EXTREMAL PROPERTIES OF APPROXIMATE METHODS OF COLLISION THEORY IN THE PRESENCE OF INELASTIC PROCESSES

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A monotonic dependence of the scattering matrix on the potential energy operator is established. It is shown that many numerical methods yield an approximate lower bound for the reactance matrix.

1. INTRODUCTION

VARIATIONAL calculation methods were formulated for collision theory [1-3] and used on the basis of the principles of stationarity of the varied functionals rather than maximality or minimality [4]. They could therefore not be applied directly to the calculation of the upper or lower bounds of the scattering phase shifts and matrices, other than stating that the error in their approximate values is quadratic relative to the error of the trial function, with the question of the sign of the error remaining open. Other approximate methods (the distorted-wave method, the method of strong coupling of a finite number of channels, the adiabatic approximation, the optical model, etc. [5,6]) yielded likewise no information whatever on the sign of the error. Inasmuch as the proposed methods for finding the upper and lower bounds of the scattering phase shift [7] turned out to be too cumbersome for extensive practical utilization, many papers were devoted to approximations by essentially the maximality or minimality methods. The Kohn method was found to provide an upper bound for the scattering length [8,9]. In the case of scattering by a short-range potential that vanishes identically outside a certain finite region, it has been possible to formulate a variational calculation method which gives the lower bound of the scattering phase shift and of the reactance matrix at zero energy [10,11].

Recently Hahn, O'Malley, and Spruch [12] (see also [10]) showed that the elastic-scattering phase shift calculated in the statistical approximation or in the strong-coupling approximation also gives a lower bound for the true scattering phase shift. They also formulated a variational method which gives a lower bound for the scattering phase shift without the need for a short-range potential [13].

In this article we consider the energy when inelastic scattering is possible in addition to elastic scattering. We show that a broad class of approximate methods gives a lower bound for the reactance matrix K, so that the scattering matrix S is connected with its approximate value S_t by a relation $S = S_t \exp(2i\gamma_t)$, where γ_t is a positive matrix [1] that approaches zero monotonically with extension of the trial-function space.

Such a regular behavior is connected with two circumstances. First, there is a monotonic connection between the potential-energy operator in the Schrödinger equation and the reactance matrix. If we subtract from the potential-energy operator a small positive operator, the reactance matrix is augmented in the form of a small positive matrix. Second, neglect of part of the possible intermediate states in the approximate calculations is equivalent to addition of a positive operator to the potential-energy operator.

2. MONOTONIC DEPENDENCE OF THE REACTANCE MATRIX ON THE POTENTIAL-ENERGY OPERATOR

The reactance matrix K, which is connected with the S matrix by the relation

$$S = (1 + iK)(1 - iK)^{-1}, \tag{1}$$

is determined by solving the Schrödinger equation:

$$L\psi = 0, \quad L \equiv \frac{1}{m}\left(\frac{d^2}{dr^2} + k^2\right) - 2V \tag{2}$$

under the following boundary conditions at infinity:

[1] A matrix (or operator) is positive if its corresponding quadratic form is not negative. [14] All eigenvalues and diagonal elements of a positive matrix are non-negative. The sum of positive matrices is positive.

$$\psi(r) \sim (m/k)^{1/2}(\sin\rho + \cos\rho\, K),$$

$$\rho = kr - l\pi/2. \tag{3}$$

In (2) and (3) $\hbar = 1$; ψ —square matrix whose columns are different linearly-independent solutions; l, m, and k —diagonal matrices whose elements are the orbital angular momenta, the reduced masses, and the wave numbers of the channels.

Let us consider two equations of the type (2) and (3) with different potentials V_1 and V_2, and let us set up the matrix

$$\int_0^r (\psi_2^T L_1 \psi_1 - \psi_1^T L_2 \psi_2)\, dr = 0. \tag{4}$$

The superscript T denotes transposition. Using (3), we integrate by parts in (4) and add the results to the transposes. Since V is self-adjoint and K is symmetrical, we obtain

$$K_2 - K_1 = \int_0^\infty [\psi_1^T (V_1 - V_2)\psi_2 + \psi_2^T (V_1 - V_2)\psi_1]\, dr. \tag{5}$$

From (5) follows the monotonic dependence of the matrix K on the potential V. If $V_1 \geq V_2$ and the matrix K varies continuously with continuous transition from V_1 to V_2, then $K_1 \leq K_2$. [Matrix (or operator) inequalities of the type $K_1 \geq K_2$ denote in the present article that the difference $K_2 - K_1$ is a positive matrix. It does not follow from this, for example, that all the elements of the matrix $K_2 - K_1$ must be positive.]

The proof is readily obtained if the potentials V_1 and V_2 differ by a very small quantity $\delta V = V_2 - V_1$. If at the same time the matrices K_1 and K_2 also differ by a very small quantity $\delta K = K_2 - K_1$, then we obtain from (5), accurate to second-order terms in δV,

$$\delta K = -2\int_0^\infty \psi_1^T \delta V \psi_1 dr. \tag{6}$$

The fact that δV is negative indicates that δK is positive.

We prove analogously the monotonicity of the matrix K^{-1}. If $V_1 \geq V_2$ and the matrix K^{-1} varies continuously under continuous transition from V_1 to V_2, then $K_1^{-1} \geq K_2^{-1}$.

Continuity is an essential requirement, for example, in the case of only one open channel $K = \tan\eta$, where η is the scattering phase shift. If the phase shift η goes through $(2n+1)\pi/2$ on going from V_1 to V_2, then K becomes infinite and the inequality $K_1 \leq K_2$ may not hold. We observe the same in the case of many channels. It is typical that violation of the continuity of the matrix K leaves the matrix K^{-1} continuous, and vice versa. This makes it possible to establish the monotonicity of the S matrix irrespective of the continuity of K or K^{-1}.

If $K_2 = K_1 + \delta K$, we obtain from (1), accurate to second-order terms in δK,

$$S_2 = (1 + iK_1)(1 - iK_1)^{-1} + 2i(1 - iK_1)^{-1}\delta K(1 - iK_1)^{-1}, \tag{7}$$

or

$$S_2 = S_1(1 + 2i\delta\gamma) \approx S_1 e^{2i\delta\gamma},$$
$$\delta\gamma \equiv (1 + iK_1)^{-1}\delta K(1 - iK_1)^{-1}. \tag{8}$$

From $\delta K \geq 0$ follows $\delta\gamma \geq 0$. We can prove analogously that when $K_2^{-1} = K_1^{-1} + \delta(K^{-1})$ it follows likewise from $\delta(K^{-1}) \leq 0$ that $\delta\gamma \geq 0$. Repeated application of these inequalities shows that $V_1 \geq V_2$ implies $S_2 = S_1 \exp(2i\gamma)$ with $\gamma \geq 0$ even if the difference $V_2 - V_1$ is not small.

3. APPROXIMATE EXPRESSIONS FOR THE OPTICAL POTENTIAL

Let us consider a calculation method in which the approximate expression for the closed-channel part of the wave function is sought among the finite-dimensional family of functions, and the open-channel part is determined in the same form as in the strong-coupling method. We shall show that the approximations of this method are equivalent to replacing the true optical potential W[15,16] by the integral operator W_t (20), and we shall investigate the conditions under which $W \leq W_t$. If this is satisfied, then the results of the preceding section lead to the inequalities between the approximate and exact values of the matrices S and K.

Let us study the scattering of particle 1 by a target containing particle 2 in the bound state. We assume that particles 1 and 2 are different, and that the energy of particle 1 is sufficient to excite the m lowest states of the target with energies ϵ_p and wave functions $\psi_p(\mathbf{r}_2)$, but is insufficient to excite other states of the target. Following[12], we introduce the projection operators P and Q = 1 − P, which separate the open- and closed-channel parts of the wave function. The operation of P on any function $f(\mathbf{r}_1, \mathbf{r}_2)$ is defined by

$$Pf(\mathbf{r}_1, \mathbf{r}_2) = \sum_{p=1}^{m} \psi_p(\mathbf{r}_2) \int \psi_p(\mathbf{r}_2) f(\mathbf{r}_1, \mathbf{r}_2)\, d\tau_2. \tag{9}$$

According to (9), the open-channel part $P\Psi$ in the wave function is of the form $\sum_{p=1}^{m} u_p(\mathbf{r}_1)\psi_p(\mathbf{r}_2)$. For an approximate representation of the closed-channel part in the form of the sum $\sum_{i=1}^{n} c_i \Phi_i$, we choose n independent square-integrable func-

tions $\Phi_i(\mathbf{r}_1, \mathbf{r}_2)$ orthogonal in the argument $\mathbf{r}_2$ to the target functions for arbitrary $\mathbf{r}_1$:

$$\int \psi_p(\mathbf{r}_2)\,\Phi_i(\mathbf{r}_1, \mathbf{r}_2)\,d\tau_2 = 0, \quad p = 1, \ldots, m. \tag{10}$$

We introduce a projection operator R, which separates from the entire function space the functions of the form

$$\Psi_t = \sum_{p=1}^{m} u_p(\mathbf{r}_1)\,\psi_p(\mathbf{r}_2) + \sum_{i=1}^{n} c_i \Phi_i(\mathbf{r}_1, \mathbf{r}_2) \tag{11}$$

with different functions $u_p(\mathbf{r}_1)$ and coefficients c_i. We seek an approximate solution of the equation

$$(H - E)\Psi = 0, \qquad H = H_1 + H_2 + V(\mathbf{r}_1, \mathbf{r}_2) \tag{12}$$

among the functions (11). To calculate $u_p(\mathbf{r}_1)$ and c_i we use the equation

$$R(H - E)R\Psi_t = 0, \tag{13}$$

which is a projection of Eq. (12) on the space of functions (11). In explicit form, Eq. (13) is a system of differential and algebraic equations

$$\sum_{q=1}^{m} L_{pq} u_q(\mathbf{r}_1) = \sum_{i=1}^{n} \int \psi_p(\mathbf{r}_2)\,V(\mathbf{r}_1, \mathbf{r}_2)\,\Phi_i(\mathbf{r}_1, \mathbf{r}_2)\,d\tau_2 c_i,$$

$$\sum_{j=1}^{n} (E N_{ij} - H_{ij})\,c_j = \sum_{q=1}^{m} \int \Phi_i(\mathbf{r}_1, \mathbf{r}_2)\,V(\mathbf{r}_1, \mathbf{r}_2)\,\psi_q(\mathbf{r}_2)\,u_q(\mathbf{r}_1)\,d\tau_1 d\tau_2,$$

$$L_{pq} = \delta_{pq}(E - H_1 - \varepsilon_p) - V_{pq}(\mathbf{r}_1),$$

$$H_{ij} = \int \Phi_i(\mathbf{r}_1, \mathbf{r}_2)\,H\Phi_j(\mathbf{r}_1, \mathbf{r}_2)\,d\tau_1 d\tau_2,$$

$$N_{ij} = \int \Phi_i(\mathbf{r}_1, \mathbf{r}_2)\,\Phi_j(\mathbf{r}_1, \mathbf{r}_2)\,d\tau_1 d\tau_2,$$

$$V_{pq}(\mathbf{r}_1) = \int \psi_p(\mathbf{r}_2)\,V(\mathbf{r}_1, \mathbf{r}_2)\,\psi_q(\mathbf{r}_2)\,d\tau_2. \tag{14}$$

In addition to the coefficients c_i in (11), the functions $\Phi_i(\mathbf{r}_1, \mathbf{r}_2)$ themselves can depend both linearly and nonlinearly on other parameters (for example scale parameters). The values of these parameters in (11), (13), and (14) are assumed fixed. They are determined not from (14) but from other considerations. A possible criterion for the best choice of the parameters may be formulas (22)—(25).

The system (14) can be simplified by eliminating the coefficients c_i. Following [15], we obtain the eigenvalues $\mathscr{E}^{(\lambda)}$ and the eigenvectors $c_j^{(\lambda)}$ of the equation

$$\sum_{j=1}^{n} (H_{ij} - \mathscr{E}^{(\lambda)} N_{ij})\,c_j^{(\lambda)} = 0. \tag{15}$$

We normalize the functions by

$$\Phi^{(\lambda)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{j=1}^{n} c_j^{(\lambda)} \Phi_j(\mathbf{r}_1, \mathbf{r}_2).$$

We write the second sum in (11) in the form $\sum_{\lambda=1}^{n} b_\lambda \Phi^{(\lambda)}(\mathbf{r}_1, \mathbf{r}_2)$ and determine b_λ from the second equation of (14)

$$b_\lambda = (E - \mathscr{E}^{(\lambda)})^{-1} \sum_{q=1}^{n} \int V_q^{(\lambda)}(\mathbf{r}_1)\,u_q(\mathbf{r}_1)\,d\tau_1,$$

$$V_q^{(\lambda)}(\mathbf{r}_1) = \int \Phi^{(\lambda)}(\mathbf{r}_1, \mathbf{r}_2)\,V(\mathbf{r}_1, \mathbf{r}_2)\,\psi_q(\mathbf{r}_2)\,d\tau_2. \tag{16}$$

Substituting (16) in the first equation of (14) we obtain for the functions $u_p(\mathbf{r}_1)$ an integro-differential equation with degenerate kernel

$$\sum_{q=1}^{m} \left[L_{pq} - \sum_{\lambda=1}^{n} \frac{V_p^{(\lambda)}(\mathbf{r}_1) \int d\tau_1 V_q^{(\lambda)}(\mathbf{r}_1)}{E - \mathscr{E}^{(\lambda)}} \right] u_q(\mathbf{r}_1) = 0. \tag{17}$$

Let us compare (17) with the equation from the theory of the optical potential [15,12]. We write (12) in the form

$$P(H - E)(P + Q)\Psi = 0,$$

$$Q(H - E)(P + Q)\Psi = 0. \tag{18}$$

Eliminating $Q\Psi$ from (18), we obtain for $P\Psi$ the equation

$$P\{E - H - HQ[Q(E - H)Q]^{-1}QH\}P\Psi = 0. \tag{19}$$

Equation (17) differs from (19) in that the optical potential

$$W = PHQ[Q(E - H)Q]^{-1}QHP$$

is replaced by its approximate value

$$W_t = \sum_{\lambda=1}^{n} (E - \mathscr{E}^{(\lambda)})^{-1} V^{(\lambda)}(\mathbf{r}) \int d\tau V^{(\lambda)}(\mathbf{r})$$

$$= PHQR(RQ(E - H)QR)^{-1}RQHP. \tag{20}$$

Thus, the approximate solution of the Schrödinger equation is equivalent to replacing the true optical potential by W_t —an integral operator with degenerate kernel.

Let us investigate the conditions when $W \leq W_t$. We introduce $T = 1 - R$ and $M = Q(H - E)Q$. From the operator identity

$$M^{-1} - R[RMR]^{-1}R = M^{-1}T[TM^{-1}T]^{-1}TM^{-1} \tag{21}$$

it follows that the inequality $W \leq W_t$ is satisfied if $TM^{-1}T \geq 0$.

The energy E lies always below the continuous spectrum of the operator QHQ. If E is lower than the lowest eigenvalue of QHQ, then the operator M is positive and the inequality $W \leq W_t$ is satisfied for any choice of the functions Φ_i. All the denominators $E - \mathscr{E}^{(\lambda)}$ in (20) are in this case negative and all the terms W_t correspond to attraction. If E is larger than the lowest of the eigenvalues QHQ, some terms of W correspond to repulsion, and the inequality $W \leq W_t$ can be proved only by limiting

the choice of the functions Φ_i. It is easy to prove that in order to satisfy the inequality $TM^{-1}T \geq 0$ it is sufficient to choose the functions Φ_i such that (15) gives as many eigenvalues $\mathscr{E}^{(\lambda)}$ lower than E as there are eigenvalues of the operator QHQ lower than E.

If these conditions are satisfied, it follows from the results of Sec. 2 that the exact and approximate values of the S matrix are related by the equation

$$S = S_t e^{2i\gamma_t}, \tag{22}$$

where $\gamma_t \geq 0$. If furthermore the matrix K varies continuously on going continuously from W_t to W, then the following inequality is satisfied

$$K \geqslant K_t. \tag{23}$$

If the matrix K^{-1} varies continuously, the following inequality is satisfied

$$K^{-1} \leqslant K_t^{-1}.$$

Assume that there are two sets of functions Φ_{i1} and Φ_{i2} with $n_2 > n_1$, and that the second set contains all the functions of the first set. If the functions of the first set satisfy the conditions under which (22) is satisfied, then the functions of the second set also satisfy these conditions and $S = S_1 \exp[2i\gamma_1] = S_2 \exp[2i\gamma_2]$ with $\gamma_1 \geq 0$ and $\gamma_2 \geq 0$. Replacing in (22) R by R_1 and M by R_2MR_2, we get

$$W \leqslant W_{t2} \leqslant W_{t1}, \qquad \gamma_1 \geqslant \gamma_2 \geqslant 0. \tag{24}$$

If the continuity conditions are satisfied, we have also

$$K \geqslant K_2 \geqslant K_1, \qquad K^{-1} \leqslant K_2^{-1} \leqslant K_1^{-1}. \tag{25}$$

4. CONCLUSION

1. In the preceding section, particles 1 and 2 were assumed different. The results remain true also if the particles are identical. It is merely necessary to choose the functions Φ_i symmetrical or asymmetrical, and replace (11) by

$$\Psi_t = \sum_{p=1}^{m} (u_p(\mathbf{r}_1)\psi_p(\mathbf{r}_2) \pm u_p(\mathbf{r}_2)\psi_p(\mathbf{r}_1)) + \sum_{i=1}^{n} c_i\Phi_i(\mathbf{r}_1, \mathbf{r}_2).$$

The results of Sec. 3 remain true also if both the target and the incident particles have additional internal degrees of freedom. This causes increases in the number of variables in (11). It is merely important to be able to excite at the energies in question only a finite number of states of the target and of the incident particle, and for the first sum in (11) to contain the wave functions of all these states.

2. In Sec. 3 there is a considerable degree of arbitrariness in the choice of the functions Φ_i, so that many approximate methods are equivalent to the solution of Eqs. (13) and (14). In particular, Eqs. (13) and (14) follow from the variational principles of collision theory[4,6], if the trial functions are chosen in the form (11) and the derivatives $\delta/\delta u_p(\mathbf{r}_1)$ and $\partial/\partial c_i$ of the varied functional are equated to zero. In this connection, the results of the variational calculations with trial functions of the form (11) satisfy inequalities (22)—(25). The equations of the method of strong coupling of a finite number of channels[5,6] are a particular case of (13) and (14), so that the results also satisfy the inequalities (22)—(25). It is essential to take into account here the coupling of all the open channels. The results obtained by allowance for a different number of closed channels are connected by inequalities (24) and (25). The equations for the coefficients $Q\Psi_t$, obtained from the variational principle[13], likewise coincide with (14) once $u_p(\mathbf{r})$ is eliminated from the latter with the aid of the Green's function.

3. The numerical solution of (17), like the solution of any integro-differential equation with degenerate kernel, reduces to a solution of the differential equations

$$\sum_{q=1}^{m} L_{pq}v_q^{(0)}(\mathbf{r}) = 0, \qquad \sum_{q=1}^{m} L_{pq}v_q^{(1)}(\mathbf{r}) = V_p^{(1)}(\mathbf{r}), \ldots,$$
$$\sum_{q=1}^{m} L_{pq}v_q^{(n)}(\mathbf{r}) = V_p^{(n)}(\mathbf{r}) \tag{26}$$

and of the algebraic equations for the determination of the coefficients of the $v_p^{(\lambda)}(\mathbf{r})$ in $u_p(\mathbf{r})$. The need for repeated solution of the equations calls for a margin of accuracy in the intermediate calculations. If we first tabulate the Green's function of the equation $\Sigma_{q=1}^{m} L_{pq}v_q(\mathbf{r}) = 0$, the solution of (26) reduces to an evaluation of integrals. We can solve the system (14) directly without first transforming it into (17).

4. Resonances appear in the calculated cross section near those values of $\mathscr{E}^{(\lambda)}$ [(15), (17)] which lie in the interval of the energies E in question.[15] The requirement that Eq. (15) give as many eigenvalues below E as there are eigenvalues of the operator QHQ is a requirement that the number of the calculated resonances below E coincide with their actual number.

5. Let n functions Φ_i be the first functions of some total set of functions. According to (24), the matrix γ_t decreases monotonically with increasing n. If only the matrices K and K^{-1} exist at the energy in question, we can always choose n

such that on going continuously from W_t to W the matrices K and K^- vary continuously. Consequently, at sufficiently large n, the inequalities (25) are always satisfied, K_t approaches the true value from below, and K_t^- from above.

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