REARRANGEMENT AND STRIPPING IN EXACTLY SOLVABLE MODELS WITH ALLOWANCE FOR MOTION OF THE NUCLEI

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Models are considered in which a particle moves in the field of two moving zero-range potentials (ZRP). Exact wave functions of the three-dimensional problem are constructed for a special choice of the ZRP trajectories. For a one-dimensional model with two uniformly moving ZRPs, stripping and rearrangement are investigated. Oscillations of a new type in the rearrangement probability are considered. In the adiabatic approximation, a general expression is obtained for these oscillations. The results of numerical calculation are compared with the results of the adiabatic approximation.

1. Introduction

Exactly solvable models play an important role in the theory of atomic collisions. The simplest and most studied models use the method of zero-range potentials [1]. Allowance for the motion of the nuclei classically leads to problems of the theory of atomic collisions with a nonstationary Schrödinger equation for the electron wave function. In slow collisions of a negative ion with a neutral atom, the energies transferred to an electron are small, and it is therefore natural to simulate the interaction of a weakly bound electron of an ion with the core of the ion and the neutral atom by means of zero-range potentials (ZRPs). However, even the use of these potentials leads to serious difficulties when attempts are made to take into account the motion of the nuclei (moving ZRPs). Usually, the complete nonstationarity of a real problem is reduced to time-dependent parameters characterizing the depth of a ZRP, and the positions of the ZRPs are left fixed [1]. In this way, the motion of the nuclei is taken into account indirectly. Such an approach is equivalent in a certain sense to the adiabatic approximation since it does not permit one, for example, to take into account the effect of momentum transfer, which is associated with a Galileo transformation.

It would seem that the first model that realistically took into account the motion of nuclei and admitted exact solution was the one-dimensional model with two uniformly moving ZRPs considered in the series of papers [2]. An exact wave function was constructed there as a series in the multiplicity of scattering of the particle on the ZRP. For the same problem in [3], the wave function was represented in integral form. In [2], the distance R_0 of nearest approach of the ZRPs was introduced and all processes calculated in the approximation of large R_0. Of course, this precluded discussion of the interesting effects considered here. In [3], no concrete calculations were made.

In this paper, we use a method that enables us to solve not only the one- but also the three-dimensional problem of the behavior of a particle in the field of two moving ZRPs. The main idea of this method is to go over from a Hamiltonian with moving centers by means of a change of variables to a Hamiltonian in which the centers are at rest. For a specially chosen trajectory of the motion of the ZRPs, one can obtain in the new variables a Schrödinger equation analogous to the one considered in the Demkov–Osherov model [4], which is solvable by the method of contour integrals.

In the region of low velocities of the ZRP motion, we make a comparison with the exact results for the one-dimensional model with the results of the adiabatic approximation (the one-dimensionality of the Hamiltonian does not play a role in the adiabatic limit). In Sec. 3, we discuss oscillations of a new type in the rearrangement probability. In the framework of the adiabatic approximation for these oscillations, we obtain a generalization of Demkov's results [5]; it leads to good agreement with the results of exact numerical calculation.

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In Sec. 4, we construct the wave functions of the "continuous spectrum", which are used to calculate the energy distribution of the outgoing particles in the one-dimensional model. The distribution obtained has one interesting feature. When the velocity of the ionized particles is equal to the ZRP velocity, the energy distribution vanishes exactly. The physical nature of this effect is clear. Particles with this velocity remain the whole time next to the ZRPs, which leads to their resonance capture in a bound state. Such an effect cannot be so clearly expressed in the three-dimensional case because the outgoing particles are distributed over angles.

2. Three-Dimensional Model

In this section, we construct the exact wave function of a three-dimensional problem with two identical ZRPs moving in the XY plane; we specify their position by the vectors $\mathbf{R}(t)$ and $-\mathbf{R}(t)$. Naturally, this problem cannot be solved for arbitrary trajectories of the ZRPs. Moreover, the very existence of an exactly solvable three-dimensional model with moving potentials is unique. The trajectory for which one can solve the nonstationary Schrödinger equation has the form of a spiral:

$$R(t)\Phi(t)=\text{const},$$

where $\Phi(t)$ is the angle between the X axis and the vector $\mathbf{R}(t)$ and $R(t)$ and $\Phi(t)$ depend as follows on the time:

$$R(t)=-vt/2,\ \Phi(t)=\rho/vt, \tag{1}$$

where ρ is the impact parameter, and v is the relative velocity of the ZRPs as $t \to -\infty$. The case $\rho = 0$ leads to the problem of a head-on collision of two ZRPs moving with constant velocity. It is easy to show that the trajectory (1) is obtained for particles attracted in a dipole manner when the square of the angular momentum is equal to the dipole moment. Of course, great interest attaches to the model in which the ZRPs move in opposite directions along parallel straight lines. However, the approach used here leads in this case to a functional equation of the form $f(x+1)+f(x-1)=F(x)f(x)$, which cannot be solved analytically for the function $f(x)$.

The wave function $\Psi(\mathbf{r}, t)$ of a particle in the field of the ZRPs satisfies the free Schrödinger equation ($m = h = 1$)

$$-{}^1/_2\Delta_r\Psi=i\frac{\partial}{\partial t}\Psi \tag{2}$$

and boundary conditions at the points corresponding to the positions of the ZRPs [1]. We replace the spherical coordinates r, ϑ, φ, and the time t by new variables r', ϑ', φ', τ:

$$r'=r/R(t),\ \vartheta'=\vartheta,\ \varphi'=\varphi-\Phi(t),\ \tau=-4/v^2t. \tag{3}$$

We represent the wave function in the form

$$\Psi(\mathbf{r},t)=t^{-3/2}\exp\left[i\frac{r^2v}{4R(t)}\right]\chi(\mathbf{r}',\tau). \tag{4}$$

The factor $t^{-3}/2$ guarantees conservation of the normalization $\chi(\mathbf{r}', \tau)$ in the new variables, and the exponential factor is due to allowance for the effect of momentum transfer (see Sec. 5). Substituting into Eq. (2) the wave function in the form (4) and going over to new variables, we obtain, using (1), the equation

$$\hat{H}_0\chi=i\frac{\partial}{\partial\tau}\chi,\quad \hat{H}_0=-{}^1/_2\Delta_{r'}-i\frac{\rho v}{4}\frac{\partial}{\partial\varphi'}, \tag{5}$$

which is identical to the Schrödinger equation for a particle in constant magnetic field with diamagnetic term ignored. The position of the ZRPs in the new variables, $\mathbf{r}_0'$ and $-\mathbf{r}_0'$ ($|\mathbf{r}_0'| = 1$), does not depend on the time. It is convenient to include the ZRPs directly in Eq. (5) and not treat them as a boundary condition. This can be done as follows:

$$\left\{\hat{H}_0-\frac{\pi v\tau}{\alpha}\left[\hat{A}_1^*|\varphi_1\rangle\langle\varphi_1|\hat{A}_1+\hat{A}_2^*|\varphi_2\rangle\langle\varphi_2|\hat{A}_2\right]\right\}\chi=i\frac{\partial}{\partial\tau}\chi, \tag{6}$$

where

$$\hat{A}_1=\frac{\partial}{\partial|\mathbf{r}'-\mathbf{r}_0'|}|\mathbf{r}'-\mathbf{r}_0'|,\quad \hat{A}_2=\frac{\partial}{\partial|\mathbf{r}'+\mathbf{r}_0'|}|\mathbf{r}'+\mathbf{r}_0'|,\quad |\varphi_1\rangle=\delta^3(\mathbf{r}'-\mathbf{r}_0'),\ |\varphi_2\rangle=\delta^3(\mathbf{r}'+\mathbf{r}_0'),$$

$\hat{A}_i^*$ is the operator which is the Hermitian conjugate of $\hat{A}_i$. The parameter $\alpha > 0$ characterizes the

depth of the isolated ZRP in the original coordinate system $\mathbf{r}$, t and $-\alpha^2/2$ is the energy of a bound state in it. Equation (6) is essentially identical to the Schrödinger equation in the Demkov–Osherov model [4]. Because the ZRPs are identical, the parity of the wave function is conserved and $\chi(\mathbf{r}', \tau)$ can be sought in symmetric, $\chi^+(\mathbf{r}', \tau)$, or antisymmetric, $\chi^-(\mathbf{r}', \tau)$, form. With allowance for this circumstance, following [4], we obtain

$$\chi^{\pm}=N^{\pm}\int g^{\pm}(E)\hat{G}(E)\left[\hat{A}_1^{*}|\varphi_1\rangle\pm\hat{A}_2^{*}|\varphi_2\rangle\right]\exp\left\{-iE\tau+\frac{i\alpha}{\pi v}\int^{E} g^{\pm}(E')\,dE'\right\}dE,$$

$$g^{\pm}(E)=\left[\langle\varphi_1|\hat{A}_1\hat{G}(E)\hat{A}_1^{*}|\varphi_1\rangle\pm\langle\varphi_1|\hat{A}_1\hat{G}(E)\hat{A}_2^{*}|\varphi_2\rangle\right]^{-1}, \tag{7}$$

where $\hat{G}(E) = (\hat{H}_0 - E)^{-1}$ is the Green's operator and $N^{\pm}$ is a normalization factor. The Green's function for the Hamiltonian $\hat{H}_0$ is given, for example, in [6].

The problem considered above has one serious shortcoming. The ZRP trajectory is also a spiral when $t \to 0$, $R(t) \to 0$. In this connection, it is natural to reformulate the problem as follows: the ZRPs move along the trajectory (1) until a certain time $t_0 < 0$, and for $t > t_0$ the motion is along the trajectory obtained by reflection in the XY plane of the original trajectory about the straight line passing through the origin and the point $\mathbf{R}(t_0)$, i.e.,

$$R(t')=R(-t'),\ \Phi'(t')=-\Phi'(-t'),$$

where $t' = t - t_0$, $\Phi' = \Phi(t) - \Phi(t_0)$. The Hamiltonian in the coordinate system with X axis along the vector $\mathbf{R}(t_0)$ then has the following symmetry property:

$$\hat{H}(x, y, z, t')=\hat{H}(x, -y, z, -t'). \tag{8}$$

To calculate the transition probability, we use the following standard device. We take two solutions of the nonstationary Schrödinger equation, $\Psi_1(\mathbf{r}, t')$ and $\Psi_2(\mathbf{r}, t')$, satisfying the conditions

$$\lim_{t'\to\infty}\Psi_1(\mathbf{r}, t')=\varphi_1(\mathbf{r}, t'),\qquad \lim_{t'\to-\infty}\Psi_2(\mathbf{r}, t')=\varphi_2(\mathbf{r}, t').$$

The matrix element

$$w=\langle\Psi_1|\Psi_2\rangle=\int\Psi_1^{*}(\mathbf{r}, t')\,\Psi_2(\mathbf{r}, t')\,d^3\mathbf{r}$$

does not depend on the time, and $|w|^2$ [8] is the probability of transition from the state φ_1 to the state φ_2 of the limit Hamiltonian. Because of the symmetry of the Hamiltonian (8), the Schrödinger equation is satisfied by the function $\Psi_1^{*}(x, -y, z, -t')$ as well as by $\Psi_1(\mathbf{r}, t')$. This enables us to calculate the transition probability using only wave functions for which the condition is posed as $t' \to -\infty$. For $t' = 0$, the matrix element w can be written as follows:

$$w=\int\Psi_1'(x, -y, z, 0)\,\Psi_2(x, y, z, 0)\,d^3\mathbf{r}.$$

The wave function $\Psi_1'(\mathbf{r}, t')$ goes over into the function $\varphi_1(\mathbf{r}, t')$ as $t' \to -\infty$. Since the motion of the ZRPs right up to $t' = 0$ is described by formula (1), the matrix elements can be calculated by means of the wave functions of the problem solved above. For example, the rearrangement probability P and the probability of occupation of the original state, Q, have the following form:

$$P=\tfrac{1}{4}|w^{+}-w^{-}|^2,\ Q=\tfrac{1}{4}|w^{+}+w^{-}|^2,\ w^{\pm}=\int\Psi^{\pm}(x, -y, z, 0)\,\Psi^{\pm}(x, y, z, 0)\,d^3\mathbf{r}.$$

The functions $\Psi^{\pm}$ are related to the functions $\chi^{\pm}$ by Eq. (4).

3. One-Dimensional Model

In the one-dimensional case, the nonstationary Schrödinger equation [2, 3]

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}-\alpha\delta\left(x-\frac{vt}{2}\right)-\beta\delta\left(x+\frac{vt}{2}\right)\right]\Psi=i\frac{\partial}{\partial t}\Psi \tag{9}$$

can be solved exactly. In contrast to the three-dimensional problem, we can here consider the nonresonance case ($\alpha \neq \beta$). We shall not give the wave functions corresponding to arbitrary time, since the wave functions for only $t = 0$ are needed to calculate the transition probability. At $t = 0$, the function $\Psi(x, t)$, which satisfies the initial condition

$$\lim_{t\to-\infty}\Psi(x,t)=\sqrt{\beta}\exp\left\{-\beta\left|x+\frac{vt}{2}\right|+i\frac{vx}{2}+i\left(\frac{\beta^2}{2}-\frac{v^2}{8}\right)t\right\},$$

can be expressed in terms of Bessel functions:

$$\Psi(x,0)=\Gamma(1/2+i\gamma)e^{-\beta|x|}[1/2\sqrt{\gamma_1\gamma_2}e^{iv|x|}]^{1/2-i\gamma}\{i\sqrt{\alpha}e^{-ivx/2}J_{1/2-i\gamma}(\sqrt{\gamma_1\gamma_2}e^{iv|x|})+\sqrt{\beta}e^{ivx/2}J_{-1/2+i\gamma}(\sqrt{\gamma_1\gamma_2}e^{iv|x|})\}, \quad (10)$$

where $\Gamma(z)$ is the gamma function, $\gamma_1=\alpha/v$, $\gamma_2=\beta/v$, $\gamma=(\gamma_2-\gamma_1)/2$. The wave function corresponding to a bound state at the other center as $t\to-\infty$ is obtained by replacing β by α and x by $-x$ in (10). The wave function (10) can be obtained either by the method developed in Sec. 2 or by the methods used in [2, 3].

We shall consider in more detail the region of small velocities v since the transferred energies are large in the case of large v and the method of zero-range potentials becomes inapplicable [7]. The behavior of the system in this region is described by the adiabatic approximation. If $\beta > \alpha > 0$, the problem has two terms $E_1(t)$ and $E_2(t)$ (instantaneous energy levels of the Hamiltonian), which are found as roots of the equation

$$(\sqrt{-2E_i(t)}-\alpha)(\sqrt{-2E_i(t)}-\beta)=\alpha\beta\exp[-v|t|\sqrt{-2E_i(t)}\,].$$

When the centers are taken infinitely far apart, $E_1(t)\to-\alpha^2/2$, and $E_2(t)\to-\beta^2/2$. As the ZRPs approach, the term $E_2(t)$ goes downward and there are few transitions from it. The term $E_1(t)$ touches the edge of the continuum at the time $t=-t_0=(\alpha+\beta)/\alpha\beta v$ and then goes onto the unphysical sheet of the energy. For $t > t_0$, the bound state corresponding to the term $E_1(t)$ again appears and it is populated through the capture of ionized particles. The amplitude for the probability of capture of outgoing particles for this situation was calculated in the adiabatic approximation by Demkov in [8]:

$$A=-\sqrt{\pi}(4t_0^3\mu^2)^{-1/4}e^{i\pi/4}, \quad M=\left|\frac{d}{dt}\sqrt{-2E_1(t)}\right|_{t=t_0}. \quad (11)$$

In the resonance case, $(\alpha=\beta)$, the parity of the wave function is conserved and the terms $E_2(t)$ and $E_1(t)$ correspond to symmetric and antisymmetric states, respectively. Figure 1 shows the results of a numerical calculation on a BÉSM-3M computer for $\alpha=\beta=1$. Here, W_u is the probability of occupation of the antisymmetric state. The dashed curve is the probability of occupation of this state due to repeated capture calculated in accordance with Eq. (11). The discrepancy between the adiabatic approximation and the exact calculation is here greater than noted in [9]. This is due to the fact that the motion of the ZRPs was not taken into account in [8, 9]. Transitions from the term $E_2(t)$ are, as we noted above, few, and the probability of occupation of the symmetric state W_g is near unity. In the region of large velocities, the influence of the ZRPs on each other is small, and in the limit $v\to\infty$ the scattering becomes purely elastic. The oscillations in the rearrangement probability, which are given for the nonresonance case $\beta\neq\alpha=1$ in Fig. 2, and for the resonance case in Fig. 1, are due to interference between the terms $E_1(t)$ and $E_2(t)$. A difference from the previously considered situation [5] is that the state corresponding to the term $E_1(t)$ decays when $|t| < t_0$. This leads to damping of the oscillations as $v\to0$. In [5], Demkov obtained the following result for the probability of rearrangement at a small departure from resonance:

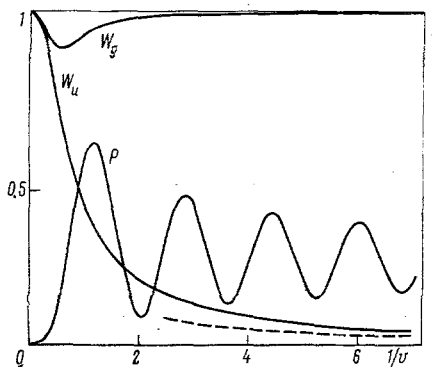

Fig. 1

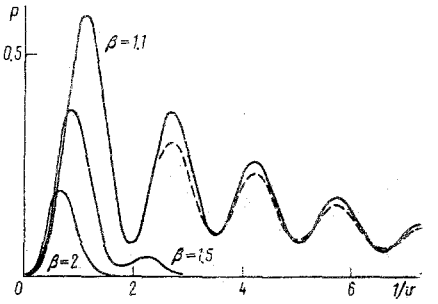

Fig. 2

$$P_{ad}=\tfrac{1}{4}\operatorname{sech}^2\left(\frac{\pi\Delta}{2v\sqrt{2J}}\right)\left|\exp\left[-i\int_{-T}^{T}E_1(t)\,dt\right]-\exp\left[-i\int_{-T}^{T}E_2(t)\,dt\right]\right|^2,\quad \Delta=\lim_{|t|\to\infty}|E_1(t)-E_2(t)|,$$

and this can be readily generalized to our case. Allowance for the decay of the upper term leads to multiplication of $\exp\left[-i\int_{-T}^{T}E_1(t)\,dt\right]$ by A, the probability amplitude of repeated capture, and after this we obtain for the rearrangement probability

$$P'_{ad}=\tfrac{1}{4}\operatorname{sech}^2\left(\frac{\pi\Delta}{2v\sqrt{2J}}\right)\left\{1+|A|^2+2|A|\cos\left[\left(\int_{-T}^{T}(E_1-E_2)\,dt\right)+\frac{5\pi}{4}\right]\right\}. \tag{12}$$

In the region $|t| < t_0$, it is necessary to set $E_1(t)$ in Eq. (12) equal to zero since the occupation of the state for $t \geq t_0$ is due to the low-energy part of the spectrum of emitted particles [8]. In [5], it was suggested that J should be taken equal to the smaller ionization potential (i.e., $J = \alpha^2/2$), but because of the form of the wave function (10) ($\Gamma(\frac{1}{2} + i\gamma)$ leads to the factor $\operatorname{sech}^2(\pi\Delta/2v\sqrt{2J})$) it can be seen that $\sqrt{2J} = (\alpha + \beta)/2$ or $\sqrt{2J} = (\sqrt{2J_1} + \sqrt{2J_2})/2$, where J_1 and J_2 are the ionization potentials of the first and the second center. The physical interpretation of Eq. (12) is simple: first, as long as the interaction between the centers is small, the system follows atomic states until the distance between the ZRPs is $R(T)$: $\sqrt{-2E_2(T)} - \sqrt{-2E_1(T)} = v$. When $R < R(T)$, the distance between the terms becomes large, there are no transitions between them, and the motion of the system takes place in accordance with the adiabatic terms $E_1(t)$ and $E_2(t)$. In Fig. 2, the dashed curve shows the rearrangement probability calculated in accordance with Eq. (12) for $\alpha = 1$ and $\beta = 1.1$. It is interesting to note that although the antisymmetric state decays almost completely (see Fig. 1) at small v, the amplitude of the oscillations in the rearrangement probability remains fairly significant. This is because the amplitude of the oscillations in the rearrangement probability is determined by the probability amplitude for capture, $A \sim \sqrt{v}$, whereas the probability of capture is $|A|^2 \sim v$. In the resonance case, $\operatorname{sech}^2(\pi\Delta/2v\sqrt{2J})=1$ and, since the antisymmetric state decays completely, $P \to \frac{1}{4}$ as $v \to 0$.

4. Energy Distribution of Outgoing Particles

The energy distribution of the outgoing particle is obtained by subtracting from the wave function $\Psi(x, t)$ as $t \to \infty$ the part corresponding to bound states at the first and the second center and projecting the remaining part of the wave function $\Psi_0(x, t)$, which describes the packet of ionized particles, onto the functions

$$\varphi_0(k, x, t)=\frac{1}{\sqrt{2\pi}}\exp\left\{ikx-i\frac{k^2}{2}t\right\}.$$

Since it is convenient to calculate the matrix elements for $t = 0$, we introduce the functions $\varphi(k, x, t)$ that satisfy the Schrödinger equation (9) and go over as $t \to \infty$ into the functions $\varphi_0(k, x, t)$. Then the matrix element $\langle\varphi|\Psi_0\rangle$ does not depend on the time and is the amplitude of the energy distribution.

We construct the functions $\varphi(k, x, t)$ for the resonance case. Here, because of conservation of parity, it is more convenient to calculate the functions $\varphi^{\pm}(k, x, t)$, which as $t \to \infty$ go over into the functions $\varphi_0^{\pm}=\tfrac{1}{2}[\varphi_0(k, x, t)\pm\varphi_0(-k, x, t)]$.

We shall seek the functions $\varphi^{\pm}$ in the form

$$\varphi^{\pm}=\Phi^{\pm}+\varphi_0^{\pm}$$

with initial condition $\Phi^{\pm} \to 0$ as $t \to \infty$. We introduce new variables $\xi = -x/vt$ and $\tau = -1/v^2t$, and for the functions $\varphi^{\pm}$ we use the representation (see Sec. 2)

$$\varphi^{\pm}=t^{-1/2}\exp\left[i\frac{x^2}{2t}\right]\chi^{\pm}(\xi, \tau).$$

The Schrödinger equation (9) then takes the form

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial\xi^2}+\frac{\alpha}{v\tau}\delta(\xi-\tfrac{1}{2})+\frac{\alpha}{v\tau}\delta(\xi+\tfrac{1}{2})\right]\chi^{\pm}=i\frac{\partial}{\partial\tau}\chi^{\pm}. \tag{13}$$

The function

$$\chi^{\pm}=\eta^{\pm}+\frac{i}{v\sqrt{2\pi\tau}}\left\{\exp\left[i\frac{|\xi+k/v|^2}{2\tau}\right]\pm\exp\left[i\frac{|\xi-k/v|^2}{2\tau}\right]\right\}$$

with

$$\eta^{\pm}=t^{1/2}\exp\left[-\frac{ix^2}{2t}\right]\Phi^{\pm}=\int_{-\infty}^{+\infty}a^{\pm}(\varkappa)\left[e^{i\varkappa|\xi+1/2|}\pm e^{i\varkappa|\xi-1/2|}\right]e^{-i\varkappa^2\tau/2}\,d\varkappa$$

satisfies Eq. (13) everywhere except at the points $\xi = \pm\frac{1}{2}$. The presence of the ZRPs at the points $\xi = \pm\frac{1}{2}$ reduces to boundary conditions, from which the functions $a^{\pm}(\varkappa)$ are determined. Integrating Eq. (13) over a small neighborhood of the point $\xi = \frac{1}{2}$, we obtain

$$\int_{-\infty}^{+\infty}\varkappa a^{\pm}(\varkappa)e^{-i\varkappa^2\tau/2}\,d\varkappa=\frac{\alpha}{v\tau}\int_{-\infty}^{+\infty}\left\{a^{\pm}(\varkappa)\left[1\pm e^{i\varkappa}\right]+\frac{1}{2\pi v}e^{i\pi/4}\left[e^{i\varkappa|k/v+1/2|}\pm e^{i\varkappa|k/v-1/2|}\right]\right\}e^{-i\varkappa^2\tau/2}\,d\varkappa. \tag{14}$$

Here, we have used the equation

$$\sqrt{2\pi i}\,\tau^{-1/2}\exp\left[i\frac{|k/v\pm 1/2|^2}{2\tau}\right]=\int_{-\infty}^{+\infty}\exp\left[-i\frac{\varkappa^2}{2}\tau+i\varkappa|k/v+1/2|\right]d\varkappa.$$

Integration over a small neighborhood of the point $\xi = -\frac{1}{2}$ leads to the same equation. After integration by parts on the right-hand side of Eq. (14) and a Fourier transformation, we obtain a first-order differential equation, from which the functions $a^{\pm}(\varkappa)$ can be readily obtained.

We give the function $\varphi^{\pm}(k, x, 0)$, which is required to calculate the energy distribution:

$$\varphi^{\pm}(k,x,0)=\frac{1}{2\sqrt{2\pi}}\left\{e^{ikx}\pm e^{-ikx}-\frac{\alpha}{v}(e^{ivx/2}\pm e^{-ivx/2})\times\right.$$

$$\left.\exp\left[i\frac{\alpha}{v}(iv|x|\pm e^{iv|x|})\right]\right\}\int_0^{|vx|}(e^{iay}\pm e^{iby})\times\exp\left[-i\frac{\alpha}{v}(iy\pm e^{iy})\right]dy.$$

where $a = |k - v/2|/v$, $b = |k + v/2|/v$. Similarly, one could obtain the functions $\varphi^{\pm}(\mathbf{k}, \mathbf{r}, t)$ of the three-dimensional problem. For a head-on collision of the ZRPs ($\rho = 0$) the functions $\varphi^{\pm}(\mathbf{k}, \mathbf{r}, 0)$ have the form

$$\varphi^{\pm}(\mathbf{k},\mathbf{r},0)=\frac{1}{2(2\pi)^{1/2}}\left\{e^{i\mathbf{kr}}\pm e^{i\mathbf{kr}}+i(e^{ivr/2}\pm e^{-ivr/2})S^{\pm}\int_0^{vr}(e^{iay}\pm e^{iby})\exp\left\{i\frac{\alpha}{v}\int_{vr}^{y}x(ix\pm e^{ix})^{-1}\,dx\right\}dy\right\},$$

where $a=|\mathbf{k}-\mathbf{v}/2|/v$, $b=|\mathbf{k}+\mathbf{v}/2|/v$, $S^{\pm}=(ivr\pm e^{ivr})^{-1}$.

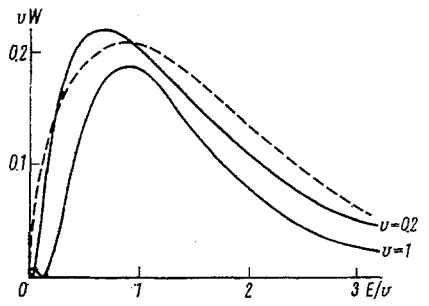

Fig. 3

In Fig. 3, we give the results of numerical calculation for the energy distribution in the one-dimensional model with $\alpha = \beta = 1$. It is interesting to note that at energy $E = v^2/8$ of the ionized particles the distribution vanishes exactly. This result is explained by the fact that at this energy the velocity of the particles is equal to the velocity of the ZRPs and because of the infinite interaction time between the particles and the ZRPs there is resonance capture into a bound state. The dashed curve shows the energy distribution calculated in the adiabatic approximation [8] for $v = 0.2$. The difference between the adiabatic approximation and the exact calculation at low energies is due to the effect of resonance capture. The difference in the behavior for large energies is explained by the fact that in [8] Demkov considered a problem in which the terms go to infinity as $t \to \infty$. In Fig. 3, we also give the energy distribution of the outgoing particles W for $v = 1$, and in the chosen scale this has a shape which differs little from the distribution for $v = 0.2$.

Conclusions

The approach used here enables us to draw some general conclusions. In [10], the problem of allowing for momentum transfer in the adiabatic approximation was considered. For the states Ψ_u and Ψ_g corresponding to the symmetric and antisymmetric terms, it was suggested that momentum transfer should be taken into account as follows: since the sum Ψ_1 and the difference Ψ_2 of the functions Ψ_u and Ψ_g go over in the resonance case into the atomic wave functions when the atoms move apart to infinity,

the adiabatic wave functions Ψ_u and Ψ_g should be replaced by the functions $\Psi^{\pm}=e^{ivr}\Psi_1 \pm e^{-ivr}\Psi_2$. On the other hand, the approach used in the present paper leads in the new variables to a problem in which the potentials are at rest, and therefore the momentum transfer effect is absent. On the transition to the new variables, the factor $\exp[ir^2v/2R(t)]$ arises in the wave function, and it is this which ensures that we obtain the correct atomic wave functions in the case of moving centers with large internuclear distances. Thus, it is natural to take into account the effect of momentum transfer for the electron functions Ψ_i corresponding to the term $E_i(t)$ by introducing this factor:

$$\Psi=\exp[ir^2v/2R(t)]\Psi_i.$$

It should however be noted that in this way one cannot take into account the part of the momentum transfer effect due to the rotation of the internuclear axis.

The three-dimensional problem considered in Sec. 2 can be used directly to calculate rearrangement and stripping processes in the collision of a negative ion A^- with a neutral atom A. Apart from these processes, the three-dimensional model can be used to study effects associated with orbiting since the choice $\Phi(t_0) = n\pi$ leads to the problem in which the centers revolve around each other n times. So far as we know, the influence of such rotation on rearrangement and stripping has not hitherto been investigated.

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