) were also employed in [10]. The nuclei d and t move over the straight-line trajectories. Making use of the Pechukas method one could change the trajectories so that the energy balance between classical and quantum motion would be kept. We would like to note that the isotope energy splitting in the reaction is

$$\triangle E = E_{t\mu} - E_{d\mu} = 48.042 \text{ eV} .$$

At low-energy collisions to solve the NFH equations one can make use of the two-level approximation. In expansions (11) the $1s$ state is kept only,

$$|\Psi_{d\mu}(t)\rangle \approx C_{1s}^{(d\mu)}(t)\Phi_{1s}^{(d\mu)}(|\vec{r}-\vec{R}_1^t|) , \tag{37}$$

$$|\Psi_{t\mu}(t)\rangle \approx C_{1s}^{(t\mu)}(t)\Phi_{1s}^{(t\mu)}(|\vec{r}-\vec{R}_2^t|) . \tag{38}$$

Thus, we obtain a set of two "hooked" equations for the unknown coefficients $C_{1s}^{(d\mu)}$ and $C_{1s}^{(t\mu)}$,

$$\begin{aligned} dC_{1s}^{(d\mu)}(t)/dt &= i\exp(i\varepsilon t)M_{11}^{(dt)}(R_t)C_{1s}^{(t\mu)}(t) , \\ dC_{1s}^{(t\mu)}(t)/dt &= i\exp(-i\varepsilon t)M_{11}^{(td)}(R_t)C_{1s}^{(d\mu)}(t) , \end{aligned} \tag{39}$$

with the initial conditions

$$C_{1s}^{(d\mu)}(-\infty)\sim 1 \quad \text{and} \quad C_{1s}^{(t\mu)}(-\infty)\sim 0 , \tag{40}$$

$$\varepsilon = E_{1s}^{(d\mu)} - E_{1s}^{(t\mu)}.$$

As we consider the Coulomb problem, a subsystem potential $V_j(x)$ in Eq. (12) is, of course, Coulombic. That is why the $\varphi_{1s}^j(\vec{x})$, for $n=1$ may be written in the form

$$\varphi_{1s}^j(\vec{x}) = \mu_j^{3/2}\pi^{-1/2}e^{-\mu_j x} . \tag{41}$$

Thus, the matrix elements in Eqs. (39) look like

$$\begin{aligned} M_{11}^{(dt)}(R_t) = -(\mu_1\mu_2)^{3/2}/\pi \int d^3r e^{-\mu_1|\vec{r}-\vec{R}_1(t)|} \\ \times \frac{1}{|\vec{r}-\vec{R}_1(t)|} e^{-\mu_2|\vec{r}-\vec{R}_2(t)|} , \end{aligned} \tag{42}$$

$$\begin{aligned} M_{11}^{(td)}(R_t) = -(\mu_2\mu_1)^{3/2}/\pi \int d^3r e^{-\mu_2|\vec{r}-\vec{R}_2(t)|} \\ \times \frac{1}{|\vec{r}-\vec{R}_2(t)|} e^{-\mu_1|\vec{r}-\vec{R}_1(t)|} . \end{aligned} \tag{43}$$

These integrals are analytically calculated [10] to have the form

$$\begin{aligned} M_{11}^{(dt)}(R_t) = \frac{8(\mu_1\mu_2)^{3/2}}{\mu_1^2-\mu_2^2} \\ \times \left(\frac{2\mu_2}{R_t}\frac{e^{-\mu_2R}-e^{-\mu_1R}}{\mu_2^2-\mu_1^2} + e^{-\mu_2R}\right) . \end{aligned} \tag{44}$$

Hence, to obtain $M_{11}^{(td)}$ one should do transformations $\mu_1 \to \mu_2$ and $\mu_2 \to \mu_1$ in the formula for $M_{11}^{(dt)}$.

Thus, we obtain the following result:

$$\begin{aligned} M_{11}^{(td)}(R_t) = \frac{8(\mu_2\mu_1)^{3/2}}{\mu_2^2-\mu_1^2} \\ \times \left(\frac{2\mu_1}{R_t}\frac{e^{-\mu_1R}-e^{-\mu_2R}}{\mu_1^2-\mu_2^2} + e^{-\mu_1R}\right) . \end{aligned} \tag{45}$$

As regards the quantum effective potential $\mathcal{V}(R(t))$ between deiterium and tritium one should note that the limit $t \to \infty$ for defining amplitudes is equivalent to $t = t''$. Hence, from Eq. (28) we have

$$T_{\alpha\beta}[\vec{R}_t] = \langle\alpha|\beta(t',t'')\rangle . \tag{46}$$

The quantum state $|\alpha\rangle$ falls in line with the moving $(t\mu)_{1s}$-atom wave function when $t \to \infty$,

$$|\alpha\rangle = |\Phi_{1s}^{(t\mu)}(|\vec{r}-\vec{R}_2^t|)\rangle|_{t\to\infty} . \tag{47}$$

In turn, $|\beta(t',t'')\rangle$ corresponds to the total wave function of a three-particle system,

$$\begin{aligned} |\beta(t',t'')\rangle &= |\Psi(t)\rangle|_{t\to\infty} \\ &\approx C_{1s}^{(d\mu)}(\infty)|\Phi_{1s}^{(d\mu)}(|\vec{r}-\vec{R}_1^t|)\rangle|_{t\to\infty} \\ &\quad + C_{1s}^{(t\mu)}(\infty)|\Phi_{1s}^{(t\mu)}(|\vec{r}-\vec{R}_2^t|)\rangle|_{t\to\infty} . \end{aligned} \tag{48}$$

Consequently, for the rearrengement channel the following result can be written

$$T_{\alpha\beta}[\vec{R}_t] = C_{1s}^{(t\mu)}(\infty) , \tag{49}$$

and

$$\mathcal{W}_{\rm quant}(R_t) = {\rm Re}\frac{C_{1s}^{d\mu}(\infty)}{C_{1s}^{t\mu}(\infty)}\left\{\left\langle \Phi_{1s}^{t\mu}(y)\left|\frac{\hat{p}^2}{2\mu_1}+V_1(x)\right|\Phi_{1s}^{(d\mu)}(x)\right\rangle + \langle\Phi_{1s}^{t\mu}(y)|V_2(y)|\Phi_{1s}^{(d\mu)}(x)\rangle\right\}$$
$$+{\rm Re}\left\{\left\langle \Phi_{1s}^{t\mu}(y)\left|\frac{\hat{p}^2}{2\mu_2}+V_2(y)\right|\Phi_{1s}^{(t\mu)}(y)\right\rangle + \langle\Phi_{1s}^{t\mu}(y)|V_1(x)|\Phi_{1s}^{(t\mu)}(y)\rangle\right\}\ , \tag{50}$$

where

$$\vec{y}=\vec{r}-\vec{R}_2^t\ , \quad \vec{x}=\vec{r}-\vec{R}_1^t\ .$$

Thus,

$$\mathcal{W}_{\rm quant}(R_t) = {\rm Re}\frac{C_{1s}^{(d\mu)}(\infty)}{C_{1s}^{t\mu}(\infty)}\int d^3r(\Phi_{1s}^{t\mu}(y))^*\frac{1}{y}\Phi_{1s}^{(d\mu)}(x)$$
$$-\int d^3r\left(\Phi_{1s}^{(t\mu)}(y)\right)^*\frac{1}{x}\Phi_{1s}^{(t\mu)}(y)\ . \tag{51}$$

In so far as such integrals are calculated analytically [10], we can obtain a final result

$$\mathcal{W}_{\rm quant}(R_t) = {\rm Re}\frac{C_{1s}^{(d\mu)}(\infty)}{C_{1s}^{(t\mu)}(\infty)}\exp[i(E_{1s}^{(t\mu)}-E_{1s}^{(d\mu)})t]$$
$$\times M_{11}^{td}(R_t)-\frac{1-e^{-2\mu_2 R_t}}{2R_t}\ . \tag{52}$$

III. RESONANCE CHARGE EXCHANGE OF PROTONS ON HYDROGEN ATOMS

In the preceding section a method for solving the Faddeev-Hahn equations is offered in the framework of the self-consistent approach [12].

Let us now consider the resonance charge exchange of protons on hydrogen atoms,

$$p_1+(p_2,e)_{1s}\to(p_2,e)_{1s}+p_1\ . \tag{53}$$

The proton motion is described classically while the electron dynamics is treated quantum mechanically by means of the time-dependent Faddeev-Hahn equations (5). To solve the equations the two-level approximation is employed.

In expansions (11) only the $1s$ state is kept,

$$|\Psi_1(t)\rangle \approx C_{1s}^{(1)}(t)\Phi_{1s}^{(1)}(|\vec{r}-\vec{R}_1^t|)\ , \tag{54}$$

$$|\Psi_2(t)\rangle \approx C_{1s}^{(2)}(t)\Phi_{1s}^{(2)}(|\vec{r}-\vec{R}_2^t|)\ . \tag{55}$$

Thus, we obtain a set of two "hooked" equations for the unknown coefficients $C_{1s}^{(1)}$ and $C_{1s}^{(2)}$

$$dC_{1s}^{(1)}(t)/dt = i\exp(i\varepsilon t)M_{11}^{(12)}(R_t)C_{1s}^{(2)}(t)\ ,$$
$$dC_{1s}^{(2)}(t)/dt = i\exp(-i\varepsilon t)M_{11}^{(21)}(R_t)C_{1s}^{(1)}(t)\ , \tag{56}$$

with the initial conditions

$$C_{1s}^{(1)}(-\infty)\sim 1 \quad \text{and} \quad C_{1s}^{(2)}(-\infty)\sim 0, \tag{57}$$

$$\varepsilon = E_{1s}^{(1)}-E_{1s}^{(2)}.$$

Bearing in mind that a mass of proton $m_p \gg m_e$, one can put $\varepsilon = 0$ and then for slow collisions

$$M_{11}^{(12)}(R_t) = M_{11}^{(21)}(R_t) = \exp(-R_t)(R_t+1)\ , \tag{58}$$

where

$$\vec{R}_t = \vec{R}_1^t - \vec{R}_2^t.$$

Hence, atomic units are used : $e=\hbar=m_0=1$.

Fortunately, in such a case Eqs. (56) are solved analytically and we obtain

$$C_{1s}^{(1)}(t) = \cos\left(\int_{-\infty}^{t}\exp(-R_t)(R_t+1)dt\right)\ , \tag{59}$$

$$C_{1s}^{(2)}(t) = i\sin\left(\int_{-\infty}^{t}\exp(-R_t)(R_t+1)dt\right)\ . \tag{60}$$

As a consequence of the Pechukas variational principle (23) we find that for the two-level approximation of the quantum task a correct trajectory of heavy classical particles is Coulombic.

Taking into account that

$$dt = \frac{MRdR}{\sqrt{2MR^2[E-U(R)]-J^2}}\ , \tag{61}$$

where $U(R)$ is the Coulomb potential between protons $U(R)=1/R$, for Coulombic classical scattering a cross section is [17]

$$\left(\frac{d\sigma}{d\Omega}\right)_{\rm cl} = \left(\frac{1}{4E\sin^2(\theta/2)}\right)^2. \tag{62}$$

A final result for the three-particle rearrangement cross section may be written in the following way

TABLE I. Values for cross sections of the resonance charge exchange of protons on hydrogen atoms ($\rm cm^2$), $a_0 = 0.529\times10^{-8}$ cm.

E (eV)	[20]	[21]	Present paper
1.0	4.7×10^{-15}	4.5×10^{-15}	4.5×10^{-15}
5.0		3.7×10^{-15}	3.8×10^{-15}
10.0	$40.7\pi a_0^2$		$40.2\pi a_0^2$
100.0	$29.1\pi a_0^2$		$28.6\pi a_0^2$

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4E\sin^2(\theta/2)}\right)^2 \sin^2\left(2M\int_{r_m}^{+\infty} \frac{e^{-R}R(R+1)dR}{\sqrt{2MR^2(E-1/R)-2MEb^2(\theta)}}\right), \tag{63}$$

where the impact parameter $b(\theta)$ is [17]

$$b(\theta) = \frac{\cot(\theta/2)}{2E}. \tag{64}$$

Of course, the total cross section for the exchange reaction is

$$\sigma_{ex}(E) = 2\pi\int_0^{\pi} d\theta\sin(\theta)\left(\frac{1}{4E\sin^2(\theta/2)}\right)^2 \sin^2\left(2M\int_{r_m}^{+\infty} \frac{e^{-R}R(R+1)dR}{\sqrt{2MR^2(E-1/R)-2MEb^2(\theta)}}\right). \tag{65}$$

Table I lists the results of calculations of total cross sections $\sigma_{ex}(E)$ for resonance charge exchange of protons on hydrogen atoms (53) at low energies in comparison with the results of other authors [20, 21].

IV. CONCLUSION

In conclusion, we can state that the proposed time-dependent semiclassical description of the Coulomb three-particle systems is decomposed into two one-particle tasks.

(i) A quantum task—NFH Eqs. (5) for a light particle dipped in the field of two heavy moving particles.

(ii) A classical task for determining the trajectories of heavy particles having a reduced mass M and interacting by means of the quantum potential (29) and (30).

It is necessary to point out that a self-consistent solution of these problems leads to a correct description of the three-particle scattering process, and the energy balance between classical and quantum motion in the time-dependent theory is kept.

Moreover, to calculate the total cross sections of the exchange reaction σ_{ex} and elastic scattering σ_{el} one has to integrate over the whole scattering angle θ in expressions (34), (35), or (63). As a matter of fact this method effectively takes into account the whole quantum momenta between heavy particles.

The main problem arising in solving Eqs. (5) is the number of states to be taken into account in expansion (11). It is quite reasonable to expect that for low incident energies only a few functions φ_n^j with little n values are dominated.

In addition, the pseudostates [22, 23] or Sturman representation [24] can be used to effectively take the contribution of the continuous spectra into account.

We hope that this semiclassical method could be applied to four-particle systems (two light particles and two heavy ones) in the framework of the Yakubovsky equations [25].

ACKNOWLEDGMENTS

I would like to thank the Alexander von Humboldt Foundation (Germany), which makes it possible to continue my research in Physikalisches Institut of Bonn University.

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