JOURNAL OF COMPUTATIONAL PHYSICS 6, 333–335 (1970)

Irregular Solution of a System of Coupled Schrödinger Equations

In some problems of quantum mechanics where it is necessary to solve a system of coupled Schrödinger equations, it is sufficient to know only the regular solution X_{r} and its derivative dX_{r}/dx (e.g., channel coupling theory of nuclear reactions [1]), while in other problems we need also the irregular solution X_{i} and its derivative dX_{i}/dx (e.g., the penetrability in the α radioactive decay [2], the optical penetrability in the theory of isobaric analogue resonances and R-matrix theory [3]). In [4] we derived the regular solution and its derivative for this system of coupled equations. Now, in this note, on the basis of the method exposed in [4], analytical formulas for the irregular solution of the system and its derivative are obtained. As examples of application of these formulas we deduce the irregular solution for the optical model equation and the irregular Coulomb function [5] and their derivatives.

In the framework of the variant III, analyzed in detail in [4], the irregular solution of coupled Schrödinger equations and its derivative can be written as follows [4, formula 21]:

$$\begin{aligned} X_{\mathrm{i}} &= X_{\mathrm{r}} Q \ln x + T G_{12} x^{-\lambda} \\ \frac{dX_{\mathrm{i}}}{dx} &= \frac{dX_{\mathrm{r}}}{dx} Q \ln x + (B_{11} T G_{12} + G_{22})\, x^{-\lambda}. \end{aligned} \tag{1}$$

The same notations as in [4] were used ($Q \equiv U_{12}$, $\lambda I \equiv \Lambda_1$). For the G_{11}^t and G_{21}^t matrices we derived in [4] recurrence relations:

$$\begin{aligned} G_{11}^{t+1} &= \Big[2\lambda P_{11} G_{11}^t + \sum_{s=0}^{t-1} V^s G_{11}^{t-s-1}\Big] \Big/ (t+1)(t+2\lambda), \\ G_{21}^t &= (t+1)\, T G_{11}^{t+1} - P_{11} T G_{11}^t\,. \end{aligned} \tag{2}$$

There are similar recurrence relations for the G_{12}^t and G_{22}^t matrices:

$$\begin{aligned} (t-1)(t-2\lambda)\, G_{12}^t &= 2\lambda T P_{11} T G_{12}^{t-1} + \sum_{s=0}^{t-2} T V^s T G_{12}^{t-s-2} \\ &\quad - [(t-1)T + (t-2\lambda)]\, G_{11}^{t-2\lambda} Q^{2\lambda-1}, \\ G_{22}^t &= (t+1-2\lambda)\, T G_{12}^{t+1} - P_{11} T G_{12}^t + G_{11}^{t+1-2\lambda} Q^{2\lambda-1}. \end{aligned} \tag{3}$$

If the system of equations is reduced to only one, the irregular solution and its derivative for the optical model equation are obtained

$$\chi_i = \chi_r Q \ln x + G_{12} x^{-\lambda}$$
$$\frac{d\chi_i}{dx} = \frac{d\chi_r}{dx} Q \ln x + (B_{11} G_{12} + G_{22})\, x^{-\lambda} \qquad (4)$$

with the following recurrence relations:

$$(t-1)(t-2\lambda)\, G_{12}^t = \beta G_{12}^{t-1} + \sum_{s=0}^{t-2} V^s G_{12}^{t-s-2} - Q(2t-2\lambda-1)\, G_{11}^{t-2\lambda},$$
$$G_{22}^t = (t+1-2\lambda)\, G_{12}^{t+1} - \frac{\beta}{2\lambda} G_{12}^t + Q G_{11}^{t+1-2\lambda}, \qquad (5)$$
$$G_{12}^0 = 0, \qquad G_{22}^0 = 1, \qquad G_{12}^{2\lambda} = 0, \qquad Q = \frac{\beta}{2\lambda} G_{12}^{2\lambda-1} + G_{22}^{2\lambda-1}.$$

In these formulas the terms multiplied by Q vanish for $0 \leqslant t \leqslant 2\lambda$.

If one sets $V^0 = -1$, $V^{s\neq 0} = 0$, in (4) and (5), the irregular part of the Coulomb function $G\gamma$ and its derivative, must be obtained. So we obtain the well-known formulas (17), (18), (22), (19), (20), and (22)–(24) from [5] for the irregular part of the $G\gamma$ function and its derivative, and for the recurrence relations respectively:

$$(G_\gamma)_1 = F_\gamma Q \ln x + G_{12} x^{-(\gamma+1)}$$
$$(G_\gamma')_1 = F_\gamma' Q \ln x + \left[\frac{\beta}{2(\gamma+1)} G_{12} + \frac{(\gamma+1)}{x} G_{12} + G_{22}\right] x^{-(\gamma+1)} \qquad (6)$$

$$(t-1)(t-2\gamma-2)\, G_{12}^t = \beta G_{12}^{t-1} - G_{12}^{t-2} - Q(2t-2\gamma-3)\, G_{11}^{t-2\gamma-2}$$
$$G_{22}^t = (t-2\gamma-1)\, G_{12}^{t+1} - \frac{\beta}{2(\gamma+1)} G_{12}^t + Q G_{11}^{t-2\gamma-1}. \qquad (7)$$

Acknowledgment

The author wishes to thank to Prof. A. Săndulescu for pointing out the necessity of solving this problem.

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RECEIVED: December 8, 1969
REVISED: March 12, 1970

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