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Эффект отдачи и кинематика молекулярной модели в реакциях с передачей

В работе рассматриваются кинематические свойства адиабатического (молекулярного) представления волновой функции задачи трех тел, которое может быть использовано при исследовании квазимолекулярных эффектов в реакциях с тяжелыми ионами. Построены матричные преобразования гамильтониана в адиабатическом представлении, которые позволяют поставить граничные условия задачи рассеяния и учесть эффект отдачи при передаче нуклона (кластера) от одного остова к другому.

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Recoil Effect and Kinematics of the Molecular States Approach to Heavy-Ion Transfer Reactions

The kinematic properties of the adiabatic representation of the total wave function which can be useful to demonstrate the molecular features in the heavy-ion transfer reactions are discussed. The matrix transformation of the adiabatic Hamiltonian which simplifies its asymptotic form is then constructed. This allows one to treat the recoil effect in the form of a simple matrix transformation of the adiabatic S-matrix.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

Some experimental data on heavy ion scattering may be described in the framework of nuclear molecular orbitals. The qualitative ideas which serve to introduce this model were used much earlier in atomic physics where this approach is usually referred to as the "perturbed stationary states" method[1] or the adiabatic states representation[2]. The usefulness of the adiabatic representation is unquestionable in the atomic physics, nevertheless, its defects are still being discussed[1,3,4]. These defects become more important with increasing mass of a particle transferred in the course of the reaction. The origin of the problem lies in the fact that a simple one or two-state approximation of the adiabatic representation fails to be successful for some problems. Therefore we need to include more states of the adiabatic basis or, in other words, to take into account the adiabatic corrections. There exists a good illustration of this problem namely, the calculations of the mesoatomic processes in the adiabatic representation when due to the large mass of a muon in comparison with that of an electron for atomic problems the role of the adiabatic corrections may become decisive[5]. This fact was recognized also by many investigators of the heavy-ion transfer problems (refs.[6-8]). The purpose of this paper is to present some recent results on the studies of the properties of the adiabatic representation and to refine upon the treatment of the so-

called recoil effect in the adiabatic representation [6]. This effect (translational exponential factor in atomic physics (refs. [1,3,4])) is initiated also by the finite mass of the valence (transferred) particle. Our treatment will clearly demonstrate the kinematic nature of the difficulties which appear in the adiabatic representation. This encourages us to discuss the problem without specifying the type of the particle interaction, we only suppose that the two-center nuclear problem can be resolved thus providing the basis for the adiabatic representation of the total wave function.

Typical processes to which our model considerations can be applied are discussed in the recent paper of Becker et al. [7] and in the review article of von Oertzen and Bohlen [8].

The review paper of E.Elbaz [6] gives a clear presentation of the treatment of the recoil effect in heavy-ion transfer reaction calculations for other models.

2. COORDINATES AND RECOIL OPERATORS

We restrict ourselves to the analysis of the reactions in which one of the interacting nuclei is described in terms of a structureless core plus a valence nucleon, the other being a bare structureless core. We suppress spin variables. Let $\vec{R}^{(1)}, \vec{R}^{(2)}$ be the coordinate vectors of the cores and $\vec{R}^{(3)}$ that of the valence particle. Then if m_1, m_2 and m_3 are masses of three particles the coordinate transformation

$$\begin{aligned} \vec{\mathcal{R}} &= (m_1\vec{R}^{(1)} + m_2\vec{R}^{(2)} + m_3\vec{R}^{(3)})/\mu, \\ \vec{r} &= \vec{R}^{(3)} - (m_1\vec{R}^{(1)} + m_2\vec{R}^{(2)})/(m_1 + m_2), \\ \vec{R} &= \vec{R}^{(2)} - \vec{R}^{(1)}, \quad \mu = m_1 + m_2 + m_3 \end{aligned} \tag{1}$$

enables us to separate the motion of the CM of the system and gives the internal Hamiltonian of the form

$$H = -\frac{1}{2M}\Delta_{\vec{R}} + V_{12} + H_0 \,, \tag{2}$$

$$H_0 = -\frac{1}{2m}\Delta_{\vec{r}} + V_{13}(r_1) + V_{23}(r_2) \tag{2a}$$

and the Schrödinger CM equation

$$H\Psi(\vec{R},\vec{r}) = E\Psi(\vec{R},\vec{r}). \tag{3}$$

Here we put $\hbar=1$ and introduce the notation

$$1/M = 1/m_1 + 1/m_2\,, \quad 1/m = 1/m_3 + 1/(m_1+m_2)\,, \tag{2b}$$

$$\vec{r}_1 = \vec{R}^{(3)} - \vec{R}^{(1)}\,, \quad \vec{r}_2 = \vec{R}^{(3)} - \vec{R}^{(2)}\,.$$

This choice of variables allows one to "separate" the "molecular" two-center problem with Hamiltonian H_0. The separation is not complete as H_0 depends on R.

We are going to study the exchange reaction

$$(c_1 + n) + c_2 \to c_1 + (c_2 + n) \tag{4}$$

starting with eq. (3). Unfortunately the CM variables $(\vec{R},\vec{r})$ are natural neither for the direct nor for the rearrangement channels of the process (4). The appropriate CM coordinates for the nonreactive scattering channels are $(\vec{R}_1,\vec{r}_1)$, where $\vec{r}_1$ is the position vector of the nucleon with respect to core c_1, and $\vec{R}_1$ is the position vector of core c_2 with respect to the CM of the system (c_1+n). The boundary conditions for the left-hand side of the process (4) have a simple form only in these variables /7/. We perform the transformation from the $(\vec{R},\vec{r})$ coordinates to the $(\vec{R}_1,\vec{r}_1)$ coordinates in two steps by the scheme $(\vec{R},\vec{r}) \to (\vec{R},\vec{r}_1) \to (\vec{R}_1,\vec{r}_1)$.

which can be effected by the unitary operator

$$T_1 = \exp(\beta_1 \vec{r}_1 \nabla_{\vec{R}}) \exp(\alpha_1 \vec{R} \nabla_{\vec{r}}) \qquad (5)$$

with $\alpha_1 = m_2/(m_1+m_2)$ and $\beta_1 = -m_3/(m_1+m_3)$. For the rearrangement channels we use the operator

$$T_2 = \exp(\beta_2 \vec{r}_2 \nabla_{\vec{R}}) \exp(\alpha_2 \vec{R} \nabla_{\vec{r}}) \qquad (6)$$

with $\alpha_2 = -m_1/(m_1+m_2)$ and $\beta_2 = m_3/(m_2+m_3)$. It is easy to verify that T_1 and T_2 operators do accomplish necessary coordinate transformations

$$\begin{aligned} T_i \vec{r} T_i^{-1} &= \vec{r}_i \ , \\ T_i \vec{R} T_i^{-1} &= \vec{R}_i \ , \quad i = 1,2. \end{aligned} \qquad (7)$$

Next we apply T_i transformations to the Schrödinger eq. (3) to receive

$$H_i \Psi_i(\vec{R}_i, \vec{r}_i) = E \Psi_i(\vec{R}_i, \vec{r}_i) \qquad (8)$$

with

$$\begin{aligned} H_i &= T_i H T_i^{-1}, \\ \Psi_i(\vec{R}_i, \vec{r}_i) &= T_i \Psi(\vec{R}, \vec{r}). \end{aligned} \qquad (9)$$

It follows from the definition of T_i that H_i are "good" channel Hamiltonians, thus eqs. (5) and (6) give what can be called the recoil operators as they account for the recoil effect /6-8/. One should expect /9/ that in terms of the adopted basis states the recoil operators have the form of infinite matrices (cf. the discussion of the translational exponential factor in refs. /3,4/).

3. ADIABATIC REPRESENTATION

We use spherical polar coordinates R, θ, Φ for the internuclear vector $\vec{R}$ and write the Hamiltonian (2) in the usual way

$$H=-\frac{1}{2M}\left(\frac{1}{R}+\frac{\partial}{\partial R}\right)^2-\frac{1}{2MR^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\Phi^2}\right\}+V_{12}+H_0. \tag{10}$$

Since potentials in H_0 have the axial symmetry around the axis joining two cores it is helpful to transform the nucleon coordinates to the "body-fixed" coordinate system by the rotation

$$D(\Phi,\theta,0)=\exp(-i\Phi\ell_z)\exp(-i\theta\ell_y). \tag{11}$$

At this step the origin of the nucleon coordinates is taken to be the CM of the nuclei. The transformation to the "geometric center of nuclei" nucleon coordinates may also be useful when introducing the two-center basis. Thus we need an operator of the finite translation

$$T=\exp\left(-i\kappa\frac{R}{2}p_z\right),\quad \kappa=(m_2-m_1)/(m_2+m_1). \tag{12}$$

It can be verified[3] that the effect of the transformations (11) and (12) is reduced to the substitutions in the Hamiltonian (10) of the transformed partial derivatives[3]

$$\begin{aligned}
A^{-1}\frac{\partial}{\partial\theta}A &= \frac{\partial}{\partial\theta}-i\left(\ell_y+\frac{\kappa R}{2}p_x\right),\\
A^{-1}\frac{\partial}{\partial\phi}A &= \frac{\partial}{\partial\phi}-i\left[\ell_z\cos\theta-\left(\ell_x-\frac{\kappa R}{2}p_y\right)\sin\theta\right],\\
A^{-1}\frac{\partial}{\partial R}A &= \frac{\partial}{\partial R}-i\frac{\kappa}{2}p_z,
\end{aligned} \tag{13}$$

with

$$A=TD. \tag{14}$$

The final form of the Hamiltonian

$$\bar{H} = A^{-1} H A \tag{15}$$

can also be obtained by other methods [2,3,7]. This Hamiltonian has a lot of terms and can be partitioned in a number of different ways.

Now we are ready to introduce the adiabatic representation of our problem (4). That means that in the Schrödinger equation

$$\bar{H}\bar{\Psi}(\vec{R},\vec{r}) = E\bar{\Psi}(\vec{R},\vec{r}) \tag{16}$$

we try to expand the total wave function in the form

$$\bar{\Psi}(\vec{R},\vec{r}) = \sum_{\alpha} \psi_{\alpha}^{(1)}(\vec{R})\phi_{\alpha}^{(1)}(\vec{r};R) + \sum_{\beta}\psi_{\beta}^{(2)}(\vec{R})\phi_{\beta}^{(2)}(\vec{r};R), \tag{17}$$

where $\phi_{\alpha}^{(1)}(\vec{r};R)$ and $\phi_{\beta}^{(2)}(\vec{r};R)$ are the solutions of the fixed cores (two-center) problem

$$H_0\phi_{\alpha}^{(i)}(\vec{r};R) = E_{\alpha}^{(i)}(R)\phi_{\alpha}(\vec{r};R). \tag{18}$$

Two summations in (17) represent two types of solutions of equation (18) which account for the valence nucleon forming either $(c_1+n)+c_2$ or $(c_2+n)+c_1$ system in the limit of large R. One may say that the expansion (17) defines the two component form of the wave function. The substitution of (17) into eq. (16) with further integration over nucleon coordinates converts equation (16) into the system of equations for $\psi_{\alpha}^{(i)}(\vec{R})$

$$\bar{H}_{\alpha\beta}^{(ij)}\psi_{\beta}^{(j)}(\vec{R}) = E\psi_{\alpha}^{(i)}(\vec{R}), \tag{19}$$

where

$$\bar{H}_{\alpha\beta}^{(ij)} = -\frac{1}{2M}\{(<\frac{\partial}{\partial R}> + \frac{1}{R})^2\}_{\alpha\beta}^{ij} -$$

$$- \frac{1}{2MR^2}\{\frac{1}{\sin\theta}<\frac{\partial}{\partial\theta}>\sin\theta<\frac{\partial}{\partial\theta}> - \frac{1}{\sin^2\theta}<\frac{\partial}{\partial\Phi}>^2\}^{ij}_{\alpha\beta} + \quad (20)$$

$$+ \{V_{12}\}^{ij}_{\alpha\beta} + E^i_\alpha(R)\delta_{ij}\delta_{\alpha\beta}.$$

The structure of matrices $<\frac{\partial}{\partial R}>$, $<\frac{\partial}{\partial\theta}>$ and $<\frac{\partial}{\partial\Phi}>$ is defined by the right-hand sides of eqs. (13). To put the proper boundary conditions, we need to examine the $R \to \infty$ limit of $\bar{H}^{(ij)}_{\alpha\beta}$. It is easy to observe that the only general simplification we receive in this limit is the degeneration of the matrix Hamiltonian into the two component form

$$\bar{H}^{(ij)}_{\alpha\beta} \to \begin{pmatrix} H^{(11)} & 0 \\ 0 & H^{(22)} \end{pmatrix}. \quad (21)$$

It follows from the different asymptotic character of two subsets $\phi^{(1)}_\alpha(\vec{r};\infty)$ and $\phi^{(2)}_\beta(\vec{r};\infty)$ of the two-center basis and leads to the asymptotic Schrödinger equation of the form

$$\begin{pmatrix} H^{(11)} & 0 \\ 0 & H^{(22)} \end{pmatrix}\begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix} = E\begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix}. \quad (22)$$

The asymptotic Hamiltonians in eq. (22) still have a complicated structure but it is clear that in the adiabatic representation the direct and rearrangement channels can be treated separately in the asymptotic region [3,4]. This is due to the fact that we require different coordinate systems to study the direct and rearrangement channels.

4. ASYMPTOTICALLY ADAPTED ADIABATIC REPRESENTATION

Any coordinate system can be used to derive physical quantities thus in principle it is possible to obtain a formula for the scattering amplitude in the adiabatic representation. But we should expect this formula to have a complicated form due to the fact that coordinates used are unnatural for the asymptotic description of the system. Our aim is to construct an asymptotically simple Hamiltonian.

The specific form of the Hamiltonian (20) which persists to appear in the $R\to\infty$ limit was introduced by the transformation (15). Thus, to diagonalize the operator of the kinetic energy in the asymptotic region we should construct the inverse transformation

$$A_\infty = D_\infty T_\infty \tag{23}$$

with two-component matrices

$$T_\infty = \begin{pmatrix} T_\kappa^{(1)} & 0 \\ 0 & T_\kappa^{(2)} \end{pmatrix} \tag{23a}$$

and

$$D_\infty = \begin{pmatrix} D^{(1)} & 0 \\ 0 & D^{(2)} \end{pmatrix}, \tag{23b}$$

where

$$T_\kappa^{(j)} = \exp(i\kappa \frac{R}{2} < p_z^j >_\infty) \tag{24a}$$

and

$$D^{(j)} = \exp(i\theta < \ell_y^j >_\infty) \exp(i\phi < \ell_z^j >_\infty). \tag{24b}$$

Matrices $\langle p_z^j \rangle_\infty$, $\langle \ell_y^j \rangle_\infty$ and $\langle \ell_z^j \rangle_\infty$ are $R \to \infty$ limits of the equivalent adiabatic matrices.

Thus, if instead of the Schrödinger system (19) with the Hamiltonian $\bar{H}$ we use the transformed Hamiltonian

$$\hat{H} = A_\infty^{-1} \bar{H} A \tag{25}$$

and the wave function

$$\hat{\psi} = A_\infty^{-1} \psi \tag{26}$$

then it follows from (15) and (25) that $\hat{H}$ is reduced in the $R \to \infty$ limit to

$$\hat{H}_{\alpha\beta}^{(ij)}(\infty) = -\frac{1}{2M}\left(\frac{\partial}{\partial R} + \frac{1}{R}\right)^2 - \frac{1}{2MR^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + A_\infty^{-1} E^{(i)}(\infty) A_\infty . \tag{27}$$

This asymptotic Hamiltonian is much simpler than that in the adiabatic representation. The price to be paid for this simplicity is that the "potential energy" matrix becomes to be a function of the orientation angles of the intercore axis. This accounts for the fact that in the decomposition of the total wave function we used the two-center basis which was quantized with respect to the intercore axis and now we treat the collision problem with asymptotic states quantized with respect to an axis fixed in space. The helicity amplitude representation discussed recently by Becker et al.[7] is an alternative approach to the same problem.

The calculation of matrix A is straightforward and can be accomplished analytically for the Coulomb[3] oscillator[10] and separable[14] interactions.

5. RECOIL CORRECTIONS

In the preceding section we have found the Hamiltonian of the asymptotically adapted adiabatic representation for the rearrangement collision problem (4). The asymptotic form of this matrix Hamiltonian is given by eq. (27) and implies that radial and angular parts of the wave function $\hat{\psi}(R)$ should be separated by substituting

$$\hat{\psi}^{(j)}(\vec{R}) = \chi^{(j)}(R) Y_{LM}(\theta, \phi)/R. \qquad (28)$$

Further integration over angular variables produces the system of radial equations which are still coupled in the $R \to \infty$ limit. The direct diagonalization of this radial asymptotic Hamiltonian, which can be accomplished by the constant matrix leads to the asymptotically uncoupled system of equations. This matrix depends on the magnitude of the intercore orbital momentum L (and spin variables). For the sake of simplicity we shall omit its discussion that can be justified to some extent if we restrict our analysis to the case of slow collision and in both the subsets of the expansion (17) choose only degenerate in the $R \to \infty$ limit solutions of the two-center problem. This ansatz forces the asymptotic Hamiltonian to be diagonal. Naturally it leads to the partial omission of the recoil corrections what we shall discuss below.

In this case the Hamiltonian given above in the limit allows us to formulate the boundary conditions in the usual way. This means that the scattering matrix can be found from the asymptotic form of the wave function

$$\Psi(\vec{r}, \vec{R}) \underset{R \to \infty}{\longrightarrow} \frac{1}{2i} \sum_L (2L+1) P_L(\cos\theta) \times \qquad (29)$$

$$\times [(-1)^{L+1} \underline{\psi_L^{(-)}(R)}\, \underline{\phi(\vec{r}, \infty)} + \underline{\psi_L^{(+)}(R)}\, \underline{\phi(\vec{r}; \infty)} S_L^a] \gamma.$$

Here the underlined entities are diagonal matrices and γ is a coefficient matrix. This formula is a direct generalization of the usual three-dimensional partial wave representation of the wave function for our particular case/11/. Now, as follows from the notation (26) and the properties of $\phi_\alpha^{(j)}(\vec{r};R)$ from eq. (18)

$$\phi_\alpha^{(j)}(\vec{r};\infty) = \tilde{\phi}_\alpha^{(j)}(\epsilon_j \vec{r}_j) , \qquad (30)$$

with $\tilde{\phi}_\alpha^{(1)}$ and $\tilde{\phi}_\alpha^{(2)}$ being the wave functions of the free (c_1+n) and (c_2+n) systems, and $\epsilon_j = m/m_{j3}$, where m_{j3} is the reduced mass of the respective pair

$$1/m_{j3} = 1/m_j + 1/m_3 , \qquad (31)$$

Becker et al./7/ have also discussed this property of the two-center basis, and Matveenko and Ponomarev/9/ have already demonstrated in a simple case how this difficulty can be overcome.

Formula (30) gives rise to recoil corrections of the first type which are purely mass dependent and can be taken into account by a matrix of the scale transformation C

$$\underline{\tilde{\phi}^{(j)}(\epsilon_j \vec{r}_j)} = \underline{\tilde{\phi}^{(j)}(\vec{r}_j)} C^{(j)} \qquad (32)$$

which persists to have the two-component form

$$C = \begin{pmatrix} C^{(1)} & 0 \\ 0 & C^{(2)} \end{pmatrix} , \qquad (33)$$

different $C^{(j)}$ acting in different channel subspaces.

Another origin of recoil corrections is the following relations for vector R

$$\vec{R} = (-1)^{(j)}[\vec{R}_j - \vec{r}_j m_3/(m_j + m_3)] \qquad (34)$$

which initiate in the asymptotic region

$$R \approx R_j - m_{j3}/m_j(\vec{R}_j \vec{r}_j)/R_j \ . \qquad (35)$$

This produces the form factor type matrix transformation F

$$\exp[iK^{(j)}(m_{j3}/m_j)(\vec{R}_j \vec{r}_j)/R_j]\underline{\tilde{\phi}^{(j)}(\vec{r}_j)} = \underline{\tilde{\phi}^{(j)}(\vec{r}_j)}F, \qquad (36)$$

again F has the two-component form

$$F = \begin{pmatrix} F^{(1)} & 0 \\ 0 & F^{(2)} \end{pmatrix}. \qquad (37)$$

So we can represent the asymptotic wave function (29) in the form

$$\Psi(R,r) \xrightarrow[R\to\infty]{} \frac{1}{2i}\sum_L (2L+1)P_L(\cos\theta)[(-1)^{L+1}\psi^{(-)}\phi + \psi^{(+)}\phi S_L]\tilde{\gamma} \qquad (38)$$

with the "proper" S-matrix

$$S_L = F^* C S^a_L C^{-1} F^{-1} \qquad (39)$$

and $\tilde{\gamma}$ being a new coefficient matrix.

We have thus transformed the S^a scattering matrix found in the asymptotically adapted adiabatic representation to the equivalent S-matrix which acts between asymptotic states in proper coordinates. The transformation matrices C and F account for the recoil corrections originated by the recoil operators (5) and (6). Their specific forms (32) and (33) could be introduced due to the asymptotic property of the two-center basis given by eq. (30). In the general case both matrices C and F have infinite dimensions, and the finite state decomposition of the wave function introduced earlier should be tested. It follows from our discussion that the finite state ansatz may be expected to be reliable for small mass of the valence particle and for low collision energies. But, in general, different processes should be analysed separately.

6. CONCLUSION

The essential point of our discussion is the suggestion that the two-center problem (quasimolecule) (18) can be solved. The first example when this can be done is the celebrated molecular hydrogen ion[12]. The other example which is more relevant for nuclear problems is the "two-center oscillator", where the complete set of solutions in three dimensions can be constructed, as it was proposed in ref.[13]. A powerful method for solving the two-center problem with separable particle-core interaction has been proposed[14]. This model is especially interesting for the heavy-ion problems. In these particular cases all the matrices introduced in this paper can be computed[3,6,10]. This puts our scheme on some footing. Becker et al.[7] (among others [8]) use the linear combination of separate nucleon orbitals instead of the two-center basis. This formulation can be more practical than ours, nevertheless, it appears to be less convenient to present the essence of the method.

When the molecular features and the exchange are expected to be important in the reaction to be studied, then the program presented in this paper can be realized if a proper two-center basis can be produced. This task becomes much simpler in the two-state approximation[7,8] when almost all the matrices introduced in the text degenerate into diagonal matrices.

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