PHYSICAL REVIEW A VOLUME 9, NUMBER 6 JUNE 1974

Addendum to "Variational formulation of the R-matrix method for multichannel scattering"*

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(Received 11 February 1974)

Our recently published variational treatment of the R-matrix method for multichannel scattering requires computations involving unsymmetric matrices. An alternative derivation by Schlessinger and Payne has shown that the method can be reformulated in terms of symmetric matrices. Special techniques applicable to symmetric matrices simplify the computations and improve numerical accuracy.

In a recent paper[1] (referred to hereafter as I) a variational version of the R-matrix theory[2,3] was derived and applied to a two-channel model scattering problem with long-range potentials. The variational approach uses basis functions that are not constrained by a particular boundary condition at r_0, the R-matrix boundary radius. Removing this constraint significantly improves convergence of the variational expansion and makes it possible to use basis functions that greatly simplify the integrals required by the method. However, as formulated in I, the method requires inversion of an unsymmetric matrix whose dimension is the number of basis functions. Numerical difficulties are encountered as the number of basis functions increases, since this matrix becomes singular.

More recently, Schlessinger and Payne[4] have proposed a new method for computing scattering solutions of the Schrödinger equation, which turns out to be equivalent to the variational R-matrix method. This can be seen by comparing the equations given by Schlessinger and Payne with those to be derived here by reformulating the method of I in terms of symmetric matrices. Because special computational techniques are available for symmetric matrices, this revised formulation is preferable to that originally presented. This computational advantage is illustrated here by applying the revised method to a model problem considered in I.

The revised method is derived by replacing Eq. (16) of I by the equivalent equations

$$\sum_q \sum_\beta Q^{pq}_{\alpha\beta} c^{qn}_\beta = \tfrac{1}{2}\eta^p_\alpha(r_0)\lambda_{pn}, \quad \text{all } p, n, \qquad (16')$$

where, in the notation of I, a symmetric matrix Q is defined by

$$Q^{pq}_{\alpha\beta} = M^{pq}_{\alpha\beta} + \tfrac{1}{2}\eta^p_\alpha(r_0)\eta^{p\prime}_\beta(r_0)\delta_{pq}$$
$$= \int_0^{r_0}\left\{\frac{1}{2}\eta^{p\prime}_\alpha\eta^{q\prime}_\beta\delta_{pq} + \eta^p_\alpha\left[\left(\frac{l_p(l_p+1)}{2r^2} - \frac{1}{2}k_p^2\right)\delta_{pq} + V_{pq}\right]\eta^q_\beta\right\} dr .$$

This is the multichannel generalization of the matrix H_{mn} defined by Eq. (2.21) of Ref. 4.

Subsequent equations in I are to be replaced by

$$\sum_q\sum_\beta Q^{pq}_{\alpha\beta}\gamma^{qs}_\beta = \tfrac{1}{2}\eta^p_\alpha(r_0)\delta_{ps}, \qquad (19')$$

$$\rho_{pq}(r) = \frac{1}{2}\sum_\alpha\sum_\beta \eta^p_\alpha(r)(Q^{-1})^{pq}_{\alpha\beta}\eta^q_\beta(r_0), \qquad (20')$$

$$c^{pm}_\alpha = \sum_\sigma \gamma^{p\sigma}_\alpha\lambda_{\sigma m}, \qquad (22')$$

$$u_{pm}(r_0) = \sum_\sigma \rho_{p\sigma}(r_0)\lambda_{\sigma m}, \qquad (23')$$

$$v_{pm}(r_0) = \sum_\sigma \rho_{pq}(r_0)v'_{qm}(r_0), \qquad (24')$$

$$v'_{pm}(r_0) = \sum_q \rho^{-1}_{pq}(r_0)v_{qm}(r_0). \qquad (25')$$

Since Q is a real symmetric matrix, $\rho_{pq}(r_0)$ as defined by Eq. (20′) can be evaluated by a special triangular factorization algorithm[5] that is numerically stable and involves significantly less computation than either inversion or diagonalization of Q. This algorithm was used for the model calculations reported here.

TABLE I. Cross sections Q_{ij}, in units a_0^2, as in Table I of Ref. 1. Numerical results are given in column A. For columns B and D, N = 10 and $r_0 = 8$ and 12, respectively. For columns B′ and D′, N = 16 and $r_0 = 8$ and 12, respectively.

k_1^2		A	B	B′	D	D′
0.1	Q_{11}	18.589	18.593	18.589	18.635	18.595
0.2	Q_{11}	15.539	15.538	15.536	15.559	15.543
0.5	Q_{11}	7.998	7.997	7.997	7.998	7.998
0.7	Q_{11}	5.589	5.588	5.589	5.585	5.588
0.749	Q_{11}	5.170	5.169	5.170	5.165	5.168
0.751	Q_{11}	5.154	5.153	5.154	5.149	5.152
	Q_{12}	0.000	0.000	0.000	0.000	0.000
	Q_{22}	0.260	0.260	0.260	0.260	0.260
0.8	Q_{11}	4.770	4.770	4.770	4.765	4.770
	Q_{12}	0.008	0.008	0.008	0.008	0.008
	Q_{22}	3.741	3.741	3.741	3.741	3.741
1.0	Q_{11}	3.522	3.522	3.522	3.516	3.521
	Q_{12}	0.065	0.065	0.065	0.065	0.065
	Q_{22}	4.044	4.044	4.044	4.044	4.044
1.5	Q_{11}	1.791	1.791	1.791	1.773	1.790
	Q_{12}	0.180	0.180	0.180	0.177	0.180
	Q_{22}	1.884	1.883	1.884	1.889	1.884

The revised variational method has been applied to the two-channel model problem of Matese and Henry,[6] with parameters appropriate to the results given in Table I of I. The new results are given in columns B′ and D′ of Table I, here, with columns A, B, and D copied from I. Column A gives values of cross sections obtained by direct numerical integration; column B gives cross sections computed in I with $r_0 = 8$ and N (the number of monomial basis functions) = 10; for column B′, $r_0 = 8$ and $N = 16$; for column D, copied from I, $r_0 = 12$ and $N = 10$; for column D′, $r_0 = 12$ and $N = 16$. In the calculations reported in I, numerical instabilities began to appear for $N > 10$, and this made it difficult to achieve adequate convergence for $r_0 > 8$. The revised method, as indicated by the results shown in columns B′ and D′ of Table I, can achieve adequate convergence for $r_0 = 12$. The required number of basis functions appears to increase in proportion to r_0. When $N = 10$, the revised method gives results identical with those of the original method, shown as columns B and D in Table I.

*Work supported in part by the Office of Naval Research under Contract No. N0014-72-C0051.

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