Alternative parametrization of *R*-matrix theory

C. R. Brune
Edwards Accelerator Laboratory, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701
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An alternative parametrization of ***R***-matrix theory is presented which is mathematically equivalent to the standard approach, but possesses features that simplify the fitting of experimental data. In particular, there are no level shifts and no boundary-condition constants which allow the positions and partial widths of an arbitrary number of levels to be easily fixed in an analysis. These alternative parameters can be converted to standard ***R***-matrix parameters by a straightforward matrix diagonalization procedure. In addition, it is possible to express the collision matrix directly in terms of the alternative parameters.

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I. INTRODUCTION

The ***R***-matrix theory of reactions has proven over the course of time to be very useful in nuclear and atomic physics, both for the fitting of experimental data and as a tool for theoretical calculations. In this paper we explore a mathematically equivalent alternative formulation of ***R***-matrix theory which will be especially useful for the fitting of experimental nuclear physics data.

In a recent paper an alternative parametrization ***R***-matrix theory was described by Angulo and Descouvemont [1]. In their framework there are no level shifts and it is straightforward to incorporate known information about level energies and partial widths. They presented an approximate iterative relation between the alternative parameters and the standard ***R***-matrix parameters. In addition consideration was limited to the single-channel case with a boundary-condition constant of zero. Some aspects of these alternative parameters have also been discussed in a paper by Barker [2]. In this paper we further develop the concept of an alternative ***R***-matrix parametrization. The description is generalized to allow nonzero boundary-condition constants and an arbitrary number of channels. We present an exact method for converting the alternative parameters to the standard ***R***-matrix parameters which only requires a matrix diagonalization. We also found a rather surprising result, that the collision matrix can be calculated directly from the alternative parameters using alternative formulations of the level matrix or ***R*** matrix. We then discuss the solution of the nonlinear eigenvalue equation required to extract the alternative parameters from the standard parametrization, and demonstrate some of these ideas using a simple example. Finally we briefly discuss the application of the alternative parametrization to γ rays and β decays.

II. REVIEW OF STANDARD *R*-MATRIX THEORY

We begin by reviewing some of the notation and results of standard ***R***-matrix theory as described by Lane and Thomas (LT) [3]. The ***R*** matrix is a function of the energy E and is defined by

$$R_{c'c}=\sum_{\lambda}\frac{\gamma_{\lambda c'}\gamma_{\lambda c}}{E_\lambda-E}, \tag{1}$$

where E_λ are the level energies, $\gamma_{\lambda c}$ are the reduced width amplitudes, λ is the level label, and c is the channel label. We will assume that the numbers of levels and channels are finite and given by N_λ and N_c, respectively. One must also specify the constants B_c, which determine the boundary conditions satisfied by the underlying eigenfunctions.

In order to calculate physical observables one must employ various combinations of the Coulomb wave functions, evaluated at the channel radius $r_c=a_c$. The quantities I_c and O_c are defined by (LT, Eq. II.2.13). For closed channels the outgoing solution O_c is taken to be the exponentially-decaying Whittaker function (LT, Eq. II.2.17). In addition one defines $\Omega_c=(I_c/O_c)^{1/2}$ and

$$L_c=\left(\frac{a_c}{O_c}\frac{\partial O_c}{\partial r_c}\right)_{a_c}=S_c+iP_c, \tag{2}$$

where the shift factor S_c and penetration factor P_c are real quantities. The collision matrix $\boldsymbol{U}$ is an $N_c\times N_c$ matrix which determines the observable quantities; it is related to the $\boldsymbol{R}$ matrix via (LT, Eq. VII.1),

$$\boldsymbol{U}=2\mathrm{i}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}[\mathbf{1}-\boldsymbol{R}(\boldsymbol{L}-\boldsymbol{B})]^{-1}\boldsymbol{R}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}+\boldsymbol{I}\boldsymbol{O}^{-1}, \tag{3}$$

where $\boldsymbol{O}$, $\boldsymbol{I}$, $\boldsymbol{L}$, $\boldsymbol{B}$, and $\boldsymbol{\rho}$ are purely diagonal with elements O_c, I_c, L_c, B_c, and $k_c a_c$, respectively; $\mathbf{1}$ is the unit matrix, and k_c is the wave number.

It is convenient to form the level-space column vector $\boldsymbol{\gamma}_c$ from the $\gamma_{\lambda c}$, and to then form the rectangular matrix $\boldsymbol{\gamma}$ from the $\boldsymbol{\gamma}_c$ such that the matrix $\boldsymbol{\gamma}$ has N_λ rows and N_c columns. In addition, the diagonal matrix $\boldsymbol{e}$ is defined by

$$e_{\lambda\mu}=E_\lambda\delta_{\lambda\mu}. \tag{4}$$

The $\boldsymbol{R}$ matrix defined by Eq. (1) can now be written succinctly as

$$\boldsymbol{R}=\boldsymbol{\gamma}^T(\boldsymbol{e}-E\mathbf{1})^{-1}\boldsymbol{\gamma}. \tag{5}$$

The collision matrix can also be expressed as

$$\boldsymbol{U}=2\mathrm{i}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}\boldsymbol{\gamma}^T\boldsymbol{A}\boldsymbol{\gamma}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}+\boldsymbol{I}\boldsymbol{O}^{-1}, \tag{6}$$

where $\boldsymbol{A}$ is an $N_\lambda\times N_\lambda$ matrix defined by its inverse,

$$\boldsymbol{A}^{-1}=\boldsymbol{e}-E\mathbf{1}-\boldsymbol{\gamma}(\boldsymbol{L}-\boldsymbol{B})\boldsymbol{\gamma}^T. \tag{7}$$

The equivalence of these two forms for the collision matrix is discussed in (LT, Sec. IX.1) and in the Appendix. In addition the elements of the collision matrix connecting open channels in Eq. (6) can also be expressed as

$$U_{c'c}=\Omega_{c'}\Omega_c[\delta_{c'c}+2\mathrm{i}(P_{c'}P_c)^{1/2}\boldsymbol{\gamma}_{c'}^T\boldsymbol{A}\boldsymbol{\gamma}_c], \tag{8}$$

using the definitions of the Coulomb functions.

An interesting feature of $\boldsymbol{R}$-matrix theory is that the collision matrix is invariant under changes in the B_c, provided that the E_λ and $\gamma_{\lambda c}$ are suitably adjusted. This result remains true even for the case of finite N_λ [4]. The transformation is most easily described using matrix equations in level space. Let us consider the transformation $B_c \to B_c'$, $E_\lambda \to E_\lambda'$, and $\gamma_{\lambda c}\to\gamma_{\lambda c}'$. One first constructs the real and symmetric matrix $\boldsymbol{C}$ defined by

$$\boldsymbol{C}=\boldsymbol{e}-\sum_c \boldsymbol{\gamma}_c\boldsymbol{\gamma}_c^T(B_c'-B_c), \tag{9}$$

which is diagonalized by the orthogonal matrix $\boldsymbol{K}$ such that $\boldsymbol{D}=\boldsymbol{KCK}^T$, with $D_{\lambda\mu}=D_\lambda\delta_{\lambda\mu}$. The necessary transformation of the $\boldsymbol{R}$-matrix parameters is then given by [4]

$$E_\lambda'=D_\lambda \tag{10}$$

and

$$\boldsymbol{\gamma}_c'=\boldsymbol{K}\boldsymbol{\gamma}_c. \tag{11}$$

It is straightforward to verify by substitution into Eqs. (6) and (7) that these transformations leave $\boldsymbol{U}$ invariant.

III. THE ALTERNATIVE PARAMETRIZATION

A. Definition of the parametrization

We begin by defining the real and symmetric matrix $\boldsymbol{\mathcal{E}}$:

$$\boldsymbol{\mathcal{E}}=\boldsymbol{e}-\sum_c \boldsymbol{\gamma}_c\boldsymbol{\gamma}_c^T(S_c-B_c), \tag{12}$$

and consider the eigenvalue equation

$$\boldsymbol{\mathcal{E}}\boldsymbol{a}_i=\tilde{E}_i\boldsymbol{a}_i, \tag{13}$$

where $\tilde{E}_i$ is the eigenvalue and $\boldsymbol{a}_i$ is the corresponding eigenvector. Note that $\boldsymbol{\mathcal{E}}$ is implicitly dependent upon $\tilde{E}_i$ through S_c, so the eigenvalue problem is nonlinear. We will assume for convenience that the eigenvectors are normalized so that $\boldsymbol{a}_i^T\boldsymbol{a}_i=1$.

Before proceeding further we would like to point out two important properties of this eigenvalue equation: (1) The eigenvalues $\tilde{E}_i$ are invariant if the B_c are changed and the E_λ and $\gamma_{\lambda c}$ are changed according to Eqs. (10) and (11). This result is easily shown by substituting Eqs. (9)–(11) into Eqs. (12) and (13). (2) If $B_c=S_c(E_\lambda)$, the matrix $\boldsymbol{\mathcal{E}}$ is diagonal for the energy E_λ and hence E_λ is an eigenvalue. For this choice of B_c the $\boldsymbol{R}$-matrix level energy E_λ is often taken to be the "observed resonance energy." This definition is particularly useful in the present context and we will thus adopt the $\tilde{E}_i$ as the observed resonance energies. The $\tilde{E}_i$ also correspond exactly to the level energies found using boundary-condition constant transformations yielding $B_c=S_c(E_\lambda)$ such as described by Barker [2] and Azuma *et al.* [5].

In addition one can define a new set of reduced width parameters $\tilde{\gamma}_{ic}$ via

$$\tilde{\gamma}_{ic}=\boldsymbol{a}_i^T\boldsymbol{\gamma}_c. \tag{14}$$

These new reduced width parameters are also invariant under changes in B_c. When $B_c=S_c(E_\lambda)$, we have also $\tilde{\gamma}_{\lambda c}=\gamma_{\lambda c}$. The quantities $\tilde{E}_i$ and $\tilde{\gamma}_{ic}$ can be taken as an alternative parametrization of $\boldsymbol{R}$-matrix theory. We will derive below efficient methods to convert $\tilde{E}_i$ and $\tilde{\gamma}_{ic}$ into the standard $\boldsymbol{R}$-matrix parameters E_λ and $\gamma_{\lambda c}$, or to the collision matrix $\boldsymbol{U}$. Also note that $\tilde{E}_i$ and $\tilde{\gamma}_{ic}$ are equivalent to the "superscript (λ)" parameters of Barker [2], and essentially equivalent to the "observed" $\boldsymbol{R}$-matrix parameters described by Angulo and Descouvemont [1].

Our Eq. (13) is closely related to the complex eigenvalue equation introduced by Hale, Brown, and Jarmie [6] to locate the poles of the collision matrix—in fact it is just the real part of their eigenvalue equation. For bound states our $\tilde{E}_i$ are thus equivalent to the eigenvalues discussed in Ref. [6] since $P_c=0$. For these states we can also introduce the asymptotic normalization constant C_{ic} which is given by [7]

$$C_{ic}^2=\frac{2\mu_c a_c}{\hbar^2 O_c^2}\left[\frac{\tilde{\gamma}_{ic}^2}{1+\sum_c \tilde{\gamma}_{ic}^2\left(\frac{dS_c}{dE}\right)_{\tilde{E}_i}}\right], \tag{15}$$

where μ_c is the reduced mass. This quantity is simply related to the pole residues described by Eq. (4) of Ref. [6]. For unbound states there appears to be no simple relation between $\tilde{E}_\lambda$ and $\tilde{\gamma}_{\lambda c}$ and the pole parameters of Ref. [6]. One may, however, define the observed partial width of a level in terms of our parameters by

$$\Gamma_{ic}=\frac{2P_c\tilde{\gamma}_{ic}^2}{1+\sum_c \tilde{\gamma}_{ic}^2\left(\frac{dS_c}{dE}\right)_{\tilde{E}_i}} \tag{16}$$

(see LT, Eqs. XII.3.5 and XII.3.6). One should bear in mind, however, that there are many different definitions of observed resonance energies and widths in use; generally the differences between definitions are significant only for broad states.

B. Relation to standard parameters

We will next show the method to convert $\tilde{E}_\lambda$ and $\tilde{\gamma}_{\lambda c}$ to standard $\boldsymbol{R}$-matrix parameters. It is assumed that the eigenvalues are distinct, so that $\tilde{E}_i\neq\tilde{E}_j$ provided $i\neq j$. Note that if this were not the case the levels with the same $\tilde{E}_i$ could be combined into a single level. The eigenvectors of Eq. (13) are not orthogonal; using the eigenvalue equation with two different eigenvalues one finds

$$\boldsymbol{a}_j^T(\boldsymbol{\mathcal{E}}_j-\boldsymbol{\mathcal{E}}_i)\boldsymbol{a}_i=(\tilde{E}_j-\tilde{E}_i)\boldsymbol{a}_j^T\boldsymbol{a}_i, \tag{17}$$

where $\boldsymbol{\mathcal{E}}_i$ is used to denote the matrix $\boldsymbol{\mathcal{E}}$ evaluated for the energy $\tilde{E}_i$. Using Eqs. (12) and (14) with this result we obtain

$$\boldsymbol{a}_j^T\boldsymbol{a}_i=-\sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc}\frac{S_{ic}-S_{jc}}{\tilde{E}_i-\tilde{E}_j}, \tag{18}$$

where S_{ic} denotes the shift function S_c evaluated at $\tilde{E}_i$. By similarly evaluating $\boldsymbol{a}_j^T(\boldsymbol{\mathcal{E}}_j+\boldsymbol{\mathcal{E}}_i)\boldsymbol{a}_i$, one finds that

$$\boldsymbol{a}_j^T\boldsymbol{e}\boldsymbol{a}_i=\frac{\tilde{E}_i+\tilde{E}_j}{2}\boldsymbol{a}_j^T\boldsymbol{a}_i+\sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc}\left(\frac{S_{ic}+S_{jc}}{2}-B_c\right). \tag{19}$$

These results are summarized in the matrices $\boldsymbol{M}$ and $\boldsymbol{N}$,

$$\boldsymbol{a}_j^T\boldsymbol{a}_i\equiv M_{ij}=\begin{cases}1 & i=j\\ -\sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc}\dfrac{S_{ic}-S_{jc}}{\tilde{E}_i-\tilde{E}_j} & i\neq j\end{cases} \tag{20}$$

and

$$\boldsymbol{a}_j^T\boldsymbol{e}\boldsymbol{a}_i\equiv N_{ij}=\begin{cases}\tilde{E}_i+\sum_c \tilde{\gamma}_{ic}^2(S_{ic}-B_c) & i=j\\ \sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc}\left(\dfrac{\tilde{E}_iS_{jc}-\tilde{E}_jS_{ic}}{\tilde{E}_i-\tilde{E}_j}-B_c\right) & i\neq j.\end{cases} \tag{21}$$

Note that the construction of $\boldsymbol{N}$ requires the adoption of specific B_c values.

The eigenvectors of Eq. (13) can be arranged into a square matrix $\boldsymbol{a}$ such that Eq. (14) becomes

$$\tilde{\boldsymbol{\gamma}}_c=\boldsymbol{a}^T\boldsymbol{\gamma}_c. \tag{22}$$

The matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ defined above can then be written as $\boldsymbol{M}=\boldsymbol{a}^T\boldsymbol{a}$ and $\boldsymbol{N}=\boldsymbol{a}^T\boldsymbol{e}\boldsymbol{a}$. From Eq. (4) the matrix $\boldsymbol{e}$ trivially satisfies the eigenvalue equation

$$\boldsymbol{e}\boldsymbol{u}_\lambda=E_\lambda\boldsymbol{u}_\lambda. \tag{23}$$

Upon substitution of $\boldsymbol{u}_\lambda=\boldsymbol{a}\boldsymbol{b}_\lambda$ and multiplying from the left by $\boldsymbol{a}^T$ this equation becomes

$$\boldsymbol{N}\boldsymbol{b}_\lambda=E_\lambda\boldsymbol{M}\boldsymbol{b}_\lambda. \tag{24}$$

This eigenvalue equation holds the key for transforming from the $\tilde{E}_i$-$\tilde{\gamma}_{ic}$ representation to the standard $\boldsymbol{R}$-matrix parameters E_λ and $\gamma_{\lambda c}$. The real, symmetric, and energy-independent matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ are completely determined by $\tilde{E}_i$, $\tilde{\gamma}_{ic}$, and B_c using Eqs. (20) and (21). The E_λ can thus be determined by finding the eigenvalues of a generalized eigenvalue equation. If the matrix $\boldsymbol{M}$ is also positive definite then Eq. (24) is known as the symmetric-definite eigenvalue problem and has N_λ real eigenvalues (see Sec. 8.7 of Ref. [8]). The off-diagonal elements of $\boldsymbol{M}$ are $\approx-\Sigma_c\tilde{\gamma}_{ic}\tilde{\gamma}_{jc}(dS_c/dE)$ which is typically small compared to unity; $\boldsymbol{M}$ will be positive definite provided the $\tilde{\gamma}_{ic}$ are not too large and the energy dependences of S_c are not too great. Further if $\boldsymbol{M}$ is not positive definite, the eigenvectors $\boldsymbol{a}_i$ are not real and the transformation to standard $\boldsymbol{R}$-matrix parameters is not defined. We thus conclude that for physically reasonable $\tilde{\gamma}_{ic}$, $\tilde{E}_i$, and S_{ic}, the matrix $\boldsymbol{M}$ will be positive definite; in practice we have found this condition to be easily fulfilled. Finally note that $\boldsymbol{M}$ is automatically positive definite for any given set of standard parameters since $\boldsymbol{M}=\boldsymbol{a}^T\boldsymbol{a}$.

The eigenvectors of Eq. (24) $\boldsymbol{b}_\lambda$ can be arranged into a square matrix $\boldsymbol{b}$ which satisfies the relations

$$\boldsymbol{b}^T\boldsymbol{M}\boldsymbol{b}=\boldsymbol{1} \tag{25}$$

and

$$\boldsymbol{b}^T\boldsymbol{N}\boldsymbol{b}=\boldsymbol{e}. \tag{26}$$

We therefore have $\boldsymbol{b}=\boldsymbol{a}^{-1}$ and from Eq. (22) the standard $\boldsymbol{R}$-matrix reduced widths are given by

$$\boldsymbol{\gamma}_c=\boldsymbol{b}^T\tilde{\boldsymbol{\gamma}}_c. \tag{27}$$

The simultaneous diagonalization of $\boldsymbol{M}$ and $\boldsymbol{N}$ thus provides all of the standard $\boldsymbol{R}$-matrix parameters. Note that any B_c can be chosen; the collision matrix $\boldsymbol{U}$ will be invariant provided the same B_c are used in Eq. (21) and in Eqs. (3) or (7). The numerical solution of Eq. (24) is discussed in Sec. 8.7.2 of Ref. [8]; we have have utilized the LAPACK [9] routine DSYGV.

IV. FURTHER DEVELOPMENT

It is fruitful to investigate alternative forms for the level matrix and the $\boldsymbol{R}$ matrix which allow the collision matrix to be calculated directly from the alternative parameters.

A. The alternative level matrix

We define the alternative level matrix $\tilde{\boldsymbol{A}}$ implicitly via

$$\boldsymbol{\gamma}_{c'}^T\boldsymbol{A}\boldsymbol{\gamma}_c\equiv\tilde{\boldsymbol{\gamma}}_{c'}^T\tilde{\boldsymbol{A}}\tilde{\boldsymbol{\gamma}}_c. \tag{28}$$

In order for this relation to hold, we must have

$$\boldsymbol{a}\tilde{\boldsymbol{A}}\boldsymbol{a}^T=\boldsymbol{A}, \tag{29}$$

or equivalently

$$\tilde{\boldsymbol{A}}^{-1}=\boldsymbol{a}^T\boldsymbol{A}^{-1}\boldsymbol{a}, \tag{30}$$

where we have used Eq. (22). We can now substitute Eq. (7) for $\boldsymbol{A}^{-1}$, and again use Eq. (22) to obtain

$$\tilde{\boldsymbol{A}}^{-1} = \boldsymbol{a}^T \boldsymbol{e}\boldsymbol{a} - E\boldsymbol{a}^T\boldsymbol{a} - \sum_c \tilde{\boldsymbol{\gamma}}_c \tilde{\boldsymbol{\gamma}}_c^T (S_c - B_c + \mathrm{i}P_c) \tag{31}$$

$$= \boldsymbol{N} - E\boldsymbol{M} - \sum_c \tilde{\boldsymbol{\gamma}}_c \tilde{\boldsymbol{\gamma}}_c^T (S_c - B_c + \mathrm{i}P_c). \tag{32}$$

The elements of this matrix can now be determined entirely from the alternative parameters with the aid of Eqs. (20) and (21),

$$(\tilde{\boldsymbol{A}}^{-1})_{ij} = (\tilde{E}_i - E)\,\delta_{ij} - \sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc}(S_c + \mathrm{i}P_c) + \sum_c \begin{cases} \tilde{\gamma}_{ic}^2 S_{ic} & i=j \\ \tilde{\gamma}_{ic}\tilde{\gamma}_{jc} \dfrac{S_{ic}(E-\tilde{E}_j) - S_{jc}(E-\tilde{E}_i)}{\tilde{E}_i - \tilde{E}_j} & i \neq j. \end{cases} \tag{33}$$

Note that the boundary-condition constants B_c have now canceled out—a not unexpected result since the alternative parameters and the collision matrix are independent of B_c. We can now express the collision matrix directly in terms of the alternative parameters using Eqs. (8) and (28)

$$U_{c'c} = \Omega_{c'}\Omega_c[\delta_{c'c} + 2\mathrm{i}(P_{c'}P_c)^{1/2}\tilde{\boldsymbol{\gamma}}_{c'}^T \tilde{\boldsymbol{A}} \tilde{\boldsymbol{\gamma}}_c]. \tag{34}$$

B. The alternative *R* matrix

The matrix $\tilde{\boldsymbol{R}}$ is an alternative to the standard $\boldsymbol{R}$ matrix and is defined implicitly via

$$[\boldsymbol{1} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1}\boldsymbol{R} \equiv (\boldsymbol{1} - \mathrm{i}\tilde{\boldsymbol{R}}\boldsymbol{P})^{-1}\tilde{\boldsymbol{R}}, \tag{35}$$

where $\boldsymbol{P}$ is a purely diagonal matrix with elements P_c. By comparison with Eqs. (3) and (34) we must have

$$(\boldsymbol{1} - \mathrm{i}\tilde{\boldsymbol{R}}\boldsymbol{P})^{-1}\tilde{\boldsymbol{R}} = \tilde{\boldsymbol{\gamma}}^T \tilde{\boldsymbol{A}} \tilde{\boldsymbol{\gamma}}. \tag{36}$$

We proceed by assuming that $\tilde{\boldsymbol{R}}$ can be written in the form

$$\tilde{\boldsymbol{R}} = \tilde{\boldsymbol{\gamma}}^T \boldsymbol{Q} \tilde{\boldsymbol{\gamma}}. \tag{37}$$

In the Appendix we describe a method to derive the level matrix form for the collision matrix [Eq. (6)] from the channel matrix form [Eq. (3)]. This reasoning can also be applied to $\tilde{\boldsymbol{R}}$ and $\tilde{\boldsymbol{A}}$. We find that in order to satisfy Eq. (36) we must have

$$\boldsymbol{Q}^{-1} = \tilde{\boldsymbol{A}}^{-1} + \mathrm{i}\tilde{\boldsymbol{\gamma}}\boldsymbol{P}\tilde{\boldsymbol{\gamma}}^T. \tag{38}$$

A formula for the elements of $\boldsymbol{Q}^{-1}$ in terms of the alternative parameters can then be found using Eqs. (33) and (38),

$$(\tilde{\boldsymbol{Q}}^{-1})_{ij} = (\tilde{E}_i - E)\,\delta_{ij} - \sum_c \tilde{\gamma}_{ic}\tilde{\gamma}_{jc} S_c + \sum_c \begin{cases} \tilde{\gamma}_{ic}^2 S_{ic} & i=j \\ \tilde{\gamma}_{ic}\tilde{\gamma}_{jc} \dfrac{S_{ic}(E-\tilde{E}_j) - S_{jc}(E-\tilde{E}_i)}{\tilde{E}_i - \tilde{E}_j} & i \neq j. \end{cases} \tag{39}$$

Using Eqs. (3) and (35) the collision matrix can now be written as

$$\boldsymbol{U} = 2\mathrm{i}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1}(\boldsymbol{1} - \mathrm{i}\tilde{\boldsymbol{R}}\boldsymbol{P})^{-1}\tilde{\boldsymbol{R}}\boldsymbol{\rho}^{1/2}\boldsymbol{O}^{-1} + \boldsymbol{I}\boldsymbol{O}^{-1}. \tag{40}$$

With the $\tilde{\boldsymbol{R}}$ matrix defined by Eqs. (37) and (39) this equation also gives $\boldsymbol{U}$ in terms of the alternative parameters without reference to the boundary-condition constants.

C. Relative merits of $\tilde{R}$ and $\tilde{A}$

The $\tilde{\boldsymbol{R}}$ matrix is more complicated than $\boldsymbol{R}$ and the calculation of $\boldsymbol{U}$ via Eq. (40) requires inverting a real $N_\lambda \times N_\lambda$ matrix in addition to a complex $N_c \times N_c$ matrix. When calculating $\boldsymbol{U}$ via the alternative level matrix one must invert a single complex $N_\lambda \times N_\lambda$ matrix—using the alternative $\boldsymbol{R}$-matrix approach may thus offer a modest computational advantage in comparison when $N_\lambda \gg N_c$. Note, however, that if it is necessary to calculate $\boldsymbol{U}$ for several energies and $N_\lambda > N_c$ it will probably be more computationally efficient to diagonalize Eq. (24) once and then use the standard $\boldsymbol{R}$-matrix parameters in Eq. (3) to calculate $\boldsymbol{U}$, as Eq. (3) only requires inverting a single complex $N_c \times N_c$ matrix.

We would also like to point out that this alternative parametrization, using $\tilde{E}_i$ and $\tilde{\gamma}_{ic}$ with Eq. (34) or (40), may be of formal interest since no arbitrary boundary-condition constants are required, but the equations are mathematically equivalent to the standard $\boldsymbol{R}$-matrix approach. The alternative parameters, in fact, correspond to eigenfunctions satisfying energy-dependent boundary conditions—the real part of the Kapur-Peierls or Siegert boundary conditions see (LT, Sec. IX.2).

V. SOLUTION OF THE NONLINEAR EIGENVALUE EQUATION

The transformation from $\tilde{E}_{ic}$ and $\tilde{\gamma}_{ic}$ to the standard $\boldsymbol{R}$-matrix parameters E_λ and $\gamma_{\lambda c}$ can be carried out in a straightforward manner using the methods discussed above in Sec. III B. We will now discuss the inverse transformation, i.e., the solution of the nonlinear eigenvalue problem Eq. (13). At this point it is instructive to introduce a concrete example: in Table I we show a simple well-documented set of standard $\boldsymbol{R}$-matrix parameters taken from Azuma *et al.* [5].

We consider the *linear* eigenvalue equation

$$\boldsymbol{\mathcal{E}}(E)\hat{\boldsymbol{a}}_i = \hat{E}_i \hat{\boldsymbol{a}}_i, \tag{41}$$

TABLE I. Standard $\boldsymbol{R}$-matrix parameters from Table III of Ref. [5] which describe $J^{\pi}=1^{-}$ reactions in the ^{16}O system, and the alternative parameters derived from them. The channel labels α and γ describe $^{12}\mathrm{C}+\alpha$ and $^{16}\mathrm{O}+\gamma$, respectively. The channel radius is 6.5 fm and the boundary condition constant is chosen so that the level shift vanishes for $E=E_1$. The β-decay feeding amplitudes $\mathcal{B}_\lambda$ are equivalent to the quantities $A_{\lambda 1}\gamma_{\lambda 1}^{-1}N_{\alpha}^{-1/2}$ of Ref. [5].

λ	1	2	3
E_λ (MeV)	-0.0451	2.845	11.71
$\gamma_{\lambda\alpha}$ (MeV$^{1/2}$)	0.0793	0.330	1.017
$\gamma_{\lambda\gamma}$ (MeV^{-1})	8.76×10^{-6}	-2.44×10^{-6}	-2.82×10^{-6}
$\mathcal{B}_\lambda$	1.194	0.558	-0.629
$\tilde{E}_\lambda$ (MeV)	-0.0451	2.400	8.00
$\tilde{\gamma}_{\lambda\alpha}$ (MeV$^{1/2}$)	0.0793	0.471	0.912
$\tilde{\gamma}_{\lambda\gamma}$ (MeV^{-1})	8.76×10^{-6}	-3.20×10^{-6}	-2.50×10^{-6}
$\tilde{\mathcal{B}}_\lambda$	1.194	0.408	-0.781

where $\boldsymbol{\mathcal{E}}$, the eigenvalues $\hat{E}_i$, and eigenvectors $\hat{\boldsymbol{a}}_i$ depend upon on the energy parameter E. The solutions to the original nonlinear problem Eq. (13) thus occur when $\hat{E}_i(E)=E$ in which case $E=\tilde{E}_i$. From inspection of Eqs. (9) and (12) we see that the eigenvalues $\hat{E}_i$ also correspond to a set of standard $\boldsymbol{R}$-matrix level energies, transformed from the original parameter values to $B_c=S_c(E)$.

We will next investigate how the $\hat{E}_i$ depend on E. Starting with

$$\hat{E}_i=\hat{\boldsymbol{a}}_i^T\boldsymbol{\mathcal{E}}\hat{\boldsymbol{a}}_i \tag{42}$$

differentiation with respect to E yields

$$\frac{d\hat{E}_i}{dE}=\hat{\boldsymbol{a}}_i^T\frac{d\boldsymbol{\mathcal{E}}}{dE}\hat{\boldsymbol{a}}_i+\frac{d\hat{\boldsymbol{a}}_i^T}{dE}\boldsymbol{\mathcal{E}}\hat{\boldsymbol{a}}_i+\hat{\boldsymbol{a}}_i^T\boldsymbol{\mathcal{E}}\frac{d\hat{\boldsymbol{a}}_i}{dE} \tag{43}$$

$$=-\hat{\boldsymbol{a}}_i^T\left(\sum_c \boldsymbol{\gamma}_c\boldsymbol{\gamma}_c^T\frac{dS_c}{dE}\right)\hat{\boldsymbol{a}}_i+\hat{E}_i\left(\frac{d\hat{\boldsymbol{a}}_i^T}{dE}\hat{\boldsymbol{a}}_i+\hat{\boldsymbol{a}}_i^T\frac{d\hat{\boldsymbol{a}}_i}{dE}\right). \tag{44}$$

Since by definition $\hat{\boldsymbol{a}}_i^T\hat{\boldsymbol{a}}_i=1$ we have $(d\hat{\boldsymbol{a}}_i^T/dE)\hat{\boldsymbol{a}}_i+\hat{\boldsymbol{a}}_i^T(d\hat{\boldsymbol{a}}_i/dE)=0$, and we finally find

$$\frac{d\hat{E}_i}{dE}=-\sum_c (\boldsymbol{\gamma}_c^T\hat{\boldsymbol{a}}_i)^2\frac{dS_c}{dE}. \tag{45}$$

The energy derivative of the shift function (dS_c/dE) is positive for negative-energy channels, and is $\geqslant 0$ for positive-energy channels for all cases we are aware of. This point is also discussed by (LT, p. 350); although a general proof of $(dS_c/dE)\geqslant 0$ is lacking it appears to always hold in practice and we will thus assume it is true here. Note that for any specific case it is a simple matter to verify this relation numerically.

Since $(\boldsymbol{\gamma}_c^T\hat{\boldsymbol{a}}_i)^2$ is clearly $\geqslant 0$, we can utilize $(dS_c/dE)\geqslant 0$ to conclude from Eq. (45) that

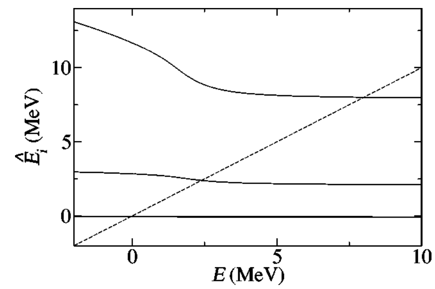

FIG. 1. The eigenvalue trajectories are shown by plotting as solid curves the eigenvalues $\hat{E}_i$ versus E; the dashed line corresponds to $\hat{E}_i=E$. The eigenvalues of Eq. (13) are given by the intersections between the solid curves and the dashed line.

$$\frac{d\hat{E}_i}{dE}\leqslant 0. \tag{46}$$

The eigenvalues $\hat{E}_i$ are thus monotonically nonincreasing functions of E. The eigenvalue trajectories for the example parameters are shown in Fig. 1 where the expected behavior is seen. We also note that the eigenvalue trajectories avoid crossing one another for the reasons given by von Neumann and Wigner [10]. The avoided-crossing behavior is most apparent when there are two nearby levels with very different reduced width amplitudes.

The nonlinear eigenvalue problem Eq. (13) and the parametric eigenvalue problem Eq. (42) are also closely related to a well-studied question in linear algebra: the modification of a symmetric matrix with known eigenvalues and eigenvectors by a positive-definite perturbation. This question is analyzed for the single-channel case in Sec. 8.5.3 of Golub and Van Loan [8] and for the multichannel case by Arbenz, Gander, and Golub [11]. The perturbation bounds on the eigenvalues derived in Ref. [11] imply that the $\hat{E}_i$ remain finite provided the S_c are finite—thus the eigenvalue trajectories do not have real poles for $|E|<\infty$.

From the lack of poles and the monotonic dependence $(d\hat{E}_i/dE)\leqslant 0$ we can conclude that each eigenvalue trajectory intersects with the line $\hat{E}_i=E$ exactly once. These intersections are shown graphically for the example in Fig. 1. We thus have the important result that the nonlinear eigenvalue problem Eq. (13) has a number of real eigenvalues exactly equal to the number of $\boldsymbol{R}$-matrix levels. A similar type of nonlinear eigenvalue problem has been investigated by Rogers [12]; it may be that the methods described in that paper could be used to develop further understanding of the present problem, e.g., to investigate inner products and/or the linear independence of the eigenvectors.

The eigenvalues of Eq. (13) satisfy the characteristic equation

$$\det(\boldsymbol{\mathcal{E}}-E\mathbf{1})=0, \tag{47}$$

which can also be written as

$$\det[\boldsymbol{e}-E\mathbf{1}-\boldsymbol{\gamma}(\boldsymbol{S}-\boldsymbol{B})\boldsymbol{\gamma}^T]=0, \tag{48}$$

TABLE II. Elements b_{ij} of the transformation matrix $\boldsymbol{b}$ corresponding to the parameters of Table I.

	j		
i	1	2	3
1	1.000	0.0373	0.0446
2	0.000	0.9781	0.2281
3	0.000	−0.1466	0.9933

where $\boldsymbol{S}$ is a purely diagonal matrix with elements S_c which depend upon E. Using the methods described in Ref. [11] one can show that

$$\det[\boldsymbol{e}-E\mathbf{1}-\boldsymbol{\gamma}(\boldsymbol{S}-\boldsymbol{B})\boldsymbol{\gamma}^T] \\ =\det(\boldsymbol{e}-E\mathbf{1})\det[\mathbf{1}-\boldsymbol{\gamma}^T(\boldsymbol{e}-E\mathbf{1})^{-1}\boldsymbol{\gamma}(\boldsymbol{S}-\boldsymbol{B})]. \quad (49)$$

The eigenvalues thus satisfy

$$\det(\boldsymbol{e}-E\mathbf{1})\det[\mathbf{1}-\boldsymbol{R}(\boldsymbol{S}-\boldsymbol{B})]=0, \quad (50)$$

which may be a computationally efficient approach for determining the eigenvalues when $N_\lambda > N_c$ since the calculation of det$(\boldsymbol{e}-E\mathbf{1})$ is trivial. Note that Eq. (50) is the multichannel arbitrary-B_c generalization of the resonance condition given by Eq. (14) of Ref. [1]. The eigenvalues also satisfy

$$\det[\mathbf{1}-\boldsymbol{R}(\boldsymbol{S}-\boldsymbol{B})]=0, \quad (51)$$

but this equation has poles in addition to zeros, and if there is a level λ with $B_c = S_c(E_\lambda)$ (at most one level can satisfy this condition) it does not produced a zero.

Rather than finding the eigenvalues by directly solving the characteristic equation, we have applied the Rayleigh quotient iteration method described in Sec. 8.2.3 of Ref. [8] to Eq. (13), as this procedure yields the eigenvectors as well as eigenvalues. Starting values for the eigenvalues and eigenvectors were taken as $\tilde{E}_i = E_i + \Sigma_c \gamma_{ic}^2[S_c(E_i)-B_c]$ and $a_{ji} = \delta_{ji}$. Due to the nonlinear nature of the problem, the matrix $\boldsymbol{\mathcal{E}}$ must be updated at each step of the iteration. These procedures were tested with several single-channel and multichannel parameter sets, and were successful in finding all of the eigenvalues in every case. We cannot rule out, however, that some cases may require more carefully chosen starting values. Once the $\tilde{E}_i$ and $\boldsymbol{a}_i$ are found, the $\tilde{\gamma}_{ic}$ can be calculated using Eq. (14). In Table I we show for the example case the alternative parameters determined from the standard $\boldsymbol{R}$-matrix parameters. Note that the alternative parameters are exactly the same as the $\boldsymbol{R}$-matrix parameters given in the last column of Table III of Ref. [5] which have been transformed to satisfy $B_c = S_c(E_\lambda)$ for other levels. As discussed in Sec. III A this equality is required due to our definition of the alternative parameters. In Table II we show the elements of the matrix $\boldsymbol{b}$ for the example parameters. Finally we would like to point out that the methods discussed in this section should be generally useful for the extraction of resonance parameters from standard $\boldsymbol{R}$-matrix parameters.

VI. APPLICATION TO γ RAYS AND β DECAYS

We will briefly discuss the application of the alternative parametrization to reactions involving γ rays and β decays. Gamma-ray decay processes are generally treated with first-order perturbation theory in $\boldsymbol{R}$-matrix theory, which implies that γ-ray channels are excluded from the sum over channels when constructing $\boldsymbol{A}$, $\tilde{\boldsymbol{A}}$, $\boldsymbol{M}$, or $\boldsymbol{N}$. Assuming that external contributions can be ignored, the collision matrix elements connecting γ-ray channels (labeled γ) and non-γ-ray channels (labeled c) are given by (LT, Eq. XIII.3.9)

$$U_{c\gamma} = 2i\Omega_c(P_cP_\gamma)^{1/2}\sum_{\lambda\mu}\gamma_{\lambda c}\gamma_{\mu\gamma}A_{\lambda\mu} \\ = 2i\Omega_c(P_cP_\gamma)^{1/2}\boldsymbol{\gamma}_c^T\boldsymbol{A}\boldsymbol{\gamma}_\gamma. \quad (52)$$

In the long-wavelength approximation the penetration factor for γ rays is given by $P_\gamma = E_\gamma^{2\ell+1}$ where ℓ is the multipolarity. The observed γ-ray widths are described by Eq. (16), where γ-ray channels are excluded from the sum in the denominator. Using the same reasoning described in Sec. IV A the alternative expression for the collision matrix elements can be obtained using the replacement

$$\boldsymbol{\gamma}_c^T\boldsymbol{A}\boldsymbol{\gamma}_\gamma = \tilde{\boldsymbol{\gamma}}_c^T\tilde{\boldsymbol{A}}\tilde{\boldsymbol{\gamma}}_\gamma, \quad (53)$$

where the alternative γ-ray reduced width amplitudes are related to the standard parameters via

$$\boldsymbol{\gamma}_\gamma = \boldsymbol{b}^T\tilde{\boldsymbol{\gamma}}_\gamma. \quad (54)$$

If the external contributions to the matrix elements are included using the formalism of Barker and Kajino [13], the expressions for the collision matrix elements and observed widths become more complicated. However, these quantities can still be written in terms of the alternative parameters using the above equations, noting that the $\gamma_{\lambda\gamma}$ above are the *internal* γ-ray reduced width amplitudes.

The extension of the alternative parametrization to the description of β-delayed particle spectra is straightforward. A multichannel formula for the particle spectrum is given by Eq. (7) of Barker and Warburton [14]; note that additional parameters must now be introduced, the β-decay feeding amplitudes $\mathcal{B}_{\lambda x}$. It is convenient to form column vectors $\boldsymbol{\mathcal{B}}_x$ from the $\mathcal{B}_{\lambda x}$, so that $\Sigma_{\lambda\mu}\mathcal{B}_{\lambda x}A_{\lambda\mu}\gamma_{\mu c}$ can be written as $\boldsymbol{\gamma}_c^T\boldsymbol{A}\boldsymbol{\mathcal{B}}_x$. Again using the reasoning of Sec. IV A we have

$$\boldsymbol{\gamma}_c^T\boldsymbol{A}\boldsymbol{\mathcal{B}}_x = \tilde{\boldsymbol{\gamma}}_c^T\tilde{\boldsymbol{A}}\tilde{\boldsymbol{\mathcal{B}}}_x, \quad (55)$$

where the alternative feeding amplitudes $\tilde{\boldsymbol{\mathcal{B}}}_x$ are related to the standard parameters via

$$\boldsymbol{\mathcal{B}}_x = \boldsymbol{b}^T\tilde{\boldsymbol{\mathcal{B}}}_x. \quad (56)$$

Note also that if $B_c = S_c(E_\lambda)$ we have $\tilde{\mathcal{B}}_{\lambda x} = \mathcal{B}_{\lambda x}$. The β-delayed particle spectrum can now be calculated directly from the alternative parameters by using Eq. (55) in Eq. (7) of Ref. [14]. One could also convert to standard $\boldsymbol{R}$-matrix parameters using Eq. (56) and the methods discussed in Sec. III B, and then calculate the spectrum using standard $\boldsymbol{R}$-matrix formulas.

In Table I we also show the standard and alternative γ-ray reduced amplitudes and β-decay feeding amplitudes for the example case.

VII. CONCLUSIONS

We have presented an alternative formulation of $\boldsymbol{R}$-matrix theory based on the parameters $\tilde{E}_i$ and $\tilde{\gamma}_{ic}$ defined in Sec. III A. This parametrization is a generalization of the ideas presented by Angulo and Descouvemont [1]. The new formulation is mathematically equivalent to the standard $\boldsymbol{R}$-matrix theory [3] but there are no boundary-condition constants or level shifts. The new parameters can be converted to standard $\boldsymbol{R}$-matrix parameters by diagonalizing Eq. (24), or be used to calculate the collision matrix directly using Eqs. (34) or (40). We have discussed the solution of the nonlinear eigenvalue problem Eq. (13) which is needed to convert standard $\boldsymbol{R}$-matrix parameters to the new parametrization. Finally we have briefly discussed the application to γ rays and β decays.

We can envision at least two uses for this new formulation in the fitting of experimental data. One application is the generation of starting parameter values from an outside source of spectroscopic information such as a level compilation or shell-model calculation. These latter sources generally do not supply standard $\boldsymbol{R}$-matrix parameters but rather resonance parameters without level shifts. In the past the methods to incorporate these types of information have not always been optimal (e.g., B_c could be chosen to make the level shift vanish for a representative energy, but not for all energies simultaneously). Another application is to use the alternative parameters as the fit parameters. The calculations can be made directly from the alternative parameters using the methods discussed in Sec. IV, or by diagonalizing Eq. (24) to find the standard $\boldsymbol{R}$-matrix parameters. The latter option may be preferable if $N_\lambda > N_c$, if observables must be calculated for many different energies. It should be noted that in data-fitting applications the collision matrix must be calculated repeatedly for different energies, and the extra computational overhead required will be negligible in comparison. With the alternative parameters it is very easy to fix known information about level energies and partial widths for any number of levels.

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APPENDIX

The equivalence of the two forms of the collision matrix given by Eqs. (3) and (6) is discussed in (LT, Sec. IX.1). The derivation is reviewed here, utilizing the matrix notation introduced in Sec. II. The same procedure is useful for the derivation of the alternative $\boldsymbol{R}$ matrix as discussed in Sec. IV B.

We define $\boldsymbol{L}_0 = \boldsymbol{L} - \boldsymbol{B}$ and note the quantity $[\boldsymbol{1} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1}$ in Eq. (3) can be written as

$$(\boldsymbol{1}-\boldsymbol{R}\boldsymbol{L}_0)^{-1} = [\boldsymbol{L}_0 - (\boldsymbol{L}_0\boldsymbol{\gamma}^T)(\boldsymbol{e}-E\boldsymbol{1})^{-1}(\boldsymbol{\gamma}\boldsymbol{L}_0)]^{-1}\boldsymbol{L}_0 . \tag{A1}$$

A useful identity is given by

$$(\boldsymbol{X}+\boldsymbol{Z}\boldsymbol{Y}\boldsymbol{Z}^T)^{-1} = \boldsymbol{X}^{-1} - \boldsymbol{X}^{-1}\boldsymbol{Z}(\boldsymbol{Y}^{-1}+\boldsymbol{Z}^T\boldsymbol{X}^{-1}\boldsymbol{Z})^{-1}\boldsymbol{Z}^T\boldsymbol{X}^{-1}, \tag{A2}$$

which holds for any square and invertible matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$ which need not be of the same dimension [15]. With the aid of this identity we obtain

$$(\boldsymbol{1}-\boldsymbol{R}\boldsymbol{L}_0)^{-1} = \{\boldsymbol{L}_0^{-1} - \boldsymbol{L}_0^{-1}(\boldsymbol{L}_0\boldsymbol{\gamma}^T)[-(\boldsymbol{e}-E\boldsymbol{1}) + (\boldsymbol{\gamma}\boldsymbol{L}_0)\boldsymbol{L}_0^{-1}(\boldsymbol{L}_0\boldsymbol{\gamma}^T)]^{-1}(\boldsymbol{\gamma}\boldsymbol{L}_0)\boldsymbol{L}_0^{-1}\}\boldsymbol{L}_0 \tag{A3}$$

$$= \boldsymbol{1} + \boldsymbol{\gamma}^T(\boldsymbol{e}-E\boldsymbol{1}-\boldsymbol{\gamma}\boldsymbol{L}_0\boldsymbol{\gamma}^T)^{-1}\boldsymbol{\gamma}\boldsymbol{L}_0 \tag{A4}$$

$$= \boldsymbol{1} + \boldsymbol{\gamma}^T\boldsymbol{A}\boldsymbol{\gamma}\boldsymbol{L}_0 , \tag{A5}$$

where in the last step we have used Eq. (7) for the definition of the level matrix $\boldsymbol{A}$.

We can then write

$$(\boldsymbol{1}-\boldsymbol{R}\boldsymbol{L}_0)^{-1}\boldsymbol{R} = (\boldsymbol{1}+\boldsymbol{\gamma}^T\boldsymbol{A}\boldsymbol{\gamma}\boldsymbol{L}_0)\boldsymbol{\gamma}^T(\boldsymbol{e}-E\boldsymbol{1})^{-1}\boldsymbol{\gamma} \tag{A6}$$

$$= \boldsymbol{\gamma}^T(\boldsymbol{e}-E\boldsymbol{1})^{-1}\boldsymbol{\gamma} + \boldsymbol{\gamma}^T\boldsymbol{A}[-\boldsymbol{A}^{-1}+(\boldsymbol{e}-E\boldsymbol{1})] \times (\boldsymbol{e}-E\boldsymbol{1})^{-1}\boldsymbol{\gamma}, \tag{A7}$$

where we have substituted $-\boldsymbol{A}^{-1}+(\boldsymbol{e}-E\boldsymbol{1})$ for $\boldsymbol{\gamma}\boldsymbol{L}_0\boldsymbol{\gamma}^T$. Simplifying this expression we finally have

$$(\boldsymbol{1}-\boldsymbol{R}\boldsymbol{L}_0)^{-1}\boldsymbol{R} = \boldsymbol{\gamma}^T\boldsymbol{A}\boldsymbol{\gamma}, \tag{A8}$$

which proves the equivalence of Eqs. (3) and (6).

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