Background phase shift in R-matrix theory

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R-matrix theory and other theories involving a division of the configuration space into an internal and an external region are derived in the frame of a projection operator formalism. The continuity condition particularly is investigated. In connection with this problem, we show that the introduction of the hard sphere phase shift is quite arbitrary and that it can be replaced by any other phase shift.

[NUCLEAR REACTIONS R-matrix theory: derivation by means of projection operator formalism. Mathematical origin of the hard sphere phase shift.]

I. INTRODUCTION

In the analysis of many resonance reactions, such as isobaric analog resonances and photonuclear reactions, the R-matrix theory[1] has been used together with the shell-model theory.[2] The respective merits of these two theories have been compared in Ref. 2. In particular, it has been stressed[3] that the main drawback of R-matrix theory is that few levels approximations are bounded to fail whenever the hard sphere phase shift differs from the experimental background phase shift. This situation may, however, be improved by allowing the external region to contain some part of the nuclear interaction, which thus modifies the nonresonant phase shift. In order to achieve a better understanding in the relationship between the two theories, it is highly desirable to have a general formulation of which the R-matrix and shell-model theories are two particular cases. Such a formulation is contained in the comprehensive formalism of Lane and Robson,[4] which has greatly clarified the existing situation. The main aim of the present paper is to construct another general formulation with the help of projection operators, which provide the advantage of writing the continuity condition in a simple way, as we shall see. The projection operators have already been used in the shell-model theory. Hence, we concentrate our attention on the formulation of the R-matrix theory by means of projection operators. More precisely, the aim of this paper is twofold.

(i) We show how to write the R-matrix equations starting from the projection operators. We also show briefly that our formulation contains, moreover, as particular cases, what we shall call the R-matrix-type theories, i.e., the theories which involve a division of the configuration space into an internal and an external region. In some sense, our work is similar to the work by Lane and Robson,[4] for the generality of the formulation, and to the work by Feshbach,[5] for the relation between the R matrix and the projection operator formalism.

(ii) We investigate how the continuity condition has been fulfilled in R-matrix theory. In connection with this problem, we show, and this is the main result of this paper, that the introduction of the hard sphere phase shift is quite arbitrary and that it can be replaced, at least formally, by any other phase shift. This, or course, changes the relation between the resonance parameters and the reduced width amplitudes. We formulate a new theory using this freedom, and exhibit its interest. In particular, we show in a numerical example the advantage of the one-level approximation in this new theory, where the nonresonant phase shift can be chosen appropriately to reproduce the background phase shift.

This work is divided as follows. Sec. II is a brief summary of the projection operators formalism. In Sec. III, we define the projection operators relevant to the R-matrix-type theories. Section IV contains the derivation of the R-matrix equations with the help of projectors. In Sec. V, we sketch the derivation of other R-matrix-type theories. In Sec. VI, we construct a new theory, which generalizes the R-matrix theory, by allowing the nonresonant part of the collision matrix to be different from the hard sphere collision matrix. As an illustration of the new theory, we study the one-level approximation in a numerical case. Section VII contains some conclusions.

II. PROJECTION OPERATORS FORMALISM

We briefly recall the principal feature of this formalism, which has been developed extensively in Ref. 5. Let us assume a Hamiltonian H and two projection operators P and Q such that

$$P^2 = P, \quad Q^2 = Q, \quad PQ = QP = 0\,, \quad P + Q = 1\,. \tag{2.1}$$

The Schrödinger equation

$$(E-H)\psi_E^c=0 \tag{2.2}$$

is equivalent to the following system of equations

$$(E-PHP)P\psi_E^c-PHQ\,Q\psi_E^c=0\,, \tag{2.3a}$$

$$(E-QHQ)Q\psi_E^c-QHP\,P\psi_E^c=0\,. \tag{2.3b}$$

We make the assumption that the asymptotic states of the system (i.e., the states which describe the splitting of the system in two subsystems that do not overlap) is entirely described by the subspace spanned by the projector Q. We assume throughout this paper that the wave function is normalized such that asymptotically we have

$$\psi_E^c\sim Q\psi_E^c\sim\sum_{c'}\frac{1}{\sqrt{v_{c'}}}(I_c\,\delta_{cc'}-S_{c'c}\,O_{c'})\,, \tag{2.4}$$

where $I_{c'}$ and $O_{c'}$ are the familiar incoming and outgoing waves, and where $v_{c'}$ is the relative velocity in channel c'.

We recall the procedure to obtain the scattering matrix from Eqs. (2.3). From Eq. (2.3b), we write

$$Q\psi_E^c=\psi_0^{c\,(+)}+\frac{1}{E^+-QHQ}\,QHP\,P\psi_E^c\,, \tag{2.5}$$

where $\psi_0^{c\,(+)}$ is the scattering wave associated with the Hamiltonian QHQ:

$$(E-QHQ)\psi_0^{c\,(+)}=0\,. \tag{2.6a}$$

The function $\psi_0^{c\,(+)}$ behaves asymptotically like

$$\psi_0^{c\,(+)}\sim\sum_{c'}\frac{1}{\sqrt{v_{c'}}}(I_c\,\delta_{cc'}-S^0_{c'c}\,O_{c'})\,. \tag{2.6b}$$

We put the value of $Q\psi_E^c$ in Eq. (2.3a) and get

$$[E-PHP-PHQ(E^+-QHQ)^{-1}QHP]\,P\psi_E^c=PHQ\psi_0^{c\,(+)}\,. \tag{2.7}$$

We solve Eq. (2.7) for $P\psi_E^c$ and substitute the result in Eq. (2.5); we obtain

$$Q\psi_E^c=\psi_0^{c\,(+)}+\frac{1}{E^+-QHQ}\,QHP\times\frac{1}{E-PHP-PHQ(E^+-QHQ)^{-1}QHP}\,PHQ\,\psi_0^{c\,(+)} \tag{2.8}$$

and for the scattering matrix

$$S_{c'c}=S^0_{c'c}+\frac{i}{\hbar}\langle\psi_0^{c'\,(-)}|\,QHP\,\frac{1}{E-PHP-PHQ(E^+-QHQ)^{-1}QHP}\,PHQ\,|\psi_0^{c\,(+)}\rangle\,. \tag{2.9}$$

We can also find another expression for the wave function in space Q by extracting $P\psi_E^c$ from Eq. (2.3) and inserting its value in Eq. (2.4). We have

$$\left(E-QHQ-QHP\,\frac{1}{E-PHP}\,PHQ\right)Q\psi_E^c=0\,, \tag{2.10}$$

whose solution is

$$Q\psi_E^c=\psi_0^{c\,(+)}+\frac{1}{E^+-QHQ-QHP\,\dfrac{1}{E-PHP}\,PHQ}\,QHP\,\frac{1}{E-PHP}\,PHQ\,\psi_0^{c\,(+)}\;. \tag{2.11}$$

Now, we have

$$\frac{1}{E^+-QHQ-QHP\,\dfrac{1}{E-PHP}\,PHQ}=\frac{1}{E^+-QHQ}+\frac{1}{E^+-QHQ-QHP\,\dfrac{1}{E-PHP}\,PHQ}\times QHP\,\frac{1}{E-PHP}\,PHQ\,\frac{1}{E^+-QHQ}\,. \tag{2.12}$$

We solve this equation for the "perturbed" Green function and we use this result in Eq. (2.11)

$$Q\psi_E^c=\psi_0^{c\,(+)}+\frac{1}{E^+-QHQ}\,\frac{1}{1-QHP\,\dfrac{1}{E-PHP}\,PHQ\,\dfrac{1}{E^+-QHQ}}\,QHP\,\frac{1}{E-PHP}\,PHQ\,\psi_0^{c\,(+)}\,. \tag{2.13}$$

For the scattering matrix, we find

$$S_{c'c}=S^0_{c'c}+\frac{i}{\hbar}\langle\psi_0^{c'\,(-)}|\,\frac{1}{1-QHP\,\dfrac{1}{E-PHP}\,PHQ\,\dfrac{1}{E^+-QHQ}}\,QHP\,\frac{1}{E-PHP}\,PHQ\,|\psi_0^{c\,(+)}\rangle\,. \tag{2.14}$$

Expression (2.9) has been used in most of the existing theories in order to derive a parametrization of the scattering matrix. This is usually achieved, as we show later, by diagonalizing the effective Hamiltonian contained in the left-hand side of Eq. (2.7). Expression (2.14) provides another parametrization of the scattering matrix. If $S^0_{cc'}$ is diagonal in the channel indices, it takes the form of a R-matrix parametrization.

Of course, expressions (2.9) and (2.14) are equivalent. This proceeds from the following relation

$$QHP\frac{1}{E-PHP-PHQ(E^+-QHQ)^{-1}QHP}=\frac{1}{1-QHP\dfrac{1}{E-PHP}PHQ\dfrac{1}{E^+-QHQ}}QHP\frac{1}{E-PHP}, \tag{2.15}$$

that we demonstrate as follows. We have

$$\frac{1}{E-PHP-PHQ\dfrac{1}{E^+-QHP}QHP}=\frac{1}{E-PHP}+\frac{1}{E-PHP}PHQ\frac{1}{E^+-QHQ}QHP\frac{1}{E-PHP-PHQ\dfrac{1}{E^+-QHQ}QHP}. \tag{2.16}$$

Multiplying this equation by QHP on the right and solving it formally, we obtain Eq. (2.15).

III. R-MATRIX TYPE THEORIES

The relevant projection operators are[5]

$$P=\sum_c |\phi_c)\theta(a_c-r_c)(\phi_c|, \tag{3.1}$$

$$Q=\sum_c |\phi_c)\theta(r_c-a_c)(\phi_c|, \tag{3.2}$$

where $\theta(x)=1$ for $x>0$, $\theta(x)=0$ for $x<0$.[6] The quantities r_c, a_c, and ϕ_c are the relative coordinate, the channel radius, and the surface function in channel c, respectively.[1] The operators P and Q fulfill the conditions (2.1) and the commutation relations

$$[H,P]=[H,Q]=0. \tag{3.3}$$

This is easily verified, since for r_c larger than a certain value, which is smaller than or equal to a_c, the Hamiltonian can be represented by

$$\sum_c |\phi_c)\left[-\frac{\hbar^2}{2M_c}\frac{\partial^2}{\partial r_c{}^2}+\frac{l(l+1)\hbar^2}{2M_c r_c{}^2}+z_1z_2\frac{e^2}{r_c}\right](\phi_c|. \tag{3.4}$$

This expresses the absence of polarizing forces beyond a certain distance: That is the basic assumption of R-matrix theory. Equation (3.3) shows that Eq. (2.2) is equivalent to

$$(E-PHP)P\psi^c_E=0, \tag{3.5a}$$

$$(E-QHQ)Q\psi^c_E=0. \tag{3.5b}$$

However, these equations must be complemented by the continuity condition which is not a consequence of the dynamics, but rather of the special structure of the P and Q spaces. The continuity condition may be written as

$$\mathcal{L}_-(b_1)P\psi^c_E=\mathcal{L}_+(b_1)Q\psi^c_E, \tag{3.5c}$$

$$\mathcal{L}_-(b_2)P\psi^c_E=\mathcal{L}_+(b_2)Q\psi^c_E, \tag{3.5d}$$

where $b_1\neq b_2$ and where $\mathcal{L}(b)$ is the Bloch operator,[7]

$$\mathcal{L}(b)=\sum_c\frac{\hbar^2}{2M_c}|\phi_c)\delta(r_c-a_c)\times\left[\frac{d}{dr_c}-\frac{(b_c-1)}{a_c}\right](\phi_c|. \tag{3.6}$$

The plus or minus signs in Eqs. (3.5) mean that the derivative should be taken from outside and inside, respectively. We show later that this is important. The quantities b_1 and b_2 are vectors in a space whose dimension is given by the number of channels. The (in)equality between b_1 and b_2 should be understood as (in)equality between vectors. The continuity condition is strictly

$$\mathcal{L}_-(0)P\psi^c_E=\mathcal{L}_+(0)Q\psi^c_E, \tag{3.7a}$$

$$\mathfrak{M}P\psi^c_E=\mathfrak{M}Q\psi^c_E, \tag{3.7b}$$

where

$$\mathfrak{M}=\sum_c\frac{\hbar^2}{2M_c}|\phi_c)\delta(r_c-a_c)(\phi_c|. \tag{3.8}$$

But, if ψ^c_E satisfies the two relations (3.7), it satisfies relation (3.5c) for *any* value of b_1. On the other hand, if ψ^c_E satisfies (3.5c) and (3.5d), i.e., the equation

$$\mathcal{L}_-(b)P\psi_E^c = \mathcal{L}_+(b)Q\psi_E^c,$$

for *two different* values of b, it satisfies (3.7a) and (3.7b).

There are many ways to rewrite Eqs. (3.5) in a form analogous to (2.3). This freedom has given rise to the variety of the R-matrix-type theories. In fact, we show below that all the freedom has not been fully exploited yet.

IV. R-MATRIX THEORY

We first rewrite Eq. (3.5a) as in Ref. 4:

$$[E - PHP + \mathcal{L}_-(b)]P\psi_E^c = \mathcal{L}_-(b)P\psi_E^c. \quad (4.1)$$

The introduction of the Hamiltonian $PHP - \mathcal{L}_-(b)$ allows to derive an expansion of $P\psi_E^c$ in terms of the eigenstates of an Hermitian Hamiltonian, namely $PHP - \mathcal{L}_-(b)$. This has been shown by Lane and Robson.[4] The continuity condition (3.5c) for $b_1 = b$ and Eq. (4.1) yield

$$[E - PHP + \mathcal{L}_-(b)]P\psi_E^c = \mathcal{L}_+(b)Q\psi_E^c. \quad (4.2a)$$

A similar procedure transforms Eqs. (3.5b) and (3.5d) in which we take $b_2 = \infty$, into

$$[E - QHQ + \mathcal{L}_+(\infty)]Q\psi_E^c = \mathcal{L}_-(\infty)P\psi_E^c. \quad (4.2b)$$

We must be careful and keep in mind that the last equation should be understood as a limiting equation, i.e.,

$$[E - QHQ + \lim_{\beta\to\infty} \mathcal{L}_+(\beta)]Q\psi = \lim_{\beta\to\infty} \mathcal{L}_-(\beta)P\psi. \quad (4.3)$$

The solution $\psi_0^{c(+)}$ of the homogeneous equation

$$[E - QHQ + \mathcal{L}_+(\infty)]\psi_0^{c(+)} = 0, \quad (4.4)$$

where QHQ is given by Eq. (3.4), is the hard sphere wave function in channel c.

We have written the R-matrix basic equations in the form (2.3)–(2.4), with the correspondence

$$PHP \to PHP - \mathcal{L}_-(b), \quad PHQ \to \mathcal{L}_+(b), \quad QHQ \to QHQ - \mathcal{L}_+(\infty), \quad QHQ \to \mathcal{L}_-(\infty). \quad (4.5)$$

Equation (2.7) becomes

$$\left[E - PHP + \mathcal{L}_-(b) - \mathcal{L}_+(b)\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\mathcal{L}_-(\infty)\right]P\psi_E^c = \mathcal{L}_+(b)\psi_0^{c(+)}. \quad (4.6)$$

We show that this equation is strictly equivalent to the equation giving the A_λ in the R-matrix theory. The latter quantities are defined by

$$P\psi_E^c = \sum_\lambda A_\lambda X_\lambda, \quad (4.7a)$$

$$A_\lambda = \langle X_\lambda | P\psi_E^c\rangle. \quad (4.7b)$$

The X_λ's are solutions of the equation

$$[E_\lambda - PHP + \mathcal{L}_-(b)]X_\lambda = 0. \quad (4.8)$$

Introducing the expansion (4.7a) in Eq. (4.6) and projecting on X_λ, we have

$$(E - E_\lambda)A_\lambda - \sum_\mu \langle X_\lambda | \mathcal{L}_+(b)\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\mathcal{L}_-(\infty)|X_\mu\rangle A_\mu = \langle X_\lambda | \mathcal{L}_+(b)|\psi_0^{c(+)}\rangle. \quad (4.9)$$

The Green's function is given by

$$\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)} = -i\sum_c |\phi_c)\frac{M_c}{\hbar^2 k_c}[I_c(r_{c<}) - \Omega_c{}^2 O_c(r_{c<})]O_c(r_{c>})(\phi_c|, \quad (4.10)$$

where $\Omega_c{}^2$ is the diagonal element of the hard sphere collision matrix. The operators $\mathcal{L}_+(b)$ and $\mathcal{L}_-(\infty)$ containing δ functions, we have to take the Green's function at r_c, $r_c' = a_c$. However, it is not the same to take $r_c = r_{c<}$, $r_c' = r_{c>}$ or $r_c = r_{c>}$, $r_c' = r_{c<}$ since the operator $\mathcal{L}_+(b)$ contains a derivative and that the derivative of the Green's function is discontinuous at $r_c = r_c'$. The indices + and − in $\mathcal{L}_+(b)$ and $\mathcal{L}_-(\infty)$ show that we *have* to take $r_c = r_{c>}$, $r_c' = r_{c<}$. Hence, Eq. (4.9) becomes

$$(E - E_\lambda)A_\lambda + i\sum_\mu\sum_c \langle X_\lambda | \mathcal{L}_+(b)|\phi_c O_c(r_c)\rangle\frac{M_c}{\hbar^2 k_c}\langle [I_c(r_c') - \Omega_c{}^2 O_c(r_c')]\phi_c | \mathcal{L}_-(\infty)|X_\mu\rangle A_\mu = v_c{}^{-1/2}\langle X_\lambda | \mathcal{L}_+(b)|(I_c - \Omega_c{}^2 O_c)\phi_c\rangle, \quad (4.11)$$

where we have used Eq. (2.6b). Using the definition (3.6), it can be shown that:

$$\langle X_\lambda | \mathcal{L}_+(b) | \phi_c O_c(r_c)\rangle\!\rangle = \frac{\hbar^2}{2M_c}\left(\frac{2M_c}{\hbar^2 a_c}\right)^{1/2} \gamma_{\lambda c} L_c^0(b) O_c(a_c), \quad (4.12)$$

$$v_c^{-1/2}\langle X_\lambda | \mathcal{L}_+(b) | \phi_c (I_c - \Omega_c{}^2 O_c)\rangle\!\rangle = -i(2\hbar)^{1/2} P_c{}^{1/2}\Omega_c \gamma_{\lambda c}. \quad (4.13)$$

For the matrix element of $\mathcal{L}_-(\infty)$, we have

$$\langle\!\langle (I_c - \Omega_c{}^2 O_c)\phi_c | \mathcal{L}_-(\infty) | X_\mu\rangle = \lim_{\beta\to\infty} \frac{\hbar^2}{2M_c}\int dr_c (u_c(\beta, r_c)\delta(r_c - a_c) \times\left(\frac{d}{dr_c} - \frac{\beta-1}{a_c}\right)\int d\mathcal{S}_c\, \phi_c^* X_\mu, \quad (4.14)$$

where $u_c(\beta, r_c)$ is the radial part of the solution of $[E - QHQ + \mathcal{L}_+(\beta)]\psi = 0$. The following relations hold:

$$\lim_{\beta\to\infty}\int d\mathcal{S}_c\, \phi_c^* X_\mu = \gamma_{\mu c}\left(\frac{2M_c a_c}{\hbar^2}\right)^{1/2}, \quad (4.15)$$

$$\lim_{\beta\to\infty} u_c(\beta, r_c)|_{r_c = a_c} = (I_c - \Omega_c{}^2 O_c)|_{r_c = a_c} = 0, \quad (4.16)$$

$$\lim_{\beta\to\infty} u_c(\beta, r_c)\frac{\beta_c}{a_c} = \frac{d}{dr_c}(I_c - \Omega_c{}^2 O_c)|_{r_c = a_c} = -2i P_c \frac{I_c(a_c)}{a_c}. \quad (4.17)$$

Taking account of all these results and of the relation

$$P_c I_c(a_c) O_c(a_c) = k_c a_c, \quad (4.18)$$

we can rewrite Eq. (4.11) as

$$(E - E_\lambda) A_\lambda + \sum_\mu\left[\sum_c L_c^0(b)\gamma_{\lambda c}\gamma_{\mu c}\right] A_\mu = -i(2\hbar)^{1/2} P_c{}^{1/2}\Omega_c \gamma_{\lambda c}, \quad (4.19)$$

which is the well-known equation for the A_λ coefficients.[1] Equations (4.19) and (2.9) yield the S matrix in terms of the level matrix.

The parametrization of the collision matrix in terms of the R matrix is obtained from Eq. (2.14). We have, using Eq. (4.5):

$$S_{c'c} = S^0_{c'c} + \frac{i}{\hbar} \times \langle \psi_0^{c'(-)} | \left[1 - \mathcal{L}_-(\infty)\frac{1}{E - PHP + \mathcal{L}_+(b)}\mathcal{L}_+(b)\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\right]^{-1} \mathcal{L}_-(\infty)\frac{1}{E - PHP + \mathcal{L}_+(b)}\mathcal{L}_+(b)|\psi_0^{c(+)}\rangle. \quad (4.20)$$

It is easy to check that the operator whose inverse is involved in this equation, when expressed in the basis ψ_0^c, is diagonal in the energy indices, but not in the channel indices. We emphasize that this is a property of R-matrix-type theories, which is due to the separability of the Green function $\{1/[E^+ - QHQ + \mathcal{L}_+(\infty)]\}$ when sandwiched between operators $\mathcal{L}_+$ and $\mathcal{L}_-$. Equation (4.16) becomes:

$$S_{c'c} = S^0_{c'c} + \frac{i}{\hbar^2}\sum_{c''}\left[\delta_{c'c''} + \sum_\lambda \langle \psi_0^{c'(-)} | \mathcal{L}_+(\infty)\left|\frac{X_\lambda\rangle\langle X_\lambda}{E - E_\lambda}\right|\mathcal{L}_+(b)|O_{c''}\phi_{c''}\rangle\right]^{-1}_{cc''} \times\sum_\lambda \langle \psi_0^{c''(-)} | \mathcal{L}_+(\infty)\left|\frac{X_\lambda\rangle\langle X_\lambda}{E - E_\lambda}\right|\mathcal{L}_+(b)|\psi_0^{c(+)}\rangle, \quad (4.21)$$

which, with the help of Eqs. (4.12) to (4.18) reduces to a well-known relation of R-matrix theory [Eq. (VII.1.6a) of Ref. 1]. As an illustration of the power of the projection operators technique, we derive in Appendix the equation (4.19) when a few levels are treated on a separate footing.

V. OTHER R-MATRIX-TYPE THEORIES

A. Freedom in R-matrix-type theories

In Secs. III and IV, we have described the main degrees of freedom contained in the R-matrix theories, i.e., the possibility of introducing mathematical parameters of which the physical quantities, mainly the collision matrix, are independent. These degrees of freedom are related to the channel radii a_c and the quantities b_1 and b_2 of Eqs. (3.5c) and (3.5d). In standard R-matrix theory, the freedom associated with a_c and b_1 has been used, while the freedom associated with b_2 has been left since one takes $b_2=\infty$. We note, incidentally, that an undeterminacy arises in the theory, when $b(=b_1)$ is taken equal to infinity, in agreement with the discussion of Sec. III. A new theory can be constructed by taking advantage of the freedom associated with b_2. We demonstrate later the interest of such a theory.

Finally, other degrees of freedom are lying in the representation of the Green functions $(E-PHP)^{-1}$ and $(E^+-QHQ)^{-1}$. In the following, we review how these degrees of freedom are used in some R-matrix-type theories.

B. Kapur-Peierls theory (Ref. 8)

This theory is differentiated from the standard R matrix by the choice of the value of b_1, namely, the one which corresponds to b in R-matrix theory. Here, the first line in Eq. (4.5) is replaced by

$$PHP\to PHP-\mathcal{L}_-(L_c),\qquad PHQ\to\mathcal{L}_+(L_c)\,. \tag{5.1}$$

Hence [see Eq. (4.12)],

$$\langle X_\lambda|\mathcal{L}_+(L_c)|\phi_c O_c(r_c)\rangle\!\rangle=0\,, \tag{5.2}$$

all other things remaining the same. We draw the attention to the fact that the two parametrizations (2.9) and (2.14) are identical in this theory.

C. Extended R-matrix theory of Tobocman (Ref. 9)

This theory differs from standard R-matrix theory in the fact that the Green's function in the internal region (or the expansion of the inner part of the wave function) is not expressed in terms of the solutions of

$$[E-PHP+\mathcal{L}_-(b)]X_\lambda=0\,, \tag{5.3}$$

but rather of the solutions of

$$[E_\lambda-RHR+\text{B.C.}]X_\lambda=0\,, \tag{5.4}$$

where R contains P $(PR=P)$ and where B.C. means any kind of boundary conditions guaranteeing the completeness of the set $\{X_\lambda\}$ and the Hermiticity of "$RHR-$B.C.." Equation (4.19) is only slightly modified. We have

$$\sum_\mu\Big[E\langle X_\lambda|X_\mu\rangle_P-\langle X_\lambda|H|X_\mu\rangle_P+\sum_c L_c^0(b)\gamma_{\lambda c}\gamma_{\mu c}\Big]A_\mu=-i\,(2\hbar)^{1/2}P^{1/2}\Omega_c\gamma_{\lambda c}\,, \tag{5.5}$$

where the subscript P means that the integration involved must be performed over the P space.

VI. GREEN'S FUNCTION IN THE EXTERNAL REGION: RELATION TO THE BACKGROUND COLLISION MATRIX

In this section, we exploit the freedom associated with the choice of b_2 in Eq. (3.5d) by leaving it unspecified. We show that the interest of such a theory is connected with the problem of the background in the one-level approximation. We note that boundary parameters $b_2\neq\infty$ have been used previously.[10] However, we introduce them in a more natural way relating them to the continuity condition and to the background phase shift.

Instead of Eq. (4.6), we have

$$\left[E-PHP+\mathcal{L}_-(b)-\mathcal{L}_+(b)\,\frac{1}{E^+-QHQ+\mathcal{L}_+(b_2)}\,\mathcal{L}_-(b_2)\right]P\psi_E^c=\mathcal{L}_+(b)\psi_0^{c(+)}\,, \tag{6.1}$$

where $\psi_0^{c(+)}$ is given by

$$\psi_0^{c(+)}=v_c^{-1/2}[I_c(r)-\Omega_c^{\,2}(b_2)O_c(r)]\,\phi_c\,. \tag{6.2}$$

The quantity $\Omega_c^{\,2}(b_2)$ is such that the logarithmic derivative of $\psi_0^{c(+)}$ on the surface is equal to b_2; hence,

$$b_2=a_c\left.\frac{(dI_c/dr_c)-\Omega_c^{\,2}(b_2)(dO_c/dr_c)}{I_c-\Omega_c^{\,2}(b_2)O_c}\right|_{r_c=a_c}\,. \tag{6.3}$$

It is easy to check that we have

$$\Omega_c^{\,2}(b_2)=\frac{[L_c^0(b_2)]^*}{L_c^0(b_2)}\,\Omega_c^{\,2}\,. \tag{6.4}$$

Equation (6.1) gives the wave function in the internal region. The transformation of Eq. (6.1) into an equation for the A_λ's is not as straightforward as in standard R-matrix theory. The reason is that the operator $\mathcal{L}_-(b_2)$ which acts on $P\psi_E^c$ contains a derivative operator at the surface. It is not allowed to commute the derivation and summation operations. However, like in standard R-matrix theory, Eq. (6.1) is useful only if $P\psi_E^c$ is given accurately by a *finite* number of components along the X_λ's. It is only in that case that Eq. (6.1) is interesting, since inverting an infinite matrix is impossible. In the following, we restrict ourselves, as it usually assumed implicitly in most of the theories, that ψ_E^c can be described accurately by a finite number of terms. Then Eq. (6.1) can, using the same method as in Sec. IV, be transformed into

$$(E-E_\lambda)A_\lambda+\sum_\mu\left(\sum_c q_c L_c^0(b)\gamma_{\lambda c}\gamma_{\mu c}\right)A_\mu = -i(2\hbar)^{1/2}P_c{}^{1/2}q_c\Omega_c\gamma_{\lambda c}\,, \quad (6.5)$$

where

$$q_c=\frac{b-b_2}{L_c^0(b_2)}\,. \quad (6.6)$$

It is easy to see that when $b_2\to\infty$, $q_c\to 1$, we recover Eq. (4.19) of standard R-matrix theory. Making $b_2=b$ (in the sense of vectors) gives rise to an undeterminacy ($q_c=0$), as we mentioned in Sec. III.

The scattering matrix reads

$$S_{c'c}=\Omega_c{}^2(b_2)\delta_{cc'}-i\Omega_{c'}q_{c'}P_{c'}{}^{1/2}\gamma_{\lambda c'}\times\sum_\mu\tilde{A}_{\lambda\mu}{}^{-1}P_c{}^{1/2}\Omega_c q_c\gamma_{\lambda c}\,, \quad (6.7)$$

where

$$\tilde{A}_{\lambda\mu}=(E-E_\lambda)\delta_{\lambda\mu}+\sum_c q_c L_c^0(b)\gamma_{\lambda c}\gamma_{\mu c}\,. \quad (6.8)$$

Equation (6.7) may be written as

$$S_{c'c}=\Omega_c{}^2(b_2)\delta_{c'c}-i\sum_{\lambda\mu}\Gamma_{\lambda c'}{}^{1/2}\tilde{A}_{\lambda\mu}{}^{-1}\Gamma_{\mu c}{}^{1/2}\,, \quad (6.9)$$

where

$$\Gamma_{\lambda c}{}^{1/2}=(2P_c)^{1/2}\Omega_c q_c\gamma_{\lambda c}\,. \quad (6.10)$$

The one-level approximation is obtained by selecting only one level λ

$$S_{c'c}=\Omega_c{}^2(b_2)\delta_{c'c}-i\,\frac{\Gamma_{\lambda c}{}^{1/2}\Gamma_{\lambda c'}{}^{1/2}}{E-\mathcal{E}_\lambda}\,, \quad (6.11)$$

where

$$\mathcal{E}_\lambda=E_\lambda-\sum_c q_c L_c^0(b)\gamma_{\lambda c}{}^2\,. \quad (6.12)$$

It can be checked that this approximation is unitary. Here, we demonstrate this property for the one-channel case only. Equations (6.11), (6.12), (6.10), and (6.6) give

$$S_{cc}=\Omega_c{}^2(b_2)-i\,\frac{2P_c\Omega_c{}^2q_c{}^2\gamma_{\lambda c}{}^2}{E-E_\lambda+q_c L_c^0(b)\gamma_{\lambda c}{}^2}\,. \quad (6.13)$$

Equations (6.6) and (6.4) yield

$$\Omega_c{}^2q_c{}^2=\Omega_c{}^2(b_2)|q_c|^2\,. \quad (6.14)$$

Hence, we have

$$S_{cc}=\Omega_c{}^2(b_2)\,\frac{E-E_\lambda+q_c L_c^0(b)\gamma_{\lambda c}{}^2-i\,2P_c|q_c|^2\gamma_{\lambda c}}{E-E_\lambda+q_c L_c^0(b)\gamma_{\lambda c}{}^2}\,. \quad (6.15)$$

Moreover, it can be checked that the following relation holds

$$\mathrm{Im}[q_c L_c^0(b)]=P_c|q_c|^2\,. \quad (6.16)$$

We are finally left with the following form for S_{cc},

$$S_{cc}=\Omega_c{}^2(b_2)\,\frac{E-E_\lambda+q_c^*L_c^0(b)^*\gamma_{\lambda c}{}^2}{E-E_\lambda+q_c L_c^0(b)\gamma_{\lambda c}{}^2}\,, \quad (6.17)$$

which is obviously unitary.

We have tested formula (6.11) in the frame of a simple model developed by Weidenmüller.[11, 12] This model describes a particle interacting with a system of two bound states $|n\rangle$, $n=1, 2$ and assumes that the wave function

$$\psi=f_1|1\rangle+f_2|2\rangle \quad (6.18a)$$

is determined by the two-channel Schrödinger

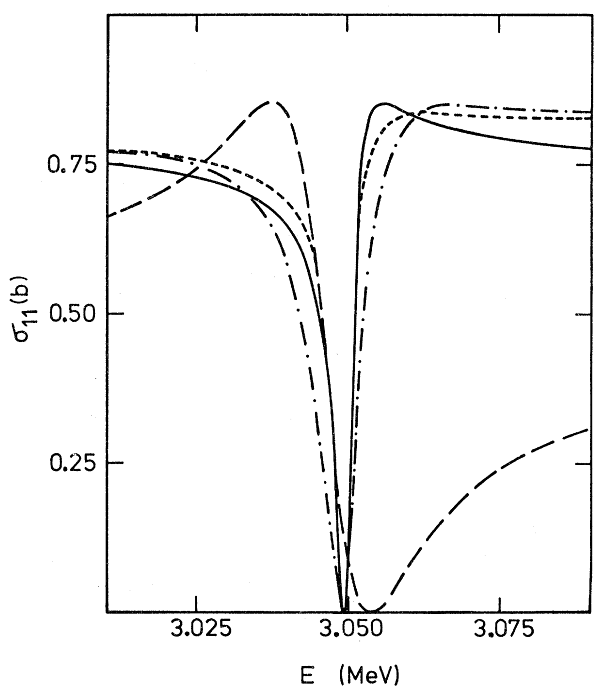

FIG. 1. Cross section in channel 1 of the model described by the Eqs. (6.18). Full curve is the exact cross section. Dashed curve is the standard R-matrix one-level approximation. Dot-and-dashed curve is the value of expression (6.11) for $b_2=1.75$ and $b=0$ in channel 1. Dotted curve is the same for $b=4.6$.

equation

$$\left[\frac{\hbar^2}{2M}\frac{d^2}{dr^2}+E-e_1-V_{11}(r)\right]-V_{12}(r)f_2(r)=0\,, \tag{6.18b}$$

$$-V_{21}(r)f_1(r)+\left[\frac{\hbar^2}{2M}\frac{d^2}{dr^2}+E-e_2-V_{22}(r)\right]f_2(r)=0\,. \tag{6.18c}$$

Moreover, the functions $V_{nm}(r)=V_{mn}(r)$ have a square well shape

$$V_{nm}(r)=V_{nm}\quad(r\leqslant r_0) \tag{6.18d}$$

$$=0\quad(r>r_0)\,. \tag{6.18e}$$

We choose the parameters $r_0=6$ fm, $e_1=0$, $e_2=6$ MeV, $V_{11}=-31$ MeV, $V_{22}=-41$ MeV, $V_{12}=V_{21}=-0.1$ MeV. The square well e_2+V_{22} has a bound state at $E=3.0512$ MeV. Because of the coupling V_{21}, this state changes into a resonance in channel 1. The Eqs. (6.18b) and (6.18c) can be solved using R-matrix techniques (for the detail, see Ref. 3). Lejeune and Mahaux,[3] in their study of this model, stressed that the one-level approximation of the standard R-matrix theory is bound to fail, whenever the hard sphere phase shift is different from the background phase shift. Figure 1 shows the comparison between the exact cross section, the result of the standard R-matrix one-level approximation, and the result of Eq. (6.11). The parameters a_c and b_c have been chosen same as in Ref. 3, namely, $a_c=6$ fm, $b_c=S_c(E_\lambda)$, $c=1,2$. The parameter b_2 $(c=1)$ has been determined by fitting the background, and is equal to 1.75. The remarkable feature of the result is that formula (6.12) not only reproduces the background, but also the width of the resonance. This is probably due to the fact that for $b_c\simeq S_c$, $|q_c|<1$ as shown by Eq. (6.6). We note that the fitting of the background does not uniquely determine the parameter b_2. In general, there are two possible values of b_2. In the numerical case above, the two values are 1.75 and 4.02. The latter one gives a good value for the background and for the width, but does not correctly reproduce the small asymmetry of the resonance, giving a small peak in the cross section below the dip and not above. On the other hand, when the value of b_2 is chosen to reproduce the background, the results are almost independent of b as indicated by the dotted curve of Fig. 1, which corresponds to b $(c=1)=4.6$. We emphasize that, for the standard R-matrix one-level approximation, this value of b yields a good value of the width, but a completely wrong value of the position of the resonance and of the background. It should, however, be noticed that the most sophisticated versions of R-matrix theory yield more satisfactory one-level approximation generally by including more than the hard sphere in the external region.

In both theories (standard R matrix and present theory), the inner wave function for the one-level approximation is practically the same (i.e., proportional to X_λ). Hence, it may be surprising that the two theories give quite different results, specially outside the resonance. We show that this difference comes from the prescription used to obtain the scattering matrix from the internal wave function. The prescription in our theory is different from that used in standard R matrix, and it actually generalizes the latter, as we will see below. The dynamical Eqs. (3.8) show that the external wave function is related to the internal wave function by

$$Q\psi=\psi_0^{c\,(+)}+\frac{1}{E^+-QHQ+\mathcal{L}_+(b_2)}\,\mathcal{L}_-(b_2)P\psi\,, \tag{6.19}$$

where the function $\psi_0^{c\,(+)}$ has a logarithmic derivative equal to b_2 on the surface. We multiply Eq. (6.19) by $\mathcal{L}_+(b_2)$ on the left. We have, with the help of Eq. (4.10) (for b_2 replacing infinity in the argument of $\mathcal{L}$),

$$\mathcal{L}_+(b_2)Q\psi=\mathcal{L}_-(b_2)P\psi\,, \tag{6.20a}$$

or

$$\left[\frac{d}{dr_{c'}}-\frac{(b_2-1)}{a_{c'}}\right]\langle\phi_{c'}|Q\psi\rangle\Bigg|_{S_{c'}}=\left[\frac{d}{dr_{c'}}-\frac{(b_2-1)}{a_{c'}}\right]\langle\phi_{c'}|P\psi\rangle\Bigg|_{S_{c'}}\,. \tag{6.20b}$$

This prescription generalizes the one used in standard R-matrix theory. The latter can be recovered by dividing Eq. (6.20b) by b_2 and making b_2 tend towards infinity. One finds easily

$$\langle\phi_{c'}|Q\psi\rangle\Big|_{S_{c'}}=\langle\phi_{c'}|P\psi\rangle\Big|_{S_{c'}}\,, \tag{6.21}$$

which amounts to equating the external and the internal wave functions on the surface.

The theory of Lane and Robson,[4] when applied to R-matrix-type theories, is entirely based on Eqs. (4.1) and (6.21). The argument above shows that this is equivalent to the Eqs. (4.2) and that the theory of Lane and Robson is implicitly contained in our formalism. We check that prescription (6.20) correctly reproduces the collision matrix for the one-level approximation. The internal wave function is given by [see Eq. (6.5)]:

$$P\psi=\frac{-i\,(2\hbar)^{1/2}P_c^{\;1/2}q_c\Omega_c\gamma_{\lambda c}}{E-E_\lambda+\sum_c q_c L_c^0(b)\gamma_{\lambda c}^{\;2}}\,X_\lambda\,, \tag{6.22}$$

and we write $Q\psi$ as

$$Q\psi=\sum_{c'}\frac{1}{\sqrt{v_{c'}}}(I_{c'}\delta_{cc'}-S_{cc'}O_{c'})\phi_{c'}\ . \tag{6.23}$$

Hence,

$$\left[\frac{d}{dr_{c'}}-\frac{b_2-1}{a_{c'}}\right](\phi_{c'}|P\psi\rangle\Bigg|_{S_{c'}}=\frac{b-b_2}{a_{c'}}(\phi_{c'}|P\psi\rangle\Bigg|_{S_{c'}}=-i\,\frac{b-b_2}{a_{c'}}\left(\frac{2M_{c'}a_{c'}}{\hbar^2}\right)^{1/2}\frac{(2\hbar)^{1/2}P_c{}^{1/2}q_c\Omega_c\gamma_{\lambda c}\gamma_{\lambda c'}}{E-E_\lambda+\sum_c q_c L_c^0(b)\gamma_{\lambda c}{}^2} \tag{6.24}$$

and

$$\left[\frac{d}{dr_{c'}}-\frac{b_2-1}{a_{c'}}\right](\phi_{c'}|Q\psi\rangle\Bigg|_{S_{c'}}=\frac{1}{a_{c'}\sqrt{v_{c'}}}\left[L_{c'}^0(b_2)^*I_{c'}(a_{c'})\delta_{cc'}-S_{cc'}L_{c'}^0(b_2)O_{c'}(a_{c'})\right]. \tag{6.25}$$

Equations (6.24) and (6.25) yield

$$S_{cc'}=\frac{[L_{c'}^0(b_2)]^*I_{c'}(a_{c'})}{L_{c'}^0(b_2)O_{c'}(a_{c'})}\delta_{cc'}-\frac{i(b-b_2)}{L_{c'}^0(b_2)}\frac{(2\hbar)^{1/2}}{O_{c'}(a_{c'})}\frac{P_{c'}{}^{1/2}\Omega_c\gamma_{\lambda c}\gamma_{\lambda c'}}{E-E_\lambda+\sum_c q_c L_c^0(b)\gamma_{\lambda c}{}^2} \tag{6.26}$$

and, with the help of Eqs. (6.4) and (4.18),

$$S_{cc'}=\Omega_c{}^2(b_2)-\frac{i(2P_{c'})^{1/2}q_{c'}\Omega_{c'}\gamma_{\lambda c'}(2P_c)^{1/2}q_c\Omega_c\gamma_{\lambda c}}{E-E_\lambda+\sum_c q_c L_c^0(b)\gamma_{\lambda c}{}^2}\,, \tag{6.27}$$

which is exactly Eq. (6.11). This shows, however, that using the continuity condition in the derivation of the collision matrix from the internal wave function is not a trivial choice as it might appear from the standard derivation of R-matrix theory.

We finally make a remark on the one-level approximation in the one-channel case. It is known, in standard R-matrix theory, that the one-level approximation yields an exact result at $E=E_\lambda$. This is related to the fact that the inner wave function is then equal to X_λ.[13] We show that this result remains in our theory. Indeed, Eqs. (6.11) gives

$$S_{cc}(E_\lambda)=\Omega_c{}^2(b_2)-\frac{i\,2P_c q_c\Omega_c}{L_c^0(b)}\,, \tag{6.28}$$

or, with the help of Eqs. (6.4) and (6.6)

$$S_{cc}(E_\lambda)=\Omega_c{}^2\,\frac{[L_c^0(b_2)]^*L_c^0(b)-2iP_c(b-b_2)}{L_c^0(b_2)L_c^0(b)}=\Omega_c{}^2\,\frac{L_c^0(b_2)[L_c^0(b)]^*}{L_c^0(b_2)L_c^0(b)}\,, \tag{6.29}$$

which is obviously independent of b_2 and is equal to the result of standard R-matrix theory.

VII. CONCLUSIONS

We have formulated the R-matrix theory in terms of projection operators, and have shown how to do the same for other R-matrix-type theories. We find two advantages of such a reformulation. Firstly, it provides a useful tool to compare different theories with each other, since we have a general formalism for all those theories. Secondly, we have exhibited the mathematical origin of the arbitrariness in the R-matrix theory and of the appearance of the hard sphere phase shift in this theory. Particularly, we have shown that the nonresonant collision matrix is quite arbitrary, and that one can choose any other unitary diagonal collision matrix instead of the hard sphere collision matrix. We have constructed a new theory making advantage of this freedom. We have proved on a numerical example, that the one-level approximation in this theory can yield a good description of the background. This is an alternative to the one-level plus constant background approximation in standard R-matrix theory or to one-level approximation of sophisticated R-matrix theory where the external region contains a part of the nuclear interaction.

We are grateful to Professor C. Mahaux for helpful discussions.

APPENDIX

Here, we derive the R-matrix equations when a few levels are treated on a separate footing. Let us divide the P space in two subspaces

$$P=P^0+P'\,, \tag{A1}$$

where P' projects on the retained levels (λ,μ) and P^0 on the unretained ones (σ,τ). Equations (4.2) can be written as

$$[E - P'HP' + \mathcal{L}_-(b)]\,P'\psi_E^c = \mathcal{L}_+(b)Q\psi_E^c\,, \tag{A2}$$

$$[E - P^0HP^0 + \mathcal{L}_-(b)]\,P^0\psi_E^c = \mathcal{L}_+(b)Q\psi_E^c\,, \tag{A3}$$

$$[E - QHQ + \mathcal{L}_+(\infty)]\,Q\psi_E^c = \mathcal{L}_-(\infty)P'\psi_E^c + \mathcal{L}_-(\infty)P^0\psi_E^c\,. \tag{A4}$$

Let us first eliminate P^0. Equations (A3) and (A4) yield

$$\left[E - QHQ + \mathcal{L}_+(\infty) - \mathcal{L}_+(\infty)\frac{1}{E - P^0HP^0 + \mathcal{L}_+(b)}\mathcal{L}_+(b)\right]Q\psi_E^c = \mathcal{L}_-(\infty)P'\psi_E^c\,. \tag{A5}$$

The solution of this equation is

$$Q\psi = \chi_c^{0+} + \mathcal{G}^+\mathcal{L}_-(\infty)P'\psi_E^c\,, \tag{A6}$$

where χ_c^{0+} is the solution of the homogeneous equation obtained from (A5) by setting the right-hand side equal to zero. The Green's function

$$\mathcal{G}^+ = \left[E - QHQ + \mathcal{L}_+(\infty) - \mathcal{L}_-(\infty)\times\frac{1}{E - P^0HP^0 + \mathcal{L}_-(b)}\mathcal{L}_+(b)\right]^{-1} \tag{A7}$$

can be written in the form

$$\mathcal{G}^+ = \frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\times\left[1 - \mathcal{L}_-(\infty)\frac{1}{E - P^0HP^0 + \mathcal{L}_-(b)}\times\mathcal{L}_+(b)\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\right]^{-1}. \tag{A8}$$

Similarly, the function χ_0^{c+} is also given by

$$\langle\chi_0^{c+}| = \langle\psi_0^{c+}|\left[1 - \mathcal{L}_-(\infty)\frac{1}{E - P^0HP^0 + \mathcal{L}_+(b)}\times\mathcal{L}_+(b)\frac{1}{E^+ - QHQ + \mathcal{L}_+(\infty)}\right]^{-1}. \tag{A9}$$

Equations (A2) and (A6) yields

$$[E - P'HP' + \mathcal{L}_-(b) - \mathcal{L}_+(b)\mathcal{G}^+\mathcal{L}_-(\infty)]\,P'\psi_E^c = \mathcal{L}_+(b)\chi_0^{c(+)}\,. \tag{A10}$$

By projecting on the basis spanned by the X_λ, we have

$$(E - E_\lambda)A_\lambda - \sum_\mu\langle X_\lambda|\mathcal{L}_+(b)\mathcal{G}^+\mathcal{L}_-(\infty)|X_\mu\rangle A_\mu = \langle X_\lambda|\mathcal{L}_+(b)|\chi_0^{c(+)}\rangle\,. \tag{A11}$$

We now need a representation for $\mathcal{G}^+$ and $\chi_0^{c(+)}$. It is easy to see that the operator whose inverse is involved in Eqs. (A8) and (A9) is diagonal in the energy indices, when sandwiched between $\psi_c^0(E)$ and $\psi_{c'}^0(E')$. Using this fact, and the results (4.12) to (4.17), it can be shown that the Green's function $\mathcal{G}^+$, when sandwiched between a $\mathcal{L}_+$ operator on the left and a $\mathcal{L}_-$ operator on the right [as in Eq. A(10)] is given by

$$\mathcal{G}^+ = -i\sum_c|\phi_c)\frac{M_c}{\hbar^2k_c}P_c^{\,1/2}\Omega_c v_c^{\,1/2}O_c(r)\times\sum_{c''}[1 - R^0L^0(b)]^{-1}_{cc''}\times\frac{I_{c''}(r') - \Omega_{c''}^{\,2}O_{c''}(r')}{P_{c''}^{\,1/2}\Omega_{c''}v_{c''}^{\,1/2}}(\phi_{c''}|\,. \tag{A12}$$

Similarly the function $\chi_0^{c(+)}$ is given by

$$\chi_0^{c(+)} = \Omega_c P_c^{\,1/2}\sum_{c''}[1 - R^0L^0(b)]^{-1}_{cc''}\times P_{c''}^{\,-1/2}\Omega_{c''}^{-1}\psi_0^{c(+)}\,. \tag{A13}$$

In the last two equations, R^0 is given by

$$R^0_{cc'} = \sum_\sigma\frac{\gamma_{\sigma c}\gamma_{\sigma c'}}{E_\sigma - E}\,. \tag{A14}$$

Using Eqs. (A12) and (A13) and the results (4.12) to (4.17), it is easy to see that Eq. (A12) reduces to

$$(E - E_\lambda)A_\lambda + \sum_\mu\left\{\sum_{cc'}L_c^0(b)\gamma_{\lambda c}[1 - R^0L^0(b)]^{-1}_{cc'}\gamma_{\mu c'}\right\}A_\mu = -i(2\hbar)^{1/2}P_c^{\,1/2}\Omega_c\sum_{c'}(1 - R^0L^0)^{-1}_{cc'}\gamma_{\lambda c'}\,, \tag{A15}$$

which is equivalent to Eq. (IX.1.27) of Ref. 1.

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