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THE EFFECTIVE ADIABATIC APPROXIMATION OF THREE-BODY PROBLEM WITH SHORT-RANGE POTENTIALS

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1 Introduction

Nonlocal and momentum-dependent potentials are known in literature as velocity-dependent potentials and applied for a phenomenological description of the interaction between nucleons [1]. A similar kind of potentials appear in the adiabatic representation of a three-body problem [2] as a result of projection onto open channels [3]. This construction is realized by a canonical transformation which is similar to the projection of solutions of the Dirac equation on large components with the use of the well-known Foldy-Wouthuysen transformation [4]. Investigation of convergence of the proposed method and construction of the effective adiabatic approximation (EAA) with correct boundary conditions are timely problems [5]. For this kind of investigations it is convenient to use the three-body problem on a line with the short-range δ-potentials [6] because this problem has an analytic solution [7]. First steps on this way have been made in paper [8]. It was shown that the adiabatic approximation (AA) gave an upper bound for the energy and a lower bound for the elastic scattering phase. However, increase in the discrepancy between the exact phase and AA phase with increasing relative momentum up to the three-body threshold was observed. This discrepancy is caused by truncation of a system of adiabatic equations and should disappear if a complete set of adiabatic functions was taken into account. Direct investigation of this problem for the infinite system of closed-coupled equations is rather cumbersome and alternative study with the help of EAA can be useful here.

In the present paper, EAA with a momentum-dependent potential is constructed for the problem of three identical particles on a line with attractive δ-function interactions. The true asymptotics of solutions of an infinite system in the adiabatic representation are built up in the framework of EAA by extracting the asymptotic energy-dependent centrifugal potential. The latter was done by using the sum rules over a complete set of the asymptotic adiabatic basis functions. The convergence of the adiabatic expansion was checked numerically by applying saturation of the corresponding sum rules. It was shown that inclusion of the nonadiabatic coupling of channels restores the true value of the elastic phase shift in the asymptotic solutions. By direct calculations with the use of EAA, the correct behavior of the phase shift with increasing relative momentum has been demonstrated and an lower bound for the energy has been obtained.

2 Hyperspherical Adiabatic Preliminaries

For three identical particles in one dimension, we first introduce the local Jacobi map in the center-of-mass system [9]

$$\eta = \left(\frac{1}{2}\right)^{1/2}(x_1 - x_2),$$

$$\xi = \left(\frac{2}{3}\right)^{1/2}\left[\left(\frac{x_1 + x_2}{2}\right) - x_3\right], \tag{1}$$

where (x_1, x_2, x_3) are the Cartesian coordinates of the particles on a line. We use hyperspherical coordinates ρ and θ that in the considered case are usual plane polar coordinates

$$\eta = \rho\cos\theta,\ \xi = \rho\sin\theta, \quad -\pi \le \theta \le \pi. \tag{2}$$

The Schrödinger equation for a partial wave function Ψ in the hyperspherical coordinates now reads

$$-\frac{\hbar^2}{2m}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right)\Psi(\rho,\theta) + (V(\rho,\theta) - E)\Psi(\rho,\theta) = 0. \tag{3}$$

Here E is the relative energy in the center of mass and $m = (m_1m_2 + m_1m_3 + m_2m_3)/(m_1+m_2+m_3)$ is the effective mass which in our case, $m_1 = m_2 = m_3 = m$, coincides with the mass m of each particle; the potential function $V(\rho,\theta)$ is defined as a sum of the pair potentials

$$V(\rho,\theta) = V\left(\sqrt{2}\rho\left|\cos\theta\right|\right) + V\left(\sqrt{2}\rho\left|\cos(\theta - 2\pi/3)\right|\right) +$$

$$V\left(\sqrt{2}\rho\left|\cos(\theta + 2\pi/3)\right|\right). \tag{4}$$

To be able to compare with the exact solvable case [7], we choose pair potentials $V(\sqrt{2}\eta) = g\delta(|\eta|)/\sqrt{2}$ as delta-functions of a finite strength, $g = c\kappa(\hbar^2/m)$ and consider the attractive case $c = -1$, $\kappa = \sqrt{2}\pi/6$ with the reduced two-body Hamiltonian

$$h^{(0)} = -\frac{\partial^2}{\partial\eta^2} + \frac{2m}{\hbar^2}V(\sqrt{2}\eta). \tag{5}$$

Then the Schrödinger equation in a pair channel $\eta/\rho << 1$ reads as ($\hbar = m = 1$)

$$\left(-\frac{\partial^2}{\partial\eta^2} - 2\bar{\kappa}\delta(|\eta|) - \epsilon_j^{(0)}\right)\phi_j(\eta) = 0, \tag{6}$$

where $\bar{\kappa} = \kappa/\sqrt{2} = \pi/6$ is the effective strength of the pair potential, $\epsilon_j^{(0)} = 2mE_j/\hbar^2$ is the doubled energy of the two-body system. The complete set of the solutions of the discrete and continuous spectra of eq.(5) is given by [10]

$$\epsilon_0^{(0)} = -\bar{\kappa}^2, \quad \phi_0(\eta) = \sqrt{\bar{\kappa}}\exp(-\bar{\kappa}|\eta|), \quad <0|0>= \int_{-\infty}^{+\infty}\phi_0^*(\eta)\phi_0(\eta)d\eta = 1, \tag{7}$$

$$\epsilon_p^{(0)} = p^2, \quad \varphi_p(\eta) = \frac{1}{\sqrt{2\pi}}(\exp(ip\eta) + \frac{it_p}{|p|}\exp(i|p||\eta|)), \quad t_p = \frac{\bar{\kappa}|p|}{|p| - i\bar{\kappa}},$$

$$< 0|p >= \int_{-\infty}^{+\infty} \phi_0^*(\eta)\phi_p(\eta)d\eta = 0, \quad < p|p' >= \int_{-\infty}^{+\infty} \phi_p^*(\eta)\phi_{p'}(\eta)d\eta = \delta(p - p'). \qquad (8)$$

Let us extract the factor $\rho^{-1/2}$ in the solutions of equation (3), using the substitution $\Psi = \rho^{-1/2}\tilde{\Psi}$, then

$$\left[-\frac{\partial^2}{\partial\rho^2} + \bar{h}_\rho - \frac{2mE}{\hbar^2} \right] \tilde{\Psi}(\rho, \theta) = 0, \qquad (9)$$

where $\bar{h}_\rho$ is the parametric Hamiltonian defined as

$$\bar{h}_\rho = h_\rho - \frac{1}{4\rho^2}, \qquad h_\rho = h_\rho^{(0)} + \frac{2m}{\hbar^2}V(\rho, \theta), \qquad h_\rho^{(0)} = -\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}. \qquad (10)$$

We can now proceed to seek a complete orthogonal set of the adiabatic functions $B_j(\rho, \theta)$, that are solutions of the eigenvalue problem on a circle C: $-\pi \le \theta \le \pi$, with the symmetry under interchange of particles [6]

$$\bar{h}_\rho B_j(\rho, \theta) = \Lambda_j(\rho) B_j(\rho, \theta), \quad \Lambda_j(\rho) = \epsilon_j(\rho) - \frac{1}{4\rho^2}, \quad < B_i(\rho)|B_j(\rho) >_C = \delta_{ij}. \qquad (11)$$

Note, in a vicinity of the triple collision point $\rho = 0$ the matrix elements of the potential energy (4) between solutions $B_K^{(0)}(\theta)$ of the free rotated Hamiltonian $h_\rho^{(0)}$, $(2m/\hbar^2)V_{KK'}(\rho) = (c/\rho)\exp(-iK\pi/2)\exp(iK'\pi/2)$, non-vanishing for $K - K' \equiv 0(mod6)$, are negligible in compare with $< K|h_\rho^{(0)}|K' >_C = \rho^{-2}K(K+1)\delta_{KK'}$, and a set of numbers $K \equiv j(mod6)$, i.e. $K = 6j, j = 0, 1, 2, \cdots$, classifies the solutions

$$\Lambda_j(\rho) \to \Lambda_K^{(0)}(\rho) = \frac{K^2 - 1/4}{\rho^2}, \qquad B_j(\rho, \theta) \to B_K^{(0)}(\theta) = \frac{1}{\sqrt{2\pi}}\exp(iK\theta). \qquad (12)$$

For large ρ we can reveal local asymptotic solutions corresponding to a pair channel solutions $\phi_j(\eta)$ of equation (6). In particular, the eigenfunctions of Hamiltonian h_ρ tend to the solutions of a pair channel, when $j = 0$

$$\epsilon_0(\rho) \to \epsilon_0^{(0)}, \quad B_0(\rho, \theta) \to \sqrt{\rho}\phi_0(\eta). \qquad (13)$$

However, if $j \ne 0$, we can set a countable covering $K/\rho \sim p$ and use a correspondence

$$\epsilon_j(\rho) \to \epsilon_p^{(0)}, \quad B_j(\rho, \theta) \to \sqrt{\rho}\phi_p(\eta), \qquad (14)$$

which closes a formal classification of the unsymmetrized sets under consideration.

By using the above correspondence at small and large values of ρ we can set the global adiabatic, K-harmonic and local Jacobi representations of a partial wave function Ψ in coordinates (ρ,θ) and (ρ,η), respectively

$$\Psi(\rho,\theta)=\rho^{-1/2}\sum_j B_j(\rho,\theta)\,\chi_j(\rho)\rightarrow\begin{cases}\rho^{-1/2}\sum\limits_{K=-\infty}^{+\infty}B_K^{(0)}(\theta)\chi_K^{(0)}(\rho),\\ \phi_0(\eta)\chi_0(\rho)+\int\limits_{-\infty}^{+\infty}dp\phi_p(\eta)\chi_p(\rho).\end{cases}\tag{15}$$

Averaging equation (9) over $B_K^{(0)}(\theta)$ leads to a set of the coupled K-harmonic equations ($\hbar=m=1$)[9]

$$\left(-\frac{d^2}{d\rho^2}+\Lambda_K^{(0)}(\rho)-2E\right)\chi_K^{(0)}(\rho)+\sum_{K'}V_{KK'}(\rho)\chi_{K'}^{(0)}(\rho)=0.\tag{16}$$

Alternatively, averaging (9) over $B_i(\rho,\theta)=B_K^{(0)}(\theta)U_{Ki}(\rho)$, where $U(\rho)$ is an unitary operator $U_{Ki}(\rho)=<B_K^{(0)}|B_i(\rho)>_C$, leads to a set of the coupled adiabatic equations

$$\left(-\frac{d^2}{d\rho^2}+\Lambda_i(\rho)-2E\right)\chi_i(\rho)+\sum_j\left(-A_{ij}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{ij}(\rho)+H_{ij}(\rho)\right)\chi_j(\rho)=0,\tag{17}$$

where

$$A_{ij}(\rho)=<B_i(\rho)|\frac{\partial}{\partial\rho}B_j(\rho)>_C,\quad H_{ij}(\rho)=<\frac{\partial}{\partial\rho}B_i(\rho)|\frac{\partial}{\partial\rho}B_j(\rho)>_C.\tag{18}$$

Note that $A=\{A\}_{ij}$ is anti-Hermitian and $H=\{H\}_{ij}$ is Hermitian

$$A_{ij}(\rho)=\sum_K U_{iK}^{-1}(\rho)\frac{\partial}{\partial\rho}U_{Kj}(\rho),\quad H_{ij}=-(A^2)_{ij}=-\sum_{j'}A_{ij'}A_{j'j}.\tag{19}$$

Then, eq.(17) can be written in the matrix form [2]

$$\left(-(1\otimes\frac{d}{d\rho}+A(\rho))^2+\Lambda(\rho)-2E\otimes 1\right)\chi(\rho)=0.\tag{17a}$$

The graphs of potentials $\Lambda_j(\rho)$, $A_{ij}(\rho)$ and $H_{ij}(\rho)$, that were calculated with the help of relations of Appendix A are plotted in Figs.1, 2,and 3. At large ρ the asymptotic form of matrix elements $A(\rho)$ in the local representation are

$$A_{ij}(\rho)=A_{ij}^{(0)}\rho^{-1}+O(\rho^{-3}),\quad A_{ij}^{(0)}=\int\limits_{-\infty}^{+\infty}d\eta\phi_i^*(\eta)\hat{A}^{(0)}\phi_j(\eta),$$

$$\hat{A}^{(0)}=\left(\frac{1}{2}+\eta\frac{\partial}{\partial\eta}\right).\tag{20}$$

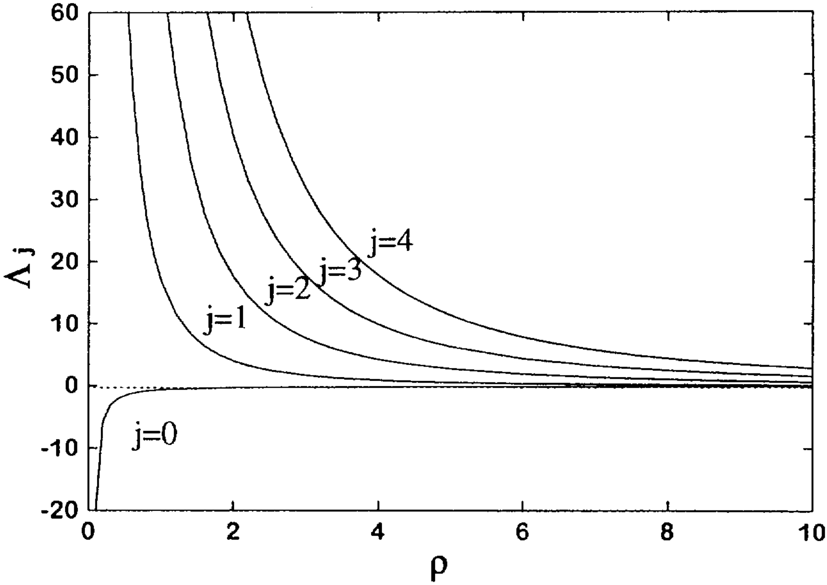


Fig.1. The adiabatic potentials Λ.

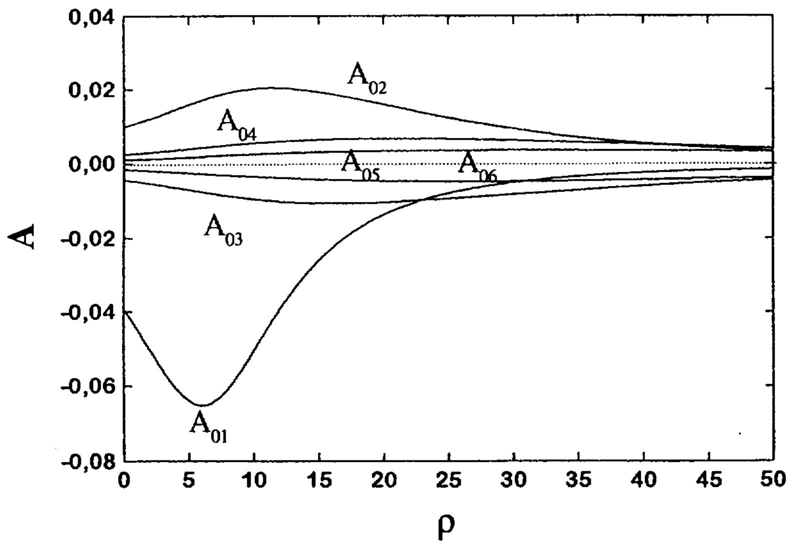


Fig.2. The off-diagonal elements of A matrix

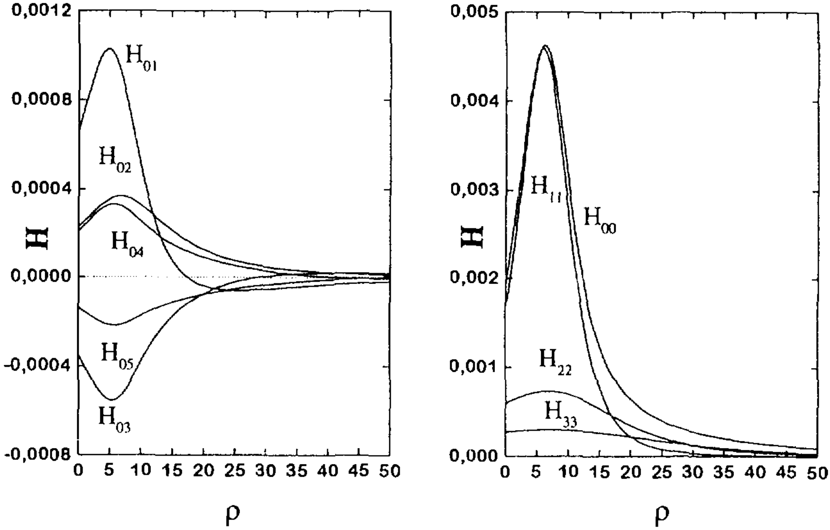


Fig 3. The diagonal and off-diagonal elements of H matrix

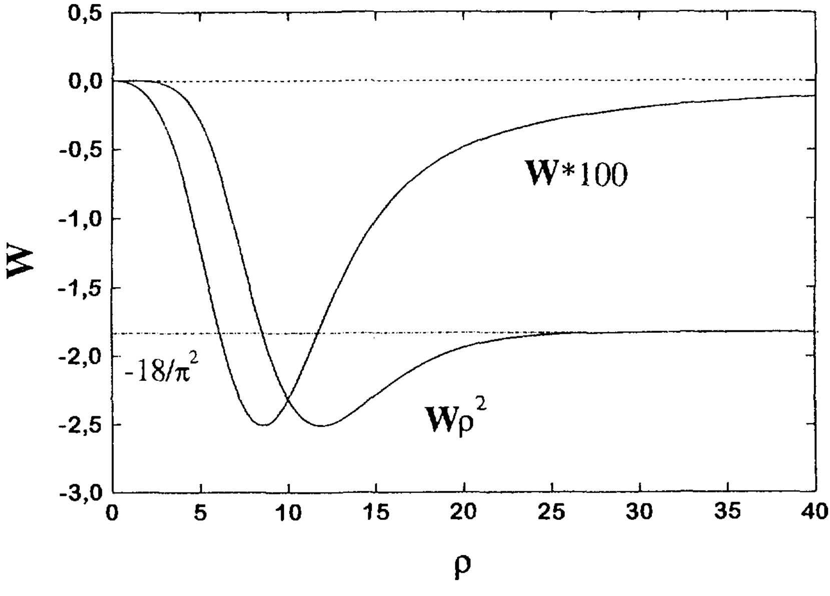


Fig 4. The effective mass correction W and it's asymptotic behavior $W\rho^2$

For matrix elements between discrete and continuous spectra of the pair channel the standard formula takes place

$$A_{ij}^{(0)} = \frac{1}{4} < \phi_i \left[\eta^2, h^{(0)}\right] \phi_j >= -\frac{1}{4}(\epsilon_i^{(0)} - \epsilon_j^{(0)}) < \phi_i|\eta^2|\phi_j > . \qquad (21)$$

The corresponding values of matrix elements $< 0|\eta^2|j >$ equal

$$< 0|\eta^2|0 >= \frac{1}{2\bar{\kappa}^2}, \quad < 0|\eta^2|p >= \sqrt{\frac{\bar{\kappa}}{2\pi}} \frac{8\bar{\kappa}p}{(\bar{\kappa}^2 + p^2)^{5/2}}. \qquad (22)$$

Owing to these equations, the following sum rule is valid, with integration substituted for summation,

$$4 \sum_{j\neq 0} \frac{A_{0j}^{(0)} A_{j0}^{(0)}}{\epsilon_0^{(0)} - \epsilon_j^{(0)}} = - < 0|\eta^2 \hat{A}^{(0)}|0 >=< 0|\eta^2|0 > . \qquad (23)$$

By substituting values (20)-(22) into the definition of the diagonal matrix element $H_{00}(\rho)$ via $A_{0j}(\rho)$ by eq.(19) and replacing the sum over j by the integration over p, the direct calculation leads to the asymptotics $H_{00}(\rho) = 1/(4\rho^2) + O(\rho^{-4})$. This provides a true asymptotic behavior of the adiabatic potential $\Lambda_0(\rho) + H_{00}(\rho) = \epsilon_0^{(0)} + O(\rho^{-4})$ and gives a test for checking of the sum rule (19) with the help of summation. Using the above asymptotics of matrix elements, we can write the asymptotic form of equations (17) in the local representation of a pair channel $|0 >$

$$\left(-\frac{d^2}{d\rho^2} + \epsilon_i^{(0)} - \epsilon_0^{(0)} - q^2\right) \chi_{i0}(\rho, q) - \frac{2}{\rho} \sum_i A_{ij}^{(0)} \frac{d}{d\rho} \chi_{j0}(\rho, q) = 0, \qquad (24)$$

where $q^2 = 2E - \epsilon_0^{(0)}$ is the relative energy which is counted off from the pair threshold of the doubled energy $\epsilon_0^{(0)} = \bar{\kappa}^2$.

3 The effective adiabatic approximation

We can define the effective adiabatic approximation (EAA) as the projection of the system of adiabatic equations (17) onto the two-body channel by using the canonical transformation [3]

$$\left(\frac{d}{d\rho}\mu^{-1}(\rho)\frac{d}{d\rho} - U_{eff}(\rho) + q^2\right) \chi_{eff}(\rho) = 0. \qquad (25)$$

The solution $\chi_{eff}(\rho) \equiv \chi_i^{new}$ is connected with the solutions $\chi_j(\rho)$ of system (17) by the relation

$$\chi_i^{new} = T_{ij}\chi_j = \sum_{jj\prime} < i \mid e^{iS^{(2)}} \mid j\prime >< j\prime \mid e^{iS^{(1)}} \mid j > \chi_j, \qquad (26)$$

where

$$\imath S^{(1)}_{ij} = \Delta^{-1}_{ij}\left(H_{ij} - A'_{ij} - 2A_{ij}\frac{d}{d\rho}\right), \quad \imath S^{(2)}_{ij} = -2\Delta^{-2}_{ij}A_{ij}V'_{jj}. \qquad (27)$$

The effective potential $U_{eff}(\rho)$ is defined as a sum of the adiabatic potential $U_{ad}(\rho)$ and effective nonadiabatic correction $\delta U(\rho)$; and $\mu(\rho)$ can be treated as effective mass that is defined as the inverse sum of unity and the effective mass correction $W(\rho)$

$$U_{eff}(\rho) = U_{ad}(\rho) + \delta U(\rho) \quad U_{ad}(\rho) = -\frac{1}{4\rho^2} + \epsilon_0(\rho) - \epsilon_0^{(0)} + H_{00}(\rho), \qquad (28)$$

$$\mu^{-1}(\rho) = 1 + W(\rho), \qquad (29)$$

$$W(\rho) = -4\sum_{j\neq 0} A_{0j}(\rho)A_{j0}(\rho)\Delta^{-1}_{0j}(\rho), \qquad (30)$$

$$\delta U(\rho) = \sum_{j\neq 0}(\Delta^{-1}_{0j}V^{(1)}_{0j} + \Delta^{-2}_{0j}V^{(2)}_{0j} + \Delta^{-3}_{0j}V^{(3)}_{0j}). \qquad (31)$$

Here the following relations are applied:

$$V^{(1)}_{0j} = H^2_{0j} - (A'_{0j})^2 - 2A_{0j}H'_{0j} - 2A_{0j}A''_{0j},$$

$$V^{(2)}_{0j} = -H_{0j}A_{0j}(\Sigma'_{0j} - \Delta'_{0j}) + A_{0j}A'_{0j}(\Sigma'_{0j} + 3\Delta'_{0j}) + A^2_{0j}(\Sigma''_{0j} + 3\Delta''_{0j}),$$

$$V^{(3)}_{0j} = A^2_{0j}(\Sigma'_{0j} + \Delta'_{0j})(\Sigma'_{0j} - 2\Delta'_{0j}),$$

$$V_{00} = V_{00}(\rho) = \Lambda_0(\rho) + H_{00}(\rho), \quad V_{jj} = V_{jj}(\rho) = \Lambda_j(\rho) + H_{jj}(\rho),$$

$$H_{00} = H_{00}(\rho) = -\sum_i A_{0i}A_{i0}, \quad H_{0j} = H_{0j}(\rho) = -\sum_i A_{0i}A_{ij},$$

$$\Delta_{0j}(\rho) = \Delta_{0j} = V_{00} - V_{jj}, \quad \Sigma_{0j}(\rho) = \Sigma_{0j} = V_{00} + V_{jj}, \qquad (32)$$

In the above formulae all of the terms except for $\epsilon_0^{(0)}$ are ρ functions and the symbol "$\prime$" denotes a derivative with respect to ρ. The graphs of the essential part $W(\rho)$, of the effective mass $\mu(\rho)$, and the saturation of the corresponding sum defined with respect to j are presented in Figs.4,and 5. The nonadiabatic correction $\delta U(\rho)$ is shown in Fig.6 . The adiabatic potential $U_{ad}(\rho) = U_{eff}(\rho) - \delta U(\rho)$ and effective adiabatic potential $U_{eff}(\rho)$ counted off from the pair threshold of the doubled energy $\epsilon_0^{(0)} = 2E_0 = -\pi^2/36$ are compared in Fig.7 . Figures 8 and 9 demonstrate the convergence of sums (19) and (31) versus the number of adiabatic state j to the true asymptotics of the adiabatic potential which tends to zero like the exponential [8] $U_{ad}(\rho) = -(\pi^2/9)exp\{-\rho\pi^2/18\}\{1 - \rho\pi^4/1944 + \pi^2/36 + 1/2\rho\}$, and the effective adiabatic potential times ρ^4 tends to constant $-18/\pi^2$. Using eqs. (20) - (23) for the description of the asymptotic behavior $A(\rho)$, we have the asymptotics of the effective mass at large ρ

$$\mu^{-1}(\rho) \sim 1 + \frac{W^{(0)}_{00}}{\rho^2}, \quad W^{(0)}_{00} = -<0|\eta^2|0> = -\frac{1}{2\bar{\kappa}^2}. \qquad (33)$$

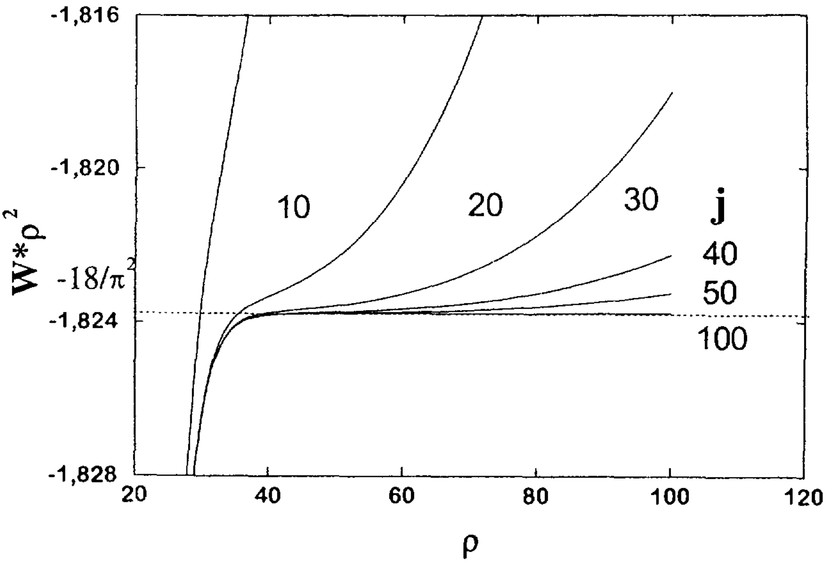


Fig.5. The asymptotic behavior of the effective mass correction W with respect to different j

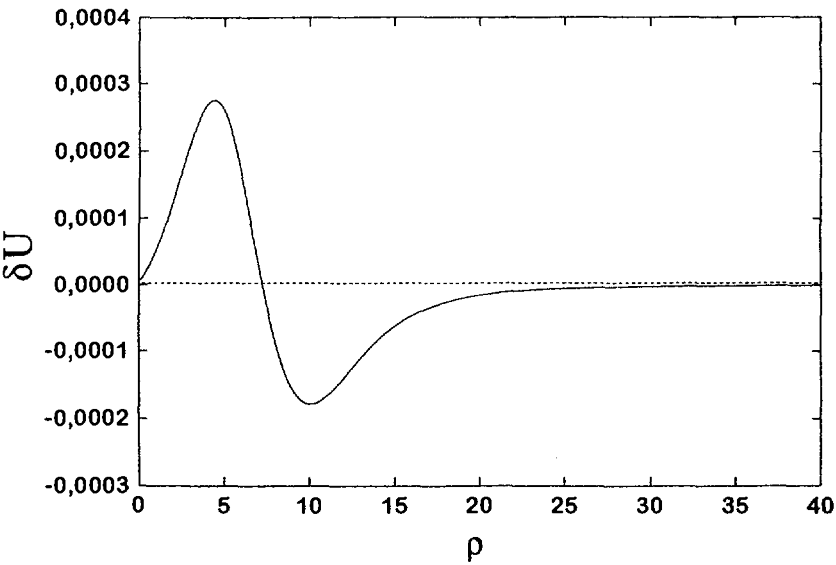


Fig.6. The nonadiabatic correction δU_{eff} to the effective adiabatic potential U_{eff}

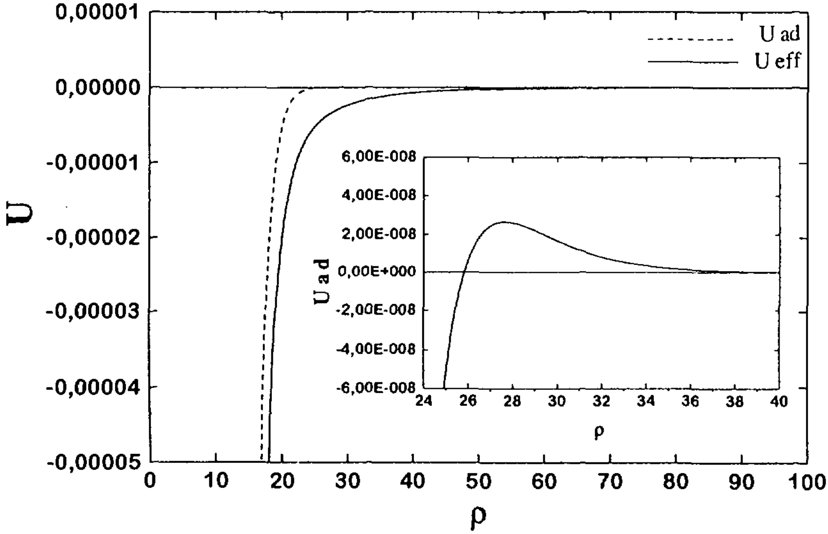


Fig.7. The adiabatic and effective adiabatic potentials U_{ad} and U_{eff}

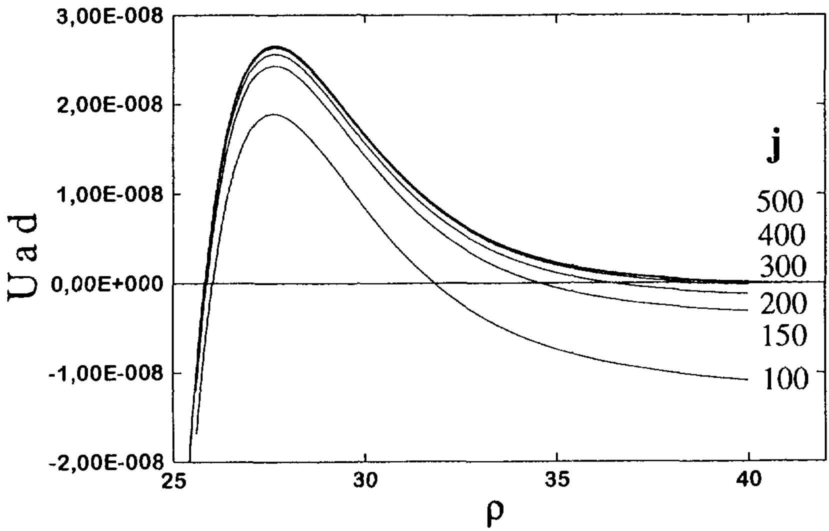


Fig.8. The adiabatic potential U_{ad} behavior with respect to different j

Figure 4 shows that the behavior of $W(\rho)$ determined by eq.(30) as $\rho \to +\infty$ is $\rho^2 W(\rho_{max}) \to -18/\pi^2$. Note that with increasing ρ the maximum value of j has to increase too to reach a given accuracy of the approximation of the sum rule eq. (23), as one can see from Fig.5 . When the compatibility conditions at large ρ

$$-A_{00}^2(\rho) - \frac{1}{4}\rho^{-2} = O(\rho^{-4}), \tag{34}$$

are included, eq. (17) takes a form

$$\left[\frac{d^2}{d\rho^2} + q^2\left(1 - \frac{W_{00}^{(0)}}{\rho^2}\right)\right]\chi_{eff}(\rho) = 0. \tag{35}$$

When $q < 0|\eta^2|0 > /(2\rho) << 1$, solutions of the continuous spectrum of eq. (25) can be given in the form

$$\chi_{eff}(\rho) \sim \sin\left[q\rho\left(1 - \frac{< 0|\eta^2|0 >}{2\rho^2}\right) + \delta\right] \sim \sin(q\rho + \delta) - q\frac{< 0|\eta^2|0 >}{2\rho}\cos(q\rho + \delta). \tag{36}$$

The solutions $\chi_j(\rho)$ of system (17) are connected with the solution $\chi_{eff}(\rho)$ of the effective eq. (25) by the inverse asymptotic transformation (26), which reveals a weak asymptotic coupling form

$$\chi_j(\rho) = T_{j0}^{-1}\chi_0^{new}(\rho) \sim \exp\left[-\frac{< j|\eta^2|0 > (1 - \delta_{j0})}{2\rho}\frac{d}{d\rho}\right]\chi_0^{new}(\rho). \tag{37}$$

After substitution (36) into this relation we have asymptotic solutions (24)

$$\chi_0(\rho) \sim \chi_0^{new}(\rho), \quad \chi_j(\rho) = T_{j0}^{-1}\chi_0^{new}(\rho) \sim -\frac{< j|\eta^2|0 > (1 - \delta_{j0})}{2\rho} q\cos(q\rho + \delta). \tag{38}$$

The partial wave function Ψ in the two-body channel $|0 >$

$$\Psi_0 = \rho^{-1/2}\sum_j |B_j >< B_j|T^{-1}|B_0 > \chi_0^{new}(\rho), \tag{39}$$

under the completeness condition

$$\sum_j |B_j >< B_j| = 1, \tag{40}$$

is defined by the relation

$$\Psi_0 \sim \rho^{-1/2} B_0\left[\sin(q\rho + \delta) - q\frac{\eta^2}{2\rho}\cos(q\rho + \delta)\right]. \tag{41}$$

When $q\eta^2/(2\rho) << 1$, we have with an accuracy of the order $O(\rho^{-1})$

$$\Psi_0(\rho, \theta) \sim \rho^{-1/2} B_0(\rho, \theta)\sin\left[q(\rho - \frac{\eta^2}{2\rho}) + \delta\right] \to \phi_0(\eta)\sin(q\xi + \delta). \tag{42}$$

It is evident that with increasing q, the role of the nonadiabatic coupling grows. In general, the discrepancy between $\xi \sim \rho(1-\eta^2/2\rho)$ and $\rho = \sqrt{\xi^2+\eta^2}$, which leads to weak asymptotic coupling (37), can be neglected only in the adiabatic limit $q \to 0$. In particular, for bound states with the normalization condition,

$$< \chi_{eff}|\chi_{eff} >= \int_0^{+\infty} \chi_{eff}(\rho)\chi_{eff}(\rho)d\rho = 1, \tag{43}$$

this coupling can be negligible too. However, to get correct results, one should be careful in special cases which can have peculiarities near the thresholds similar to a three-body zero-energy state, etc. Note that the transformation (26) changes the form of the solution, because the true value of ξ is restored only in the total solution Ψ defined by (39)-(42). This circumstance leads to the formal definition of a *mean-position* operator $\hat{\rho}_m^{new}$ in the *new* representation $\chi_0^{new} = T\chi$ of the pair channel

$$\rho_m^{new} =< \chi_0^{new}|\hat{\rho}_m^{new}|\chi_0^{new} >=< \chi|T^{-1}\hat{\rho}_m^{new}T|\chi >=< \chi|\hat{\rho}_m|\chi >= \rho_m. \tag{44}$$

Here the *mean-position* operator $\hat{\rho}_m^{new} = \rho$ corresponds asymptotically to the Jacobi variable ξ in the old representation χ, i.e. delocalization of ξ is contained in the *new* radial function $\chi_0^{new} = T\chi$. Indeed, in the old adiabatic representation χ, the *mean-position* operator $\hat{\rho}_m$ is determined by the relation

$$\hat{\rho}_m = T^{-1}\hat{\rho}_m^{new}T = T^{-1}\rho T = \rho + \delta\hat{\rho}. \tag{45}$$

Here $\delta\hat{\rho}$ corresponds to a delocalization of the variable ξ that for large $\rho >> 1$ is of an order of $< 0|\eta^2|0 > /2\rho << 1$, i.e.

$$\hat{\rho}_m = T^{-1}\rho T \sim < \xi > . \tag{46}$$

Such a construction formally determines the required *Zitterbewegung* of $\hat{\rho}_m$ around ρ with an amplitude of the order of $\delta\hat{\rho}$ and closes the definition of *mean-position operators* similar to [4] . Thus, we have not only the effective approximation (25) - (32) for the system (17) of adiabatic equations, but also a way to find the asymptotics of their solutions. For example, in the case of N-open channels one can use the projection techniques developed in [13] to build up an appropriate canonical transformation and find an effective N-channel approximation even if degeneracy of eigenvalues $\epsilon_i(\rho), i = 1, ..., N$ of a parametric Hamiltonian takes place. Note that eq. (25) can be derived also by the transformation $T_{0j}^{(2)} =< 0|\exp(\imath(S^{(1)}+S^{(2)}))|j >$ [14]. In this case, the discrepancy is only in the term $V_{0j}^{(3)}$

$$V_{0j}^{(3)} = -2A_{0j}^2\Delta'_{0j}(\Sigma'_{0j} + \Delta'_{0j}). \tag{47}$$

If we omit the nonadiabatic term in eq. (35) and take the adiabatic behavior

$$\chi_{ad} \sim \sin(q\rho + \delta^{ad}), \tag{48}$$

then we can find the obvious difference between the true and adiabatic phase shifts δ and δ^{ad}, respectively

$$\delta = \delta^{ad} + q\frac{< 0|\eta^2|0 >}{2\rho}. \qquad (49)$$

As it has been shown, the asymptotic coupling of channels in a scattering problem is in any case to be taken into account when any adiabatic approach is used. It happens since a slow variable ρ is restored completely into the needed Jacobi vector ξ only in the complete adiabatic expansion of a three-body wave function. The above reduction from the initial eq. (17) to the effective eq. (25) can be compared with an elegant method of eliminating small components of solutions of the Dirac equation via Foldy-Wouthuysen transformation [4]. Also, it gives a true probabilistic interpretation of all observable variables such as coordinate, momentum, and so on.

Note that with the standard substitution $\chi_{eff}(\rho) = \mu^{1/2}(\rho)\tilde{\chi}_{eff}(\rho)$, we can also rewrite the momentum - dependent form of eq. (25) in the energy-dependent form

$$\left(\frac{d^2}{d\rho^2} - V_{eff}(q^2, \rho) + q^2\right)\tilde{\chi}_{eff}(\rho) = 0. \qquad (50)$$

Here $V_{eff}(q^2, \rho)$ reads as

$$V_{eff}(q^2,\rho) = \left(U_{eff}(\rho) + q^2W(\rho)\right)\mu(\rho) + \Delta U_{eff}(\rho),$$

$$\Delta U_{eff}(\rho) = \frac{1}{2}W''(\rho)\mu(\rho) - \frac{1}{4}\left(W'(\rho)\mu(\rho)\right)^2, \qquad (51)$$

that is sometimes a more applicable for the analysis of solutions. This representation can give us an opportunity to compare the effective adiabatic eq. (25) with a conventional one having the potential quadratically dependent on the momentum [1]

$$\left(\frac{d}{d\rho}(1 + W(\rho))\frac{d}{d\rho} - U_{ad}(\rho) + \frac{1}{2}\frac{d^2}{d\rho^2}W(\rho) + q^2\right)\chi_{eff}(\rho) = 0, \qquad (52)$$

where the term $-(1/2)d^2W(\rho)/d\rho^2$ corresponds to the nonadiabatic effective correction $\delta U_{eff}(\rho)$. It means that we can compare now effective potential (51) with the standard definition of the energy-dependent potential [1]

$$V_{eff}^{(st)}(q^2,\rho) = \frac{U_{ad}(\rho) + q^2W(\rho)}{1 + W(\rho)} - \frac{1}{4}\left[\frac{d}{d\rho}\ln(1 + W(\rho))\right]^2,$$

where $V_{eff}^{(st)}$ is a part of eq.(50) and the second term corresponds to $\Delta U_{eff}(\rho)$ from eq.(51). These types of potentials were also under consideration in paper [11], where the analytic solutions for a square well with some modifications were found. As it follows from next sections, this brief review of the methods under consideration shows the new way to an adequate treatment of the three-body scattering problem.

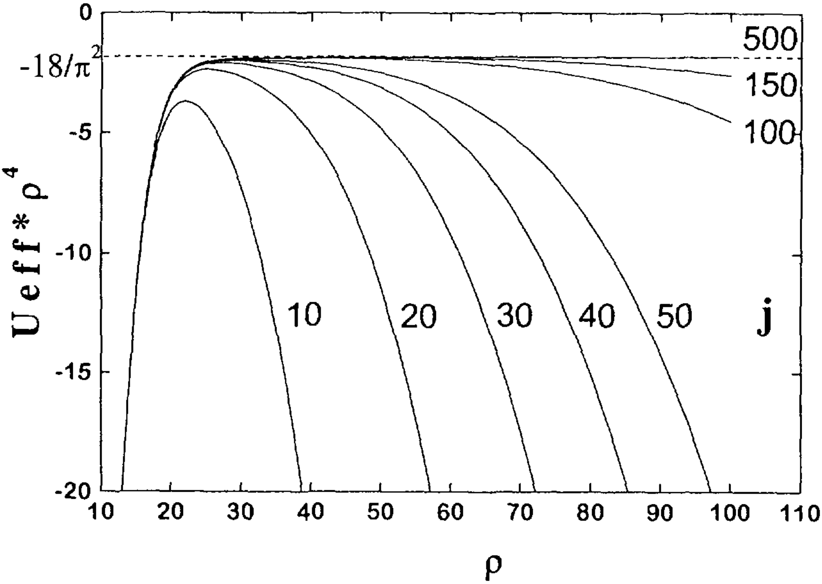


Fig.9. The asymptotic behavior of the effective adiabatic potential U_{eff} with respect to different j

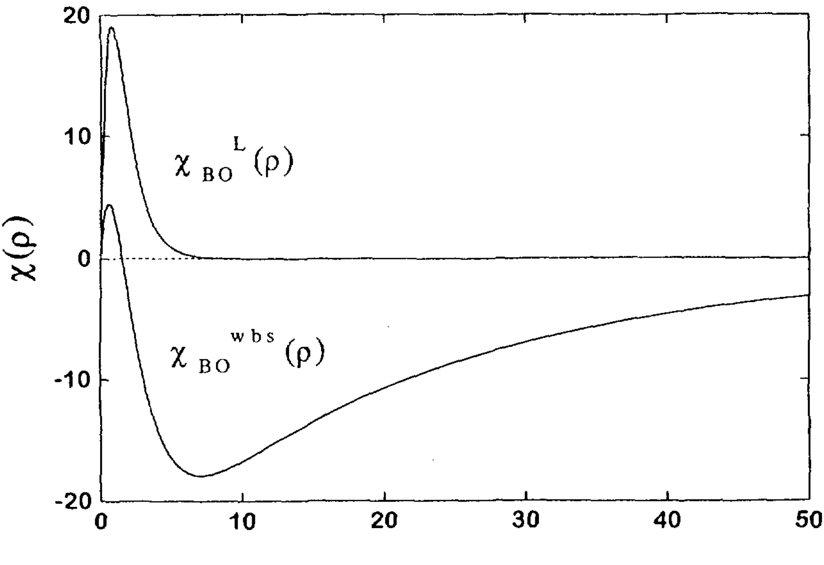


Fig.10. The radial wave functions of the ground χ^L_{BO} and weakly bound χ^{wbs}_{BO} states of the BO approximation

4 Discrete spectrum of the three-body problem

Let us consider the eigenvalue problem for the one-channel approximation

$$\left(\frac{d^2}{d\rho^2} - U(\rho) + 2E - \epsilon_0^{(0)}\right)\chi(\rho) = 0, \tag{53}$$

with the following boundary and normalization conditions:

$$\chi(0) = 0, \quad \chi(+\infty) = 0. \tag{54}$$

$$<\chi|\chi>= 1. \tag{55}$$

For $U(\rho)$ we can apply either the so-called BornOppenheimer (BO) approximation

$$U_{BO}(\rho) = -\frac{1}{4\rho^2} + \epsilon_0(\rho) - \epsilon_0^{(0)}, \tag{56}$$

or the standard adiabatic approximation (AA)

$$U_{ad}(\rho) = -\frac{1}{4\rho^2} + \epsilon_0(\rho) - \epsilon_0^{(0)} + H_{00}(\rho). \tag{57}$$

The ground $\chi^L_{BO}(\rho)$ and weakly bound $\chi^{wbs}_{BO}(\rho)$ solutions of the eigenvalue problem (53) - (55) with the BO potential (56) are represented in Fig.10 . So, the BO approximation provides lower bound E^L_{BO} of the ground state and E^{wbs}_{BO} of the artificial weakly bound state. The latter disappears in the standard AA with the potential (57) that provides also the upper bound E^U_{ad} of the ground state, as has been shown in [12] and recalculated here. To evaluate the energy in EAA, we apply the following equation:

$$\left(\frac{d}{d\rho}(1 + W(\rho))\frac{d}{d\rho} - U_{eff}(\rho) + 2E - \epsilon_0^{(0)}\right)\chi_{eff}(\rho) = 0, \tag{58}$$

where the effective potential $U_{eff}(\rho)$ and effective mass $\mu(\rho)$ were determined in the previous section. Solving of the eigenvalue problem (58), (54), and (43) leads to the new lower bound $E^L_{eff} = -1.096626(\hbar^2/2m)$ of the exact value $E_{xct} = \pi^2/9(\hbar^2/2m)$ with the deviation equal to $2.6 * 10^{-6}$. The above adiabatic $\chi^U_{ad}(\rho)$ and effective $\chi^L_{eff}(\rho)$ radial wave functions are shown in Fig.11 . The difference between $\chi^U_{ad}(\rho)$ and $\chi^L_{eff}(\rho)$ is negligible on the scale chosen here. The doubled values of the energies E_{tth}, E_{pth} of the three-body and pair thresholds, and the corresponding results of the numerical calculations of the lower BO bounds E^{wbs}_{BO} and E^L_{BO} of the weakly bound and ground states, together with the upper adiabatic (ad) and lower effective (eff) bounds E^U_{ad} and E^L_{eff} of the exact(xct) one E_{xct} are presented in Fig.12. This figure demonstrates the above-mentioned set of the lower and the upper bounds of the energy E. To solve the discrete spectrum problem, we reduced it to a finite interval $\xi \in [0, 1]$, approximated latter with the help of the finite-difference scheme of the 4th-order on an uniform grid and applied the multi-parametric continuous analog of Newton's method [15](see Appendix B).

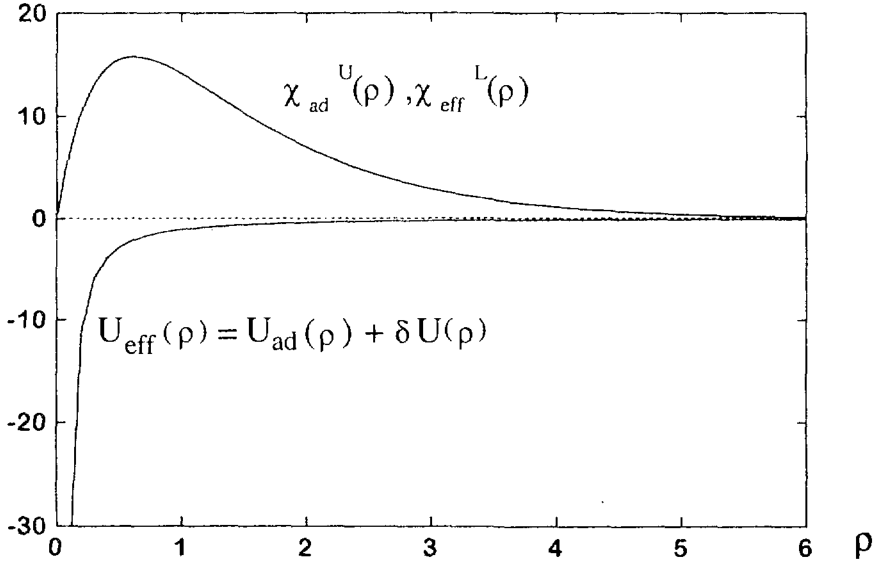


Fig.11. The effective adiabatic potential U_{eff} and radial wave functions χ_{eff}^{L} and χ_{ad}^{U}

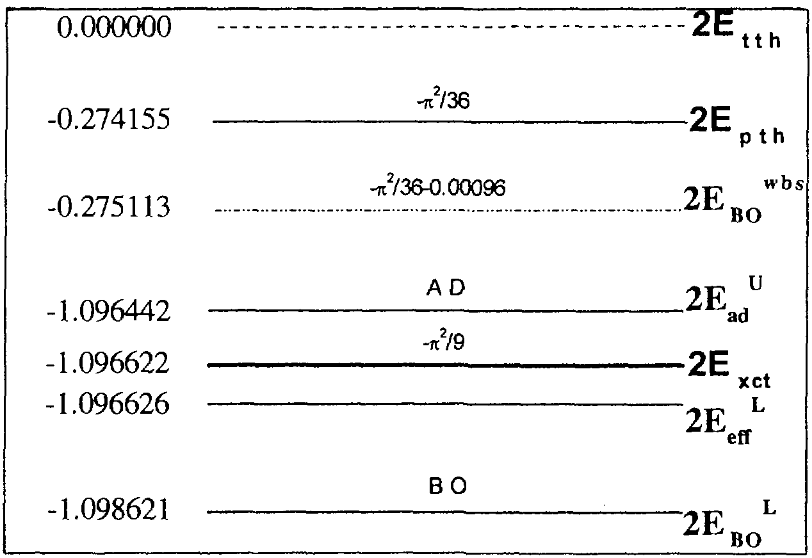


Fig.12. The doubled values of the energies E_{tth}, E_{pth} of the three-body and pair thresholds, and the corresponding results of the numerical calculations of the lower BO bounds E_{BO}^{wbs} and E_{BO}^{L} of the weakly bound and ground states, together with the upper adiabatic (ad) and lower effective (eff) bounds E_{ad}^{U} and E_{eff}^{L} of the exact(xct) one E_{xct}.

5 Continuous spectrum of the problem

In the continuous spectrum below the three-body threshold $E_0 < E < 0$ we solve the equation for the phase function in cases of AA with potential U_{ad} and of EAA with potentials $\mu(\rho)$ and $U_{eff}(\rho)$. The phase shift $\delta_{ad}(q)$ corresponding to AA (57) is determined from the equation for the phase function $\delta_{ad}(q,\rho) = \delta(q,\rho)$ [1]

$$\frac{d\delta(q,\rho)}{d\rho} = -\frac{U_{ad}(\rho)}{q}\sin^2(q\rho + \delta(q,\rho)), \quad \delta(q,0) = 0. \tag{59}$$

The phase shift $\delta(q)$ as a function of the relative momentum $q^2 = 2(E - E_0)$, $0 < q^2 < (\pi/6)^2$, is defined as

$$\delta(q) = \lim_{\rho\to+\infty} \delta(q,\rho). \tag{60}$$

The phase shift $\delta_{eff}(q)$ corresponding to EAA is determined from the momentum - dependent equation for the phase function $\delta_{eff}(q,\rho) = \delta(q,\rho)$ following from (25), (28), and (31):

$$\frac{d\delta(q,\rho)}{d\rho} = -\frac{1}{1+W(\rho)}\frac{U_{eff}(\rho) + q^2W(\rho)}{q}\sin^2(q\rho + \delta(q,\rho)) +$$

$$+\frac{1}{1+W(\rho)}\frac{dW}{d\rho}\sin(q\rho + \delta(q,\rho))\cos(q\rho + \delta(q,\rho)), \tag{61}$$

$$\delta(q,0) = 0.$$

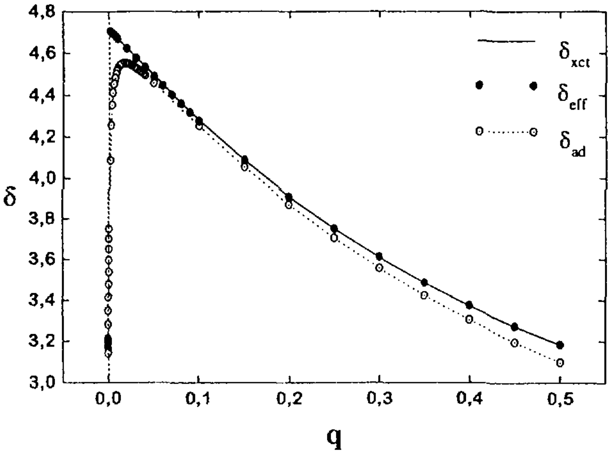
The graphs of $\delta_{xct}(q)$,$\delta_{ad}(q)$ and $\delta_{eff}(q)$ are presented in Fig.13 . Note that the results of the adiabatic phase shift $\delta_{ad}(q)$ calculation completely coincide with the results of the paper [8]. The exact phase shift δ_{xct} is defined in that paper under the assumption that one can write rigorously the wave function in the form

$$\Psi \sim \rho^{-1/2}B_0(\rho,\theta)\chi(\rho), \quad \chi(\rho) \sim \sin(q\rho + \delta_{xct}) \tag{62}$$

for large ρ, where

$$\delta_{xct} = \frac{3\pi}{2} - arctg\frac{8\sqrt{3}q/\pi}{1 - 36q^2/\pi^2}. \tag{63}$$

As it follows from the comparison with the exact phase value $\delta_{xct}(q)$, EAA ensures a correct behavior of the function $\delta_{eff}(q)$ with an accuracy of $2 * 10^{-3}$ for values of $q^2 : 4 * 10^{-6} < q^2 < (\pi/6)^2$. From Fig.13 including tabulated calculated values one can see that on the above interval of q the adiabatic phase shift $\delta_{ad}(q)$ tends to π while the effective phase shift $\delta_{eff}(q)$, in accordance with the exact one $\delta_{xct}(q)$, tends to $\pi + \pi/2$. This comparison confirms the convergence of the method under consideration and consistency with an accuracy of the order $2 * 10^{-6}$ of the lower bound of the energy of EAA. As it follows from eq. (59) and eq. (61) the phase shifts of AA and EAA are connected really by eq. (49). Note that for the continuous spectrum the above problems were reduced to the phase-function equations (59) and (61) solved by the Runge-Kutta method of the 4th-order.



q	δ ad	δ eff
.002	4.08	4.70
0.10	4.25	4.28
0.15	4.05	4.09
0.20	3.87	3.91
0.25	3.71	3.75
0.30	3.56	3.61
0.35	3.42	3.49
0.40	3.30	3.37
0.45	3.20	3.27
0.50	3.10	3.18

Fig.13. The exact δ_{xct}, adiabatic δ_{ad} and the effective adiabatic δ_{eff} phase shifts

6 Conclusion

An essential part of the proposed approach is the reduction of the system of adiabatic equations to the unique effective adiabatic equation and construction of the momentum-dependent potential with the help of the operator canonical transformation. For the problem under consideration this was realized via the analytic representation of the solutions of the parametric spectral problem on a circle. As a result, we investigated the method convergence of the adiabatic expansion and established that the appropriate sum rules saturate and satisfy the correct asymptotic behavior of the momentum-dependent potential. It was proved that the asymptotic kinematic connection of closed channels under the three-body threshold is transformed to the energy-dependent centrifugal potential proportional to the mean-square size of a pair subsystem in the ground state. This provides a correct phase shift behavior in the whole region of the relative energy below the three-body threshold except the vicinity of small relative energies of the order $4 * 10^{-6}$, which is beyond the method accuracy.

The investigation shows that in the cases when the threshold peculiarities take place, nobody can think that the standard adiabatic approximation can provide the true threshold behavior. Even if one can apply the proposed EAA, a careful investigation of the saturation of the indicated sum rules is needed, even if short-range pair potentials are considered. As it has been mentioned above, the projection of the initial problem with short-range potentials onto an effective one can be treated as a nonlocal momentum-dependent potential problem. As a consequence, the long-range potentials appear and construction of true asymptotics is required. It seems that a relation between EAA and the known approach of construction of an effective nonadiabatic potential for the exotic Coulomb three-body problems [16], [17] can be found too. As a matter of experience, one can see that the expansion for any truncated set of eigenfunctions of the pure rotation Hamiltonian on a circle, which is the essential part of K-harmonic expansion, does not provide the true asymptotics for a three-body problem with pair channels. As it follows from the presented results, the proposed EAA approach shows the new way to an adequate treatment of the three-body rearrangement scattering problem.

7 Acknowledgements

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8 Appendix A

To construct $A_{0j}(\rho)$ from eq.18, we use the following relations for the attractive case $c=-1$ with the effective strength $\bar{\kappa}=\pi/6$ (in the units $\hbar=m=1$) [12]:

$$A_{0j}(\rho)=-\frac{1}{\rho}\frac{<0|2V(\rho)|j>_C}{(\epsilon_0(\rho)-\epsilon_j(\rho))},$$

where

$$<0|2V(\rho)|j>_C=\int_{-\pi}^{\pi}B_0^*(\rho,\theta)2V(\rho,\theta)B_j(\rho,\theta)d\theta,$$

$$2V(\rho,\theta)=\frac{c\bar{\kappa}}{\rho}\sum_n\delta(\theta-\theta_n),\qquad \theta_n=n\pi/3+\pi/6,\qquad n=0,1,2,3,4,5.$$

The eigenvalues $\epsilon_0(\rho)$ and $\epsilon_j(\rho)$ are determined via reduced eigenvalues y_0 and y_j

$$\epsilon_0(\rho)=-\left(\frac{6y_0}{\rho}\right)^2,\quad \epsilon_j(\rho)=\left(\frac{6y_j}{\rho}\right)^2.$$

The roots y_0 and y_j are determined from the following transcendental equations:

$$y_0\tanh(\pi y_0)=-x,$$

$$y_j\tan(\pi y_j)=x,\qquad j-1/2<y_j<j,\qquad j=1,2,3,...,$$

where

$$x=c\frac{\bar{\kappa}}{6}\rho=c\frac{\pi}{36}\rho.$$

The corresponding eigenfunctions have the form

$$B_0(\rho,\theta)=\sqrt{\frac{y_0^2-x^2}{\pi(y_0^2-x^2)+|x|}}\cosh\left[6y_0\left(\theta-n\pi/3\right)\right],$$

$$B_j(\rho,\theta)=\sqrt{\frac{y_j^2+x^2}{\pi(y_j^2+x^2)-|x|}}\cos\left[6y_j\left(\theta-n\pi/3\right)\right],$$

for

$$n\pi/3-\pi/6\le\theta\le n\pi/3+\pi/6,\qquad n=0,1,2,3,4,5.$$

As for $\cosh(\pi y_j)$ and $\cos(\pi y_j)$, respectively, we simplify the form of eigenfunctions by using the reduced transcendental equations

$$\cos(\pi y_j)=\frac{(-1)^j y_j}{\sqrt{y_j^2+x^2}},\qquad \cosh(\pi y_j)=\frac{|y_0|}{\sqrt{y_0^2-x^2}}.$$

Finally, the equations for $A_{jj'}$ have the form

$$A_{jj'}(\rho) = \begin{cases} -\frac{c\pi}{18}\dfrac{(-1)^j y_j |y_0|}{(y_0^2 - y_j^2)\sqrt{\pi(y_j^2 + x^2) - |x|}\sqrt{\pi(y_0^2 - x^2) + |x|}}, & j' = 0, \\ \frac{c\pi}{18}\dfrac{(-1)^{j-j'} y_j y_{j'}}{(y_j^2 - y_{j'}^2)\sqrt{\pi(y_j^2 + x^2) - |x|}\sqrt{\pi(y_{j'}^2 + x^2) - |x|}}, & j \neq 0, j' \neq 0. \end{cases}$$

9 Appendix B

For numerical solving of the eigenvalue problem (53) - (55), we transform the independent variable ρ to reduce the problem from the infinite interval $[0; +\infty]$ to the finite interval $[0; 1]$

$$\zeta = \frac{\rho}{\rho + \alpha}, \quad \rho = \frac{\alpha\zeta}{1 - \zeta}, \quad 0 \leq \zeta \leq 1, \tag{64}$$

where α is the parameter of the transformation, $\alpha \geq 1$. To obtain the Dirichlet boundary condition, we go over to the function

$$y(\zeta) = \zeta\chi(\zeta).$$

For the function $y(\zeta)$ we have the equation

$$\Phi^{(1)} = \mathbf{P}_1 y(\zeta) + E y(\zeta) = 0, \tag{65}$$

where $\mathbf{P}_1$ is the differential operator of the second order

$$\mathbf{P_1} = \frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2} - \frac{(1-\zeta)^3}{\alpha^2\zeta}\frac{d}{d\zeta} + \frac{(1-\zeta)^3}{\alpha^2\zeta^2} - U(\zeta),$$

with the boundary conditions

$$\Phi^{(2)} = y(0) = 0, \quad \Phi^{(3)} = y(1) = 0, \tag{66}$$

and the normalization condition

$$\int_0^1 \frac{1}{\zeta^3(1-\zeta)^2} y^2(\zeta) d\zeta = 1. \tag{67}$$

Due to the Dirichlet boundary conditions we can use the unit normalization condition

$$\Phi^{(4)} = \int_0^1 y^2(\zeta) d\zeta = 1. \tag{68}$$

Now we rewrite the eigenvalue problem for eq. (58) in the following form:

$$\left[\frac{d}{d\rho}(1+W(\rho))\frac{d}{d\rho} - U_{eff}(\rho) + q^2\right]\chi_{eff}(\rho) = 0,$$

$$|\chi_{eff}(0)| < +\infty, \quad \chi_{eff}(+\infty) = 0,$$

$$\int_0^{+\infty} \chi_{eff}^2(\rho)d\rho = 1, \tag{69}$$

where $1 + W(\rho) = \mu^{-1}(\rho)$, $\mu(\rho)$ is the effective mass and $U_{eff}(\rho)$ is the effective potential. We perform a similar transformation and obtain the following equation:

$$\Phi^{(1)} = \mathbf{P}_2 y(\zeta) + Ey(\zeta) = 0, \tag{70}$$

where $\mathbf{P}_2$ is the differential operator of the second order

$$\mathbf{P_2} = (1+W(\zeta))\frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2} + (-(1+W(\zeta))\frac{(1-\zeta)^3}{\alpha^2\zeta} + W'_\rho(\zeta)\frac{(1-\zeta)^2}{\alpha})\frac{d}{d\zeta} +$$

$$(1+W(\zeta))\frac{(1-\zeta)^3}{\alpha^2\zeta^2} - W(\zeta)\frac{(1-\zeta)^2}{4\alpha^2\zeta^2} + W'_\rho(\zeta)\frac{(1-\zeta)(2\zeta-1)}{2\alpha\zeta} - U_{eff}(\zeta),$$

with the same boundary conditions (66) and normalization (67).

This problem is solved by a continuous analog of the Newton method

$$\Phi'_z(z)\frac{dz}{dt} = -\Phi(z), \quad z(0) = z_0,$$

where

$$\Phi(z) = \{\Phi^{(1)}(z), \Phi^{(2)}(z), \Phi^{(3)}(z), \Phi^{(4)}(z)\}, \quad z = \{y(\zeta,t), E(t)\},$$

$\Phi'_z(z)$ is the Frechet derivative and t is the continuous parameter. We introduce the following notations:

$$u = \frac{dy}{dt}, \quad e = \frac{dE}{dt},$$

and make the decomposition

$$u = u_1 + eu_2.$$

For unknown functions u_1 and u_2 we have the equations

$$\mathbf{P}u_1 + Eu_1 = -(\mathbf{P}y + Ey), \quad u_1(0) = -y(0), \quad u_1(1) = -y(1),$$

$$\mathbf{P}u_2 + Eu_2 = -y, \quad u_2(0) = 0, \quad u_2(1) = 0. \tag{71}$$

It is obvious that $u_1 = -y$, therefore from an unity boundary condition we obtain

$$e = -\frac{1}{\int_0^1 u_2 y d\zeta}. \tag{72}$$

System (71) is solved on an uniform grid ω:

$$\omega = \{\zeta = (i-1)h_\zeta, \quad i = 1, N_\zeta, \quad h_\zeta = 1/(N_\zeta - 1)\},$$

with the help of the 4th-order approximation by means of finite-difference formulae

$$y_2'' = \frac{1}{12h^2}(10y_1 - 15y_2 - 4y_3 + 14y_4 - 6y_5 + y_6) + O(h^4),$$

$$y_2' = \frac{1}{12h}(-3y_1 - 10y_2 + 18y_3 - 6y_4 + y_5) + O(h^4),$$

$$y_i'' = \frac{1}{12h^2}(-y_{i-2} + 16y_{i-1} - 30y_i + 16y_{i+1} - 6y_{i+2}) + O(h^4),$$

$$y_i' = \frac{1}{12h}(y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2}) + O(h^4),$$

$$y_{n-1}'' = \frac{1}{12h^2}(y_{n-5} - 6y_{n-4} + 14y_{n-3} - 4y_{n-2} - 15y_{n-1} + 10y_n) + O(h^4),$$

$$y_{n-1}' = \frac{1}{12h}(-y_{n-4} + 6y_{n-3} - 18y_{n-2} + 10y_{n-1} + 3y_n) + O(h^4).$$

The matrices of linear systems are reduced to a five-diagonal form and we solve the above algebraic problems with the help of LU-decomposition for the band matrices. The integrals in formula (72) are calculated by the Simpson method.

Thus, using $y^{(k)}, E^{(k)}$ we calculate $u_2^{(k)}$ solving (71). Relation (72) gives us $e^{(k)}$. The increment for the wave function is

$$u^{(k)} = -y^{(k)} + e^{(k)}u_2^{(k)}.$$

The next approximation is calculated by the formula

$$y^{(k+1)} = y^{(k)} + \tau u^{(k)}, \quad E^{(k+1)} = E^{(k)} + \tau e^{(k)},$$

where τ is the step in parameter t calculated by

$$\tau = \frac{\delta(0)}{\delta(0) + \delta(1)},$$

$$\delta(t) = \delta(y^{(k)} + tu^{(k)}, E^{(k)} + te^{(k)}) = \| \Phi(y^{(k)} + tu^{(k)}, E^{(k)} + te^{(k)}) \|_{C_2} .$$

The iteration process is completed when $\delta < \varepsilon$, ε is a given small number.

The optimal choose of the parameter α in the transformation (64) allows us to have a required number of mesh points of the grid ω in the region of essential variation of the wave function [15].

References

[1] V.V. Babikov, Phase Function Method in Quantum Mechanics (Nauka, Moscow, 1976)(in Russian).

[2] S.I. Vinitsky, B.L. Markovski, A.A. Suzko, Yadernaya Fizika, **55**, 669 (1992); (Sov. J. Nucl. Phys. **55**,371 (1992)).

[3] A.G. Abraskevich, I.V. Puzynin, Yu.S. Smirnov and S.I. Vinitsky, Hyperfine Interections, **101/102**, 381 (1996).

[4] L.L. Foldy and S.A. Wouthuysen, Phys. Rev. **78**, 29 (1950).

[5] M.B. Kadomtsev, S.I. Vinitsky, F.R. Vukajlovich, Phys. Rev. **A 36**, 4652 (1987).

[6] W. Gibson, S.Y. Larsen, J.J. Popiel, Phys. Rev. **A 35**, 4919 (1987).

[7] J.B. McGuire, J. Math. Phys. **5**, 622 (1964); **29**, 155 (1988); L.R. Dodd, J. Math. Phys. **11**, 207 (1970).

[8] A. Amaya-Tapia, S.Y. Larsen, J.J. Popiel, Few-Body Systems, **23**, 87 (1997).

[9] R.D. Amado, H.T. Coelho, Am. J. Phys. **46**, 1057 (1978).

[10] W.C. Damert, Am. J. Phys. **43**, 531 (1975).

[11] M. Razavy, G. Field, and J.S. Levinger, Phys. Rev. **125**, 269 (1962).

[12] J.J. Popiel and S.Y. Larsen, Few-Body Systems, **15**, 129 (1993).

[13] L.I. Ponomarev, S.I. Vinitsky, F.R. Vukajlovich, J. Phys. **B 13**, 847 (1980); Preprint JINR, P4-12018 (Dubna, 1978).

[14] P.R. Bunker and R.E. Moss, Mol. Phys. **33**, 417 (1977).

[15] D.V. Pavlov, I.V. Puzynin, S.I. Vinitsky, JINR E4-99-141 (Dubna, 1999).

[16] D.A. Kirzhnits, F.M. Pen'kov, ZhETP. **85**, 80 (1983).

[17] D.A. Kirzhnits, Nonadiabatic theory of interactions of Van-der-Vaals type, in "Problems of Theoretical Physics and Astrophysics", the volume devoted to 70-th anniversary of V.L. Ginzburg, Edts: L.V. Keldysh, V.Ya. Fainberg (Moscow, Nauka, 1989), p.225 - 239 (in Russian).

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