# Projection Operators in the Unified Reaction Theory*

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A simple form of the projection operators applicable for general rearrangement and exchange processes with full recoil effect is constructed for the unified reaction theory of Feshbach. Channels of different cluster configurations are not orthogonal and the overlap of their wave functions is important. Multidimensional generalization of the wave functions and corresponding wave equations takes this effect into account in a simple way without the complication of solving the integral equations with overlap kernels. Introduction of the projection operators makes it possible to reduce the multiparticle scattering problem in a natural way to that of multiclusters and the dispersive part which involves intermediate states of the compound system. The formalism is compared with the Faddeev equations for the case of three-particle two-cluster reactions, and also with other theories.

## I. INTRODUCTION

THE unified reaction theory of Feshbach[1] requires explicit forms of the projection operators for different channels. By proper choices of these operators it has been possible formally to identify various reaction theories[2] and also to give a systematic discussion of the compound and the direct reactions from a unified point of view. Once the two-body interaction is assumed, then the theoretical basis for the effective interactions between two clusters can be given and their energy dependence and nonlocal properties can be studied in detail. Absence of the interaction radius, which appears in the other theories, makes it especially useful in defining resonance parameters rather unambiguously. It may also be an attractive starting point for the development of approximation methods when the interaction between particles is explicitly given. Several applications of the theory to specific reactions have already been done.[3]

Recently the formalism has also been applied to derive bounds on the reactance matrix.[4,5] When all the open channels at a fixed total energy have been projected out, then the resulting Hamiltonian has the spectrum bounded from below and discrete in the energy region below the threshold for new channels, very much like that in the bound-state problems. Therefore, the various methods to bound the ground-state energies in the bound-state problems apply with trivial modifications. It was assumed however that necessary forms of the projection operators can be given.

Explicit derivation of the projection operators is often very difficult, however, especially when rearrangement and exchange collisions are involved with full recoil effect. Feshbach[1] and Mittleman[6] obtained the specific forms of operators for some simple problems, but even in these cases they involve one or more sets of eigenfunctions generated by the strength-eigenvalue problems associated with certain overlap kernels. It is not likely therefore that such methods can be readily applied in practice to more complicated scattering systems. On the other hand, the problem is more of a *geometrical* rather than a dynamical one in the sense that the short-range behavior of the projection operators is not uniquely defined, and thus can be modified at one's convenience as long as the asymptotic behavior of the total wave function remains unchanged.

We formulate the necessary operators and wave functions in Sec. II and show that all the essential requirements are satisfied. The result is then compared with other formulations, but their equivalence has not been shown explicitly. Our main result is the form of $P$ given by Eq. (11), and the subsequent generalizations of relevant quantities Eqs. (14), (16), and (20), (21).

## II. PROJECTION OPERATORS AND MATRIX EQUATIONS

We start with two essential remarks. Firstly, for problems involving rearrangement collisions it has been known for some time that a basis set in one channel is *not orthogonal* to sets of other channels and that their overlap is important.[7] Furthermore, this affects the nonuniqueness of solutions of the usual Lippmann-Schwinger equations and it was suggested[8] that a multi-

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component form of the wave function should improve the situation. This point has been incorporated into the three-particle scattering by Faddeev[9] and for the general case of many-particle scattering by Weinberg.[10] Secondly, as already stressed by Feshbach, choice of the projection operators is rather *arbitrary* so long as they meet certain standard properties and also give correct projections asymptotically. That is, the form of the operators within the interaction region may be adjusted at one's convenience.

For simplicity we consider only those channels with two clusters, and define the asymptotically independent (AI) channels as those which possess distinct channel Hamiltonians and the asymptotically dependent (AD) channels which do not. Rearrangement channels belong to AI, while inelastic channels without the change of cluster composition belong to the AD channels. Exchange channels involving identical particles are AI but reducible (AIR) in the sense that they do not require additional independent solutions. For formal discussion we will treat the AIR channels as AI channels, keeping the above simplification in mind in the actual application.

Two clusters in $\alpha$th AI channel are denoted by $A_\alpha$ and $B_\alpha$, and their internal Hamiltonians by $h^{A}{}_{\alpha}$ and $h^{B}{}_{\alpha}$. The projection operator of $\alpha$th channel is then given by

$$P_\alpha = P^{A}{}_{\alpha} P^{B}{}_{\alpha} = P^{B}{}_{\alpha} P^{A}{}_{\alpha}, \tag{1}$$

with

$$P_\alpha{}^2 = P_\alpha, \tag{2}$$

$$P^{A}{}_{\alpha}{}^2 = P^{A}{}_{\alpha} = \sum_{i=1}^{D_\alpha} P^{A}{}_{\alpha i}, \tag{3}$$

and

$$P_{\alpha i}{}^{A} = |A_\alpha i\rangle\langle A_\alpha i|. \tag{4}$$

The bound-state functions $|A_\alpha i\rangle$ for the cluster $A_\alpha$ are defined by

$$h^{A}{}_{\alpha}|A_\alpha i\rangle = E^{A}{}_{\alpha,i}|A_\alpha i\rangle, \tag{5}$$

and $D_\alpha$ is the number of AD channels contained in the $\alpha$th AI channel. The total Hamiltonian $H$ can be decomposed in the $\alpha$th channel in the form

$$H = H_\alpha + V_\alpha, \tag{6}$$

with

$$H_\alpha = h^{A}{}_{\alpha} + h^{B}{}_{\alpha} + T_\alpha, \tag{7}$$

where $h$ is the internal Hamiltonian and $T_\alpha$ is the kinetic energy of two clusters, and

$$[P_\alpha, H_\alpha] = 0. \tag{8}$$

The total number of open channels $C$ for a given total energy $E$ is

$$C = \sum_{\alpha=1}^{I} D_\alpha, \tag{9}$$

where $I$ is the total number of AI channels.

The main source of difficulty in deriving the projection operators of AI channels is that

$$[P_\alpha, P_\beta] \neq 0, \quad \text{for} \quad \alpha \neq \beta. \tag{10}$$

The remarks we made earlier suggest a natural way to avoid this problem. We construct the operator in the multicomponent form

$$\mathbf{P} = \begin{bmatrix} P_1 & & & & 0 \\ & P_2 & & & \\ & & P_3 & & \\ & & & \ddots & \\ 0 & & & & P_I \end{bmatrix} \tag{11}$$

and

$$\mathbf{Q} = \mathbf{1} - \mathbf{P}, \tag{12}$$

with

$$\mathbf{P}^2 = \mathbf{P}, \quad \mathbf{Q}^2 = \mathbf{Q}, \quad \text{and} \quad \mathbf{PQ} = 0. \tag{13}$$

Construction of such operators is trivial once the states $|A_\alpha i\rangle$ are separately known.

The wave function and the corresponding wave equation must also be generalized. We define

$$\mathbf{\Psi} = \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \vdots \\ \Psi_I \end{bmatrix}, \tag{14}$$

with

$$\Psi_\alpha = \sum_{i=1}^{D_\alpha} \Psi_{\alpha i} + \sum_{i=D_\alpha+1}^{\infty} \Psi_{\alpha i} \equiv P_\alpha \Psi_\alpha + Q_\alpha \Psi_\alpha. \tag{15}$$

The boundary conditions for $\Psi_{\alpha i}$ are given by

$$\Psi_{\alpha i} \rightarrow (|A_\alpha i\rangle|B_\alpha i\rangle)(a_{\alpha i}\vartheta_{\alpha i} + \sum_{\alpha' i'} a_{\alpha' i'} S_{\alpha i, \alpha' i'} \mathcal{O}_{\alpha i}),$$

where $i' \leqslant D_{\alpha'}$ and $\alpha' \leqslant I$. $\vartheta_{\alpha i}$ and $\mathcal{O}_{\alpha i}$ are the incoming and outgoing waves, respectively, while $a_{\alpha i}$ are the specified initial constant amplitudes, and $S$ is the scattering matrix. $\Psi_{\alpha i}$, with $i > D_\alpha$, goes to zero asymptotically faster than the inverse of the distance between the centers of mass of clusters $A_\alpha$ and $B_\alpha$. We also define $I \times I$ matrix operator

$$\mathbf{H} - \mathbf{E} = (H - E) \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \vdots & & & & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{bmatrix}, \tag{16}$$

which has a well-defined inverse because of the different boundary conditions for each AI channel. The form (16) is very much like the operator used by Mottleson[11] to deal with exchanges. Finally, we have

$$(\mathbf{H} - \mathbf{E})\mathbf{\Psi} = 0, \tag{17}$$

and the Feshbach formalism can be carried out exactly the same way with the operators $\mathbf{P}$ and $\mathbf{Q}$.

[9] L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)].

[10] S. Weinberg, Phys. Rev. **133**, B232 (1964).

[11] B. R. Mottleson, in the Les Houches lecture notes on *The Many-body Problem*, edited by C. DeWitt (John Wiley & Sons, Inc., New York, 1958), p. 283.

Separating out the part of $(\mathbf{H}-\mathbf{E})$ which commutes with $\mathbf{P}$ as

$$(\mathbf{H}-\mathbf{E})=\mathbf{M}+\mathbf{V}, \tag{18}$$

with

$$[\mathbf{M},\mathbf{P}]=0, \tag{19}$$

we have explicitly

$$\mathbf{M}=\begin{bmatrix} H_1-E & & & 0 \\ & H_2-E & & \\ & & \ddots & \\ 0 & & & H_I-E \end{bmatrix}, \tag{20}$$

and

$$\mathbf{V}=\begin{bmatrix} V_1 & H-E & \cdots & H-E \\ H-E & V_2 & \cdots & \vdots \\ \vdots & \vdots & \cdots & \\ H-E & H-E & \cdots & V_I \end{bmatrix}. \tag{21}$$

The interaction $\mathbf{V}$ is by construction explicitly energy-dependent. We also note that the $\mathbf{P}$ component alone gives

$$\mathbf{P}(\mathbf{H}-\mathbf{E})\mathbf{P}\Psi^P=0, \tag{22}$$

which is what one obtains by the resonating-group-structure method.[12] For the complete problem, we have, without approximation,

$$\mathbf{P}[\mathbf{H}-\mathbf{E}+\mathbf{V}\mathbf{Q}(\mathbf{Q}(\mathbf{E}-\mathbf{H})\mathbf{Q})^{-1}\mathbf{Q}\mathbf{V}]\mathbf{P}\Psi=0,$$

where $\mathbf{V}$ is given by Eq. (21).

It has been shown[4] that the exact solution of (22) gives upper bound on the inverse reactance matrix. Furthermore, the variational treatment of the $\mathbf{Q}$ component, which takes into account the effect of closed channels in which clusters are virtually excited, would monotonically improve the bound without destroying the rigor of boundedness.

The $\mathbf{Q}$ component contains the many-particle feature of the original problem, and thus a rigorous treatment of this part requires the method such as that of Faddeev and Weinberg. This is difficult to carry out for most of the physically interesting problems. On the other hand, one often has a detailed knowledge of the structure of the intermediate compound system, and thus it may be possible to develop a reasonably good and simple approximation method. In this way, the nuclear-structure problem is incorporated into the reaction theory in a very natural way.

We also stress the fact that the operators given by (20) and (21) may be a more suitable starting point for formulating the perturbation theory because of the nice asymptotic properties as well as their symmetry, even apart from the simple possibility of introducing projection operators as discussed above.

## III. REARRANGEMENT AND EXCHANGE COLLISIONS

Since exchange scattering is a special case—AIR—of the general rearrangement collisions—AI—and in which identical particles are involved, we consider the AI channels first. For simplicity of discussion we neglect the target recoil and consider the two-channel process $(I=2)$

$$\begin{aligned} 1+(2+C) &\rightarrow 1+(2+C) \\ &\rightarrow (1+2)+C, \end{aligned}$$

where the core $C$ has no internal structure and is of infinite mass, and the particles 1 and 2 are distinguishable. The positron-hydrogen scattering with the elastic and the pickup channels is an example, and Mittleman[6] obtained the explicit form for $P$ for this case, following the prescription of Feshbach.[1]

The operator $\mathbf{P}$ is required to satisfy

$$\mathbf{P}\Psi=\psi_0(r_2)u_0(r_1)+\phi_0(r)v_0(R),$$

and of course

$$\mathbf{P}^2=\mathbf{P}, \quad \mathbf{Q}=\mathbf{1}-\mathbf{P}, \quad \text{with} \quad \mathbf{PQ}=0.$$

The functions $\psi_0$ and $\phi_0$ are the ground-state wave functions of the hydrogen atom and positronium, respectively. The orthonormal sets $\{u_n\}$ and $\{v_n\}$, which are not necessarily complete, can be generated from the homogeneous coupled equations

$$u_n+\lambda_n\int K_1 v_n d\mathbf{r}_2=0,$$

$$v_n+\lambda_n\int K_2 u_n d\mathbf{r}=0,$$

where $u_n(r_1)$ and $v_n(R)$ are the strength eigenfunctions satisfying the decaying boundary conditions asymptotically, and the overlap kernels $K_1$ and $K_2$ are given by

$$K_1=\psi_0(r_2)\phi_0(r)=K_2^{\dagger}.$$

The operator $P$ is then given by

$$P=P_{11}+P_{12}+P_{21}+P_{22}, \tag{23}$$

where

$$P_{11}=|\psi_0(r_2)\rangle\left[\delta(r_1-r_1')+\sum_n \frac{u_n(r_1)u_n^*(r_1')}{\lambda_n^2-1}\right]\langle\psi_0(r_2')|,$$

$$P_{21}=|\phi_0(r)\rangle\sum_n \frac{\lambda_n}{\lambda_n^2-1}v_n(R)u_n^*(r_1')\langle\psi_0(r_2')|,$$

and similarly for $P_{12}$ and $P_{22}$. We note that the second term in $P_{11}$ and in $P_{22}$ and the entire expressions for $P_{12}$ and $P_{21}$ are of short-range character compared to the $\delta$-function term, and that these terms are necessary mainly to cancel the overlap effects of $\psi_0$ and $\phi_0$ such that $P^2=P$ is satisfied.

From the result of Sec. II, we have

$$P_1=|\psi_0(r_2)\rangle\langle\psi_0(r_2')|,$$

$$P_2=|\phi_0(r)\rangle\langle\phi_0(r')|,$$

[12] J. A. Wheeler, Phys. Rev. **52**, 1107 (1937).

and

$$\mathbf{P}=\begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix}. \tag{24}$$

The fact that $P_1P_2 \neq P_2P_1$ has no effect on the wave function since we have now

$$\mathbf{\Psi}=\begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix},$$

and thus

$$\mathbf{P\Psi}=\begin{bmatrix} \psi_0(r_2)u_0(r_1) \\ \phi_0(r)v_0(R) \end{bmatrix}.$$

The equations for $\mathbf{P\Psi}$ and for $\mathbf{P\Psi}^P$ obtained by the two methods are identical, as they should be.

Now we turn to exchange scattering, in which particles 1 and 2 are identical. Simple physical examples are the single-channel elastic $e$–H scattering and $n$-$d$ scattering. Feshbach[1] has given $P$ in the form

$$P=(\mathfrak{A}/\sqrt{2})\{(P_{11}+P_{12})\}(\mathfrak{A}/\sqrt{2}), \tag{25}$$

where

$$P_{11}=|\psi_0(r_1)\rangle\langle\psi_0(r_1')|,$$

$$P_{21}=\sum_{n,\lambda_n\neq 1}(\lambda_n-1)^{-1}|u_n(r_1)\psi_0(r_2)\rangle\langle u_n(r_2')\psi_0(r_1')|,$$

and $\mathfrak{A}$ is the antisymmetrization operator in the case of fermions. Again we observe that $P_{12}$ and $P_{21}$ are the short-range terms. According to Sec. II we have

$$\mathbf{P}=\begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix}, \quad \text{with} \quad P_2=X_{12}P_1, \tag{26}$$

where $X_{12}$ is the exchange operator. The $P$ equation is especially simple and is given by

$$P_1(H-E)(1+X_{12})P_1\Psi_1{}^P=0.$$

In case of $e$–H scattering with the proton being fixed, a much simpler form[4] $P=P_1+P_2-P_1P_2$ suffices, since $r_1$ and $r_2$ are then independent and $[P_1,P_2]=0$.

An attempt was made earlier by Corinaldesi[13] to construct a symmetric theory of $e$–H scattering. With

$$H=T_1+T_2+V_1+V_2+V_{12},$$

he writes

$$\mathbf{M}_C=\begin{bmatrix} T_1+T_2+V_2-E & 0 \\ 0 & T_1+T_2+V_1-E \end{bmatrix}, \tag{27}$$

$$\mathbf{V}_C=\tfrac{1}{2}(V_1+V_2+V_{12})\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \tag{28}$$

and

$$\mathbf{\Psi}_C=\begin{bmatrix} \Psi_{C1} \\ \Psi_{C2} \end{bmatrix}.$$

Obviously $\mathbf{M}_C$ is identical with $\mathbf{M}$ in form, while $\mathbf{V}_C$ is different from $\mathbf{V}$ given in Sec. II, i.e.,

$$\mathbf{V}=\begin{bmatrix} V_1+V_{12} & H-E \\ H-E & V_2+V_{12} \end{bmatrix}. \tag{29}$$

$\mathbf{V}_C$ is quite symmetric in particles 1 and 2, and energy-independent, but the essential complication is carried in this case by the wave function.

Still another formulation is possible, which is due to Faddeev,[8] for the special case of three-particle scattering. We consider the two cluster reactions in which one of the three mutually distinct particles is scattered by the other pair in their bound state. Total energy is restricted so that only elastic and rearrangement scatterings are possible. The total Hamiltonian $H$ is given by

$$H=T_1+T_2+T_3+V_{12}+V_{13}+V_{23},$$

and the transition operator $t$ is given by

$$\begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix}=\begin{bmatrix} t_{23} \\ t_{13} \\ t_{23} \end{bmatrix}+\begin{bmatrix} 0 & t_{23} & t_{23} \\ t_{13} & 0 & t_{13} \\ t_{23} & t_{23} & 0 \end{bmatrix}G_0\begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix},$$

where

$$G_0=(E-H_0+i\epsilon)^{-1},$$

$$t_{ij}=V_{ij}+V_{ij}G_0t_{ij}, \quad i,\ j=1,\ 2,\ \text{and}\ 3\ (i\neq j).$$

For the present purpose, we rewrite the equations for the wave functions in the form

$$\begin{bmatrix} H_0+V_{23}-E & V_{23} & V_{23} \\ V_{13} & H_0+V_{13}-E & V_{13} \\ V_{12} & V_{12} & H_0+V_{12}-E \end{bmatrix}\begin{bmatrix} \Psi_{F1} \\ \Psi_{F2} \\ \Psi_{F3} \end{bmatrix}=0, \tag{30}$$

with the asymptotic boundary conditions on $\Psi_{Fi}$ given by

$$\Psi_{Fi}\rightarrow\psi_i(r_{jk})(a_i\exp[i\mathbf{k}_i\cdot\mathbf{r}_i+i\mathbf{K}_{jk}\cdot\mathbf{R}_{jk}]+b_i\chi_i(r_i,R_{jk})),$$

with $i,\ j,\ k=1,\ 2,\ 3$ in cyclic order, and where $\chi_i$ are the outgoing scattered waves, and

$$(T_{23}+V_{23}-E_n{}^{23})\psi_1(r_{23};n)=0, \text{ etc.}$$

[13] E. Corinaldesi, Nuovo Cimento **24**, 92 and 757 (1962); **27**, 1484 (1963). His wave functions have different character in that $\Psi_{C1}$ for example is a linear combination of the solutions of the ordinary Schrödinger equations with proper symmetry and exchanges. We do not discuss further its connection here.

As before we separate the wave equations into two parts:

$$\mathbf{M}_F=\begin{bmatrix} H_0+V_{23}-E & 0 & 0 \\ 0 & H_0+V_{13}-E & 0 \\ 0 & 0 & H_0+V_{12}-E \end{bmatrix}, \quad (31)$$

and

$$\mathbf{V}_F=\begin{bmatrix} 0 & V_{23} & V_{23} \\ V_{13} & 0 & V_{13} \\ V_{12} & V_{12} & 0 \end{bmatrix}. \quad (32)$$

Again, these are compared with $\mathbf{M}$ and $\mathbf{V}$ of Sec. II. From the assumptions on the model, we have three AI channels, with the total number of open channels $C=3$. Thus we have

$$\mathbf{V}=\begin{bmatrix} V_{13}+V_{12} & H-E & H-E \\ H-E & V_{12}+V_{23} & H-E \\ H-E & H-E & V_{13}+V_{23} \end{bmatrix}, \quad (33)$$

and

$$\mathbf{M}=\mathbf{M}_F. \quad (34)$$

The projection operators $\mathbf{P}$ and $\mathbf{Q}$ are

$$\mathbf{P}=\begin{bmatrix} P_1 & 0 & 0 \\ 0 & P_2 & 0 \\ 0 & 0 & P_3 \end{bmatrix} \quad \text{and} \quad \mathbf{Q}=\mathbf{1}-\mathbf{P}, \quad (35)$$

with

$$P_i=|\psi_i(r_{jk})\rangle\langle\psi_i(r_{jk}')|\,.$$

Introduction of these operators into the Faddeev equations gives in the static approximation ($\mathbf{Q}\Psi=0$),

$$P_1(H_0+V_{23}-E)P_1\Psi_{F1}{}^P + P_1V_{23}(P_2\Psi_{F2}{}^P+P_3\Psi_{F3}{}^P)=0, \quad (36)$$

while the matrix equations of Sec. II give

$$P_1(H-E)P_1\Psi_1{}^P+P_1(H-E)(P_2\Psi_2{}^P+P_3\Psi_3{}^P)=0,$$

or,

$$P_1(H_0+V_{23}-E)P_1\Psi_1{}^P+P_1V_{23}(P_2\Psi_2{}^P+P_3\Psi_3{}^P) = -P_1(V_{12}+V_{13})P_1\Psi_1{}^P - P_1(H_0+V_{12}+V_{13})(P_2\Psi_2{}^P+P_3\Psi_3{}^P). \quad (37)$$

Thus, the two formulations give the same scattering amplitudes if the right-hand side of (37) vanishes. This difference is again of short-range character, and shows that in the region where different AI channel interactions are present the wave functions can be adjusted to suit specific purposes.

## IV. DISCUSSION

We have essentially divided the entire available configuration space into two regions such that the $P$ operator projects onto states which become asymptotically the eigenstates of $\mathbf{M}=(\mathbf{H}-\mathbf{E})_{\text{asymp}}$ outside the ranges of AI channel interactions but still within the AD channel interactions. The complexity of the results derived by Feshbach and by Mittleman arises mainly from the effort to satisfy the requirement $\mathbf{P}^2=\mathbf{P}$, and here this is trivially avoided by rearranging the short-range parts of the wave function $\Psi$ among its components $\Psi_\alpha$.

The formulation of Faddeev and Weinberg stresses the individual-particle aspect of the problem, which is essential in the construction of mathematically consistent theory of many-particle scattering. On the other hand, for the purpose of constructing a reasonably accurate and simple approximation method for the reactions which involve only a few clusters in the initial and final states, the present formulation may be much easier to work with. The multiparticle formalism requires matrix equations of dimension $\frac{1}{2}N(N-1)$, where $N$ is the total number of particles, while the matrix equations of Sec. II requires $I$ dimensions, where usually $I\ll\frac{1}{2}N(N-1)$. When the projection operators are introduced, the $\mathbf{P}$ component can be treated as an $I$-"particle" problem while the many-particle feature of the original problem is contained in the $\mathbf{Q}$ component.

Details of the cluster decomposition of the multiparticle system into multiclusters, approximation methods to solve the resulting matrix equations, and the application of the formalism to low- and high-energy reactions will be given elsewhere.

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