Completeness relation in the *R*-matrix theory of scattering

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We present the biorthogonal complement of the standing wave state and its relation to scattering operators. This establishes a completeness relation in terms of the standing wave states, and therefore completes the *R*-matrix (reactance matrix) theory of scattering. We clarify with an example that the *R*-matrix theory, in its formulation presented here, can claim its due place in addition to the standard *T*-matrix theory.

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I. INTRODUCTION

The *R*-matrix (reactance matrix) theory describes scattering phenomena in terms of standing wave states [1]. In spite of its many merits, it has not, however, enjoyed as wide use as the *T*-matrix theory. The key problem is that the standing wave states do not constitute an orthogonal basis set, and therefore that a proper completeness relation has not been known in the *R*-matrix theory [1]. In this paper we solve the above long-standing problem. We present the biorthogonal state of the standing wave state, and show that it is a solution to the equation studied by Kouri and Levin [2,3] more than three decades ago.

The plan of the paper is the following. In Sec. II, we briefly review the *T*-matrix theory with fixing the notation. In Sec. III, we explain the *R*-matrix theory where the scattering operator and the scattering state are described by $\mathcal{R}(E)$ and $|E\rangle_P$, respectively. Here we contrast the *R*-matrix to the *T*-matrix theory, and clarify what is missing in the current *R*-matrix theory. In Sec. IV, we introduce a scattering operator $\tilde{\mathcal{R}}(E)$ and a corresponding scattering state $|\tilde{E}\rangle_P$, which are closely related to $\mathcal{R}(E)$ and $|E\rangle_P$, respectively. Then, we present the main point of the present work, that $\{|\tilde{E}\rangle_P\}$ is biorthogonal to $\{|E\rangle_P\}$, which in turn gives the completeness relation via $\{|\tilde{E}\rangle_P\}$ and $\{|E\rangle_P\}$ immediately. In Sec. V, we present discussions on the basis of the above findings. We derive a spectral representation of $\tilde{\mathcal{R}}(E)$ in terms of the standing wave states, which in turn leads to a counterpart of the Low equation [1,4] in the *R*-matrix theory. By comparing the Low equations in the *T*- and *R*-matrix theories, we show that *R*-matrix version is much more tractable than the original *T*-matrix version. Finally in Sec. VI, we present a brief summary.

II. SCATTERING OPERATOR $\mathcal{T}(E)$

We consider a spinless particle described by the following Hamiltonian [1]:

$$H = H_0 + V, \tag{1}$$

where H_0 is the kinetic energy and V is the potential energy of the particle with a fixed force center. In the absence of the potential V, the particle is described by H_0 alone, of which the eigenstate with energy E is given by

$$H_0|Ea\rangle = E|Ea\rangle, \tag{2}$$

where "a" denotes additional quantum numbers. They are normalized as [1]

$$\langle E'a'|Ea\rangle = \delta(E'-E)\delta_{a'a}. \tag{3}$$

When "a" stands for the angular momentum quantum numbers lm, for example, Eq. (3) reads

$$\langle E'l'm'|Elm\rangle = \delta(E'-E)\delta_{l'l}\delta_{m'm}$$

and when "a" represents the direction $\hat{\boldsymbol{k}}=(\theta,\phi)$ of the momentum $\boldsymbol{k}$ of the particle ($E=\boldsymbol{k}^2/2m$), it reads

$$\langle E'\hat{\boldsymbol{k}}'|E\hat{\boldsymbol{k}}\rangle = \delta(E'-E)\delta(\hat{\boldsymbol{k}}'-\hat{\boldsymbol{k}}),$$

where $\delta(\hat{\boldsymbol{k}}'-\hat{\boldsymbol{k}})=\delta(\theta'-\theta)\delta(\phi'-\phi)/\sin\theta$. Then the completeness relation can be written symbolically as [1]

$$\int_0^\infty dE \sum_a |Ea\rangle\langle Ea| = 1, \tag{4}$$

from which it follows immediately

$$\sum_a |Ea\rangle\langle Ea| = \delta(E-H_0). \tag{5}$$

Now we introduce the potential V, which represents a central force of short range, and describe briefly the scattering states in the *T*-matrix theory [1]. The T operator is defined for an arbitrary E by

$$\mathcal{T}(E) = V + V\frac{1}{E-H_0+i\eta}\mathcal{T}(E) = V + V\frac{1}{E-H+i\eta}V. \tag{6}$$

The corresponding scattering state $|Ea\rangle_+$ obeys $H|Ea\rangle_+ = E|Ea\rangle_+$ with the outgoing wave boundary condition. It is given by

$$|Ea\rangle_+ = |Ea\rangle + \frac{1}{E-H_0+i\eta}V|Ea\rangle_+$$
$$= |Ea\rangle + \frac{1}{E-H_0+i\eta}\mathcal{T}(E)|Ea\rangle \tag{7}$$

and satisfies

$$V|Ea\rangle_+ = \mathcal{T}(E)|Ea\rangle. \tag{8}$$

Here we define the on-shell matrix $T(E)$ by

$$\langle a'|T(E)|a\rangle = \langle Ea'|V|Ea\rangle_+ = \langle Ea'|\mathcal{T}(E)|Ea\rangle. \tag{9}$$

Then the S matrix is given by

$$S(E) = 1 - 2\pi i\ T(E), \tag{10}$$

which is, in the angular momentum basis, the familiar expression $\langle l'm'|S(E)|lm\rangle = \delta_{l'l}\delta_{m'm}\exp[2i\delta_l(E)]$ in terms of the phase shift $\delta_l(E)$. Note here that we have to require the unitarity relation (generalized optical theorem) [1]

$$T(E) - T^\dagger(E) = -2\pi i\ T(E)T^\dagger(E) \tag{11}$$

or its operator extension

$$\mathcal{T}(E) - \mathcal{T}^\dagger(E) = -2\pi i\ \mathcal{T}(E)\delta(E-H_0)\mathcal{T}^\dagger(E) \tag{12}$$

to guarantee the unitarity of the S matrix $S(E)$.

It is well known [1] that $\{|Ea\rangle_+\}$ constitutes an orthogonal set satisfying

$${}_+\langle E'a'|Ea\rangle_+ = \delta(E'-E)\delta_{a'a} \tag{13}$$

and therefore that the completeness relation is

$$\int_0^\infty dE \sum_a |Ea\rangle_{++}\langle Ea| = 1. \tag{14}$$

Here we have employed a notation which suggests that there are no bound states for simplicity; bound states are taken into account easily by adding appropriate contributions in the summation in the above, and also in what follows.

The completeness relation of Eq. (14) can be used, for example, to give the spectral representation of Green's operator $1/(E-H+i\eta)$ as

$$\frac{1}{E-H+i\eta} = \sum_A |A\rangle_+ \frac{1}{E-E_a+i\eta}{}_+\langle A|, \tag{15}$$

where we have used a shorthand notation $|A\rangle$ for $|E_a a\rangle$ and Σ_A for $\int dE_a \Sigma_a$. By using Eq. (15) in the second equality of Eq. (6), we can immediately obtain the following spectral representation of $\mathcal{T}(E)$:

$$\langle A'|\mathcal{T}(E)|A\rangle = \langle A'|V|A\rangle + \sum_B \langle A'|\mathcal{T}(E_b)|B\rangle \times \frac{1}{E-E_b+i\eta}\langle B|\mathcal{T}^\dagger(E_b)|A\rangle, \tag{16}$$

which shows that an off-shell $(E_a \neq E,\ E_{a'} \neq E)$ matrix element of $\mathcal{T}(E)$ can be written in terms of half-on-shell matrix elements [1].

III. SCATTERING OPERATOR $\mathcal{R}(E)$

Let us turn to the R-matrix theory [1]. The R operator $\mathcal{R}(E)$ is given by

$$\mathcal{R}(E) = V + V\frac{1}{E-H_0}\mathcal{R}(E), \tag{17}$$

where the propagator $1/(E-H_0)$ is defined via the principal value. The corresponding scattering state $|Ea\rangle_P$ satisfies $H|Ea\rangle_P = E|Ea\rangle_P$ with the standing wave boundary condition. It is given by

$$|Ea\rangle_P = |Ea\rangle + \frac{1}{E-H_0}V|Ea\rangle_P = |Ea\rangle + \frac{1}{E-H_0}\mathcal{R}(E)|Ea\rangle \tag{18}$$

and has the following property:

$$V|Ea\rangle_P = \mathcal{R}(E)|Ea\rangle. \tag{19}$$

Then we define the on-shell matrix $R(E)$ as [5]

$$\langle a'|R(E)|a\rangle = \langle Ea'|V|Ea\rangle_P = \langle Ea'|\mathcal{R}(E)|Ea\rangle, \tag{20}$$

in the same way as $T(E)$ of Eq. (9).

It is appropriate here to present relations between the R- and T-matrix frameworks. They can be most simply derived as follows. By comparing $|Ea\rangle_+$ of Eq. (7) and $|Ea\rangle_P$ of Eq. (18), we can immediately see

$$\left(1 - \frac{1}{E-H_0}V\right)\{|Ea\rangle_P - |Ea\rangle_+\} = i\pi\delta(E-H_0)V|Ea\rangle_+, \tag{21}$$

where we have used $1/(E-H_0+i\eta) = 1/(E-H_0) - i\pi\delta(E-H_0)$. Let us note here, by using Eqs. (5) and (9)

$$\delta(E-H_0)V|Ea\rangle_+ = \sum_b |Eb\rangle\langle Eb|V|Ea\rangle_+ = \sum_b |Eb\rangle\langle b|T(E)|a\rangle$$

on the right-hand side of Eq. (21). Then, by dividing both sides of Eq. (21) by $1-[1/(E-H_0)]V$ and by using Eq. (18), we arrive at the following relation between the outgoing wave $|Ea\rangle_+$ and the standing wave $|Ea\rangle_P$:

$$|Ea\rangle_+ = \sum_b |Eb\rangle_P\{1 - i\pi T(E)\}_{ba}, \tag{22}$$

where $T_{ba}(E)$ means $\langle b|T(E)|a\rangle$ defined in Eq. (9). Finally, by substituting Eq. (22) in Eq. (9), we obtain the Heitler integral equation [1]

$$T(E) = R(E) - i\pi\ R(E)T(E), \tag{23}$$

which directly relates $T(E)$ and $R(E)$.

Having derived the relations (22) and (23) between the T- and R-matrix descriptions, we can easily see that the S matrix of Eq. (10) is written in terms of $R(E)$ as

$$S(E) = \frac{1 - i\pi R(E)}{1 + i\pi R(E)}. \tag{24}$$

In the partial wave decomposition, $R(E)$ becomes diagonal as $\langle lm|R(E)|lm\rangle = -(1/\pi)\tan\delta_l(E)$, to give $\langle lm|S(E)|lm\rangle = \exp[2i\delta_l(E)]$.

Note that Hermiticity of $R(E)$ [or $\mathcal{R}(E)$] alone can assure the unitarity of $S(E)$. This is a great advantage of the R matrix over the T-matrix description where $T(E)$ [or $\mathcal{T}(E)$] must satisfy the nonlinear Eq. (11) [or Eq. (12)] to be compatible with the unitarity of $S(E)$. In Sec. V, we shall see an example which illustrates this point.

This should not be, however, the whole story of the R-matrix description of scattering theory. It is well known, for example, that the spectral representation (16) of the T operator has played important roles in many aspects [1]. In the R-matrix theory, on the other hand, we do not have the counterparts to Eqs. (13)–(16) of the T-matrix theory. The point is that the standing wave states $\{|Ea\rangle_P\}$ do not form an orthogonal basis set; instead they satisfy [1], as shall also be proven later,

$$ {}_P\langle E'a'|Ea\rangle_P = \delta(E'-E)\{1+\pi^2 R^2(E)\}_{a'a}, \tag{25}$$

where $R_{a'a}(E)$ means $\langle a'|R(E)|a\rangle$ defined in Eq. (20). Consequently, it is suggested that a properly normalized standing wave state is given by [1]

$$|Ea\rangle_{P'} = \sum_b |Eb\rangle_P \{1+\pi^2 R^2(E)\}^{-1/2}_{ba}.$$

Then we may write down the completeness relation as $\Sigma_A |A\rangle_{P'}\,{}_{P'}\langle A|=1$. This is not, however, a convenient way of treating the standing wave states, first because the physical meaning of $|A\rangle_{P'}=|E_a a\rangle_{P'}$ is not clear, and second because $\langle Ea'|V|Ea\rangle_{P'}$ cannot be written as a matrix element of an appropriate scattering operator as in Eq. (20). Since a proper completeness relation is not known in the R-matrix theory, even the principal value Green's operator has been expressed as [1]

$$\frac{1}{E-H} = \sum_A |A\rangle_+ \frac{1}{E-E_a}\,{}_+\langle A|, \tag{26}$$

using the complete set $\{|A\rangle_+\}$ of the T-matrix theory as in Eq. (15). Obviously this expression is not satisfactory; we need a proper completeness relation and a spectral representation of $1/(E-H)$ in terms of the standing wave states. This is exactly what we shall establish below.

IV. SCATTERING OPERATOR $\hat{\mathcal{R}}(E)$

Having understood the unsolved problem in the R-matrix theory, we define a Hermitian operator $\tilde{\mathcal{R}}(E)$ by

$$\tilde{\mathcal{R}}(E) = V + V\frac{1}{E-H}V, \tag{27}$$

where $1/(E-H)$ is defined via the principal value. Note that $\tilde{\mathcal{R}}(E)$ is different from $\mathcal{R}(E)$ of Eq. (17) [1–3]. We introduce a corresponding scattering state $|\widetilde{Ea}\rangle_P$, that satisfies $H|\widetilde{Ea}\rangle_P = E|\widetilde{Ea}\rangle_P$ by

$$|\widetilde{Ea}\rangle_P = |Ea\rangle + \frac{1}{E-H}V|Ea\rangle, \tag{28}$$

so that we have

$$V|\widetilde{Ea}\rangle_P = \tilde{\mathcal{R}}(E)|Ea\rangle. \tag{29}$$

Note that Eqs. (27)–(29) correspond to Eqs. (17)–(19) in the R-matrix theory. We shall see later that $|\widetilde{Ea}\rangle_P$ is quite similar to the standing wave state $|Ea\rangle_P$.

Kouri and Levin [2,3] studied Eqs. (27) and (28) more than three decades ago, and showed that $\tilde{\mathcal{R}}(E)$ can give the phase shift $\delta_l(E)$ as $\mathcal{R}(E)$ does. However, their analysis did not reveal physical meanings of $\tilde{\mathcal{R}}(E)$ and $|\widetilde{Ea}\rangle_P$, which then have been left unclear to date without drawing much attention. In the following, we clarify their meanings.

We now present the key point of the present paper. $|\widetilde{Ea}\rangle_P$ defined via Eq. (28) is biorthogonal to $|Ea\rangle_P$, satisfying

$$ {}_P\langle \widetilde{E'a'}|Ea\rangle_P = \delta(E'-E)\delta_{a'a}. \tag{30}$$

The proof goes as follows. Let us note

$$\begin{aligned} {}_P\langle \widetilde{E'a'}|Ea\rangle_P &= \langle E'a'|\left\{1+V\frac{1}{E'-H}\right\}\left\{1+\frac{1}{E-H_0}\mathcal{R}(E)\right\}|Ea\rangle \\ &= \langle E'a'|Ea\rangle + \langle E'a'|\frac{1}{E-H_0}\mathcal{R}(E)|Ea\rangle \\ &\quad + \langle E'a'|V\frac{1}{E'-H}|Ea\rangle_P. \end{aligned} \tag{31}$$

By using Eq. (20), we see that the last term on the right-hand side can be written as

$$\langle E'a'|V|Ea\rangle_P \frac{1}{E'-E} = \langle E'a'|\mathcal{R}(E)|Ea\rangle\frac{1}{E'-E},$$

which cancels the second term $\langle E'a'|\mathcal{R}(E)|Ea\rangle/(E-E')$. Then the right-hand side of Eq. (31) becomes $\langle E'a'|Ea\rangle = \delta(E'-E)\delta_{a'a}$, which completes the proof of Eq. (30).

Because $\{|Ea\rangle_P\}$ constitutes a complete set for the scattering states, so does its biorthogonal set $\{|\widetilde{Ea}\rangle_P\}$. It is then clear that we have established the completeness relation in terms of the standing wave states as

$$\int dE \sum_a |Ea\rangle_P\,{}_P\langle\widetilde{Ea}| = 1, \tag{32}$$

which is to be compared to Eq. (14) in the T-matrix theory. Then we can show immediately the useful relation

$$\sum_a |Ea\rangle_P\,{}_P\langle\widetilde{Ea}| = \delta(E-H), \tag{33}$$

with which we can prove the following identity:

$$V\delta(E-H)V = \mathcal{R}(E)\delta(E-H_0)\tilde{\mathcal{R}}(E) = \tilde{\mathcal{R}}(E)\delta(E-H_0)\mathcal{R}(E), \tag{34}$$

where we have used Eqs. (19) and (29) to make $\delta(E-H_0)$ of Eq. (5).

In the following, we establish relations between $\tilde{\mathcal{R}}(E)$ and $\mathcal{R}(E)$, and between $|\widetilde{Ea}\rangle_P$ and $|Ea\rangle_P$. Let us first note the following identity [2]:

$$\frac{1}{E-H} = \frac{1}{E-H_0} + \frac{1}{E-H_0}V\frac{1}{E-H} - \pi^2\delta(E-H_0)V\delta(E-H), \tag{35}$$

which we can prove by using $1/(E-H\pm i\eta)=1/(E-H)\mp i\pi\delta(E-H)$, and the Lippmann-Schwinger equation for $1/(E-H\pm i\eta)$. Then it is easy to show that $\tilde{\mathcal{R}}(E)$ of Eq. (27) satisfies

$$\tilde{\mathcal{R}}(E) = V + V\frac{1}{E-H_0}\tilde{\mathcal{R}}(E) - \pi^2 V\delta(E-H_0)V\delta(E-H)V, \tag{36}$$

which makes a clear contrast with Eq. (17) that allows a perturbation expansion of $\mathcal{R}(E)$ in powers of V. By solving Eq. (36) for $\tilde{\mathcal{R}}(E)$, we obtain [2]

$$\tilde{\mathcal{R}}(E) = \mathcal{R}(E)\{1 - \pi^2\delta(E-H_0)V\delta(E-H)V\}, \tag{37}$$

where we have used a formal expression for $\mathcal{R}(E)$ in terms of V that derives from Eq. (17). By substituting Eq. (34) for $V\delta(E-H)V$ in Eq. (37), we arrive at the following operator relation between $\tilde{\mathcal{R}}(E)$ and $\mathcal{R}(E)$ [2]:

$$\tilde{\mathcal{R}}(E) = \frac{1}{1+\pi^2[\mathcal{R}(E)\delta(E-H_0)]^2}\mathcal{R}(E) = \mathcal{R}(E)\frac{1}{1+\pi^2[\delta(E-H_0)\mathcal{R}(E)]^2}. \tag{38}$$

It should be noted here that the Hermiticity of $\mathcal{R}(E)$ guarantees the Hermiticity of $\tilde{\mathcal{R}}(E)$, and vice versa, as can be shown by Eq. (38).

We now define the on-shell matrix $\tilde{R}(E)$ by

$$\langle a'|\tilde{R}(E)|a\rangle = \langle Ea'|V|\widetilde{Ea}\rangle_P = \langle Ea'|\tilde{\mathcal{R}}(E)|Ea\rangle, \tag{39}$$

in the same way as $T(E)$ and $R(E)$. By taking the on-shell matrix element of Eq. (38) between $\langle Ea'|$ and $|Ea\rangle$, we obtain the on-shell matrix relation

$$\tilde{R}(E) = \frac{R(E)}{1+\pi^2R^2(E)}, \tag{40}$$

where we have used Eq. (5) for $\delta(E-H_0)$.

It is easy to generalize Eq. (40) to the off-shell and half-on-shell cases. By evaluating the half-on-shell matrix element of Eq. (38), for example, we obtain

$$\langle E'a'|\tilde{\mathcal{R}}(E)|Ea\rangle = \sum_b \langle E'a'|\mathcal{R}(E)|Eb\rangle\{1+\pi^2R^2(E)\}^{-1}_{ba}, \tag{41}$$

which is the half-on-shell generalization of Eq. (40).

It is appropriate here to discuss the relation between $\tilde{R}(E)$ and $S(E)$. We can derive immediately the following matrix relation using Eqs. (24) and (40):

$$S(E) - S^\dagger(E) = -4\pi i\tilde{R}(E), \tag{42}$$

which shows that $\tilde{R}(E)$ determines the anti-Hermitian part of $S(E)$. This is naturally understood by noticing

$$\tilde{\mathcal{R}}(E) = \frac{1}{2}\{\mathcal{T}(E) + \mathcal{T}^\dagger(E)\}, \tag{43}$$

which we can prove easily using the second equality of Eq. (6). This relation shows explicitly that $\tilde{\mathcal{R}}(E)$ is the Hermitian part of $\mathcal{T}(E)$, which in turn determines the anti-Hermitian part of $S(E)$ of Eq. (10). Note also that the knowledge of $\tilde{R}(E)$ is sufficient to give the phase shift $\delta_l(E)$, because Eq. (40) becomes diagonal in the angular momentum basis as $\langle lm|\tilde{R}(E)|lm\rangle = -(1/\pi)\cos\,\delta_l(E)\sin\,\delta_l(E)$.

Let us turn to the relation between $|\widetilde{Ea}\rangle_P$ and $|Ea\rangle_P$. First, using Eqs. (35), (27), and (37) in order in Eq. (28), we can express $|\widetilde{Ea}\rangle_P$ as

$$|\widetilde{Ea}\rangle_P = \left\{1 + \frac{1}{E-H_0}\mathcal{R}(E)\right\}\{1-\pi^2\delta(E-H_0)V\delta(E-H)V\} \times|Ea\rangle. \tag{44}$$

Second, by using expressions (34) and (5) for $V\delta(E-H)V$ and $\delta(E-H_0)$, respectively, we can easily see

$$\delta(E-H_0)V\delta(E-H)V|Ea\rangle = \sum_{bc}|Eb\rangle\langle Eb|\mathcal{R}(E)|Ec\rangle\langle Ec|\tilde{\mathcal{R}}(E)|Ea\rangle = \sum_b|Eb\rangle\{R(E)\tilde{R}(E)\}_{ba}.$$

Then, we can show that Eq. (44) gives the following explicit relation between $|\widetilde{Ea}\rangle_P$ and $|Ea\rangle_P$:

$$|\widetilde{Ea}\rangle_P = \sum_b|Eb\rangle_P\{1+\pi^2R^2(E)\}^{-1}_{ba}, \tag{45}$$

where we have used Eqs. (18) and (40). In the angular momentum basis, Eq. (45) becomes

$$|\widetilde{Elm}\rangle_P = |Elm\rangle_P\cos^2\,\delta_l(E), \tag{46}$$

which shows obviously that $|\widetilde{Elm}\rangle_P$ is a standing wave state except for an overall factor [2,3].

It is very important here to note that we have expressed $|\widetilde{Ea}\rangle_P$ in two ways, i.e., first by Eq. (28) that relates $|\widetilde{Ea}\rangle_P$ to the scattering operator $\tilde{\mathcal{R}}(E)$, and second by Eq. (45) that proves by itself the biorthogonality of Eq. (30) because of Eq. (25). The crucial point is that these two definitions, (28) and (45), lead to the same $|\widetilde{Ea}\rangle_P$.

Here we make the following two points. First, because we have derived Eqs. (30) and (45) independently of Eq. (25), we can easily give a proof of Eq. (25) by combining Eqs. (30) and (45). Second, Eqs. (25) and (45) in turn give the overlap among $\{|\widetilde{Ea}\rangle_P\}$ as

$${}_P\langle\widetilde{E'a'}|\widetilde{Ea}\rangle_P = \delta(E'-E)\{1+\pi^2R^2(E)\}^{-1}_{a'a}. \tag{47}$$

In this section, we have introduced $\tilde{\mathcal{R}}(E)$ and $|\widetilde{Ea}\rangle_P$, and have clarified their meanings. We stress here that their significance originates from the fact that they provide the R-matrix theory with the completeness relation (32), but not from numerical feasibility in calculating phase shifts for a given potential V. In fact, Eq. (17) for $\mathcal{R}(E)$ is numerically more tractable than Eq. (27) for $\tilde{\mathcal{R}}(E)$. In Sec. V, we shall see how $\tilde{\mathcal{R}}(E)$ and $|\widetilde{Ea}\rangle_P$ show up as indispensable elements in numerical as well as in analytical aspects of the scattering theory.

V. DISCUSSIONS

Here we derive the spectral representation and the Low equation in the R-matrix theory. Discussions on the basis of these results show the importance of the relations obtained in Sec. IV. In particular, we will see that the Low equation is an example where the R-matrix theory is truly more appropriate than the T-matrix theory.

A. Spectral representation

We show, as an application of the completeness relation in the standing wave states, the counterpart of Eq. (16) in the R-matrix theory. It is clear that $\mathcal{R}(E)$ does not have a spectral representation because the propagator in Eq. (17) is $1/(E-H_0)$. On the other hand, $\tilde{\mathcal{R}}(E)$ of Eq. (27) is defined via $1/(E-H)$, and has a spectral representation. Using the completeness relation (32), we have

$$\frac{1}{E-H}=\sum_B |B\rangle_P \frac{1}{E-E_b}\, {}_P\langle\tilde{B}|, \tag{48}$$

which replaces Eq. (26). Then we can show immediately that Eq. (27) yields the following spectral representation:

$$\langle A'|\tilde{\mathcal{R}}(E)|A\rangle=\langle A'|V|A\rangle+\sum_B \langle A'|\mathcal{R}(E_b)|B\rangle \frac{1}{E-E_b} \times\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle. \tag{49}$$

Because the matrix elements of $\mathcal{R}(E)$ and $\tilde{\mathcal{R}}(E)$ can be transformed to each other by virtue of Eq. (38) as shown by Eqs. (40) and (41), the spectral representation of Eq. (49) plays exactly the same role in the R-matrix theory as that of Eq. (16) in the T-matrix theory.

We emphasize here that the derivation of Eq. (49) requires both expressions (28) and (45) for $|\widetilde{Ea}\rangle_P$. Suppose one starts with the knowledge the R-matrix theory summarized by Eqs. (17)–(20), (24), and (25). Then, from Eq. (25) for the overlap among $\{|Ea\rangle_P\}$, one would be led naturally to define $|\widetilde{Ea}\rangle_P$ by Eq. (45), that guarantees the biorthogonality (30) and gives the expression (48) for $1/(E-H)$. Only with $\mathcal{R}(E)$ of Eq. (17) at hand, however, one cannot proceed any further to establish Eq. (49). In order to write a spectral representation, one needs, in addition to Eq. (45), a relation between $|\widetilde{Ea}\rangle_P$ and a scattering operator defined via $1/(E-H)$. The investigation in the present work shows that the relation is exactly what is expressed by Eq. (29), and the scattering operator is $\tilde{\mathcal{R}}(E)$ defined by Eq. (27). In fact, to complete Eq. (49), we need to use ${}_P\langle\tilde{B}|V|A\rangle=\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle$ that derives from Eq. (29). The above observation clearly shows that if we had, to express $|\widetilde{Ea}\rangle_P$, either Eq. (28) or Eq. (45) only, we could not have arrived at the spectral representation (49).

B. Low equation

Having established the spectral representation (49), we now derive for the first time the Low equation [1,4] in the R-matrix theory in the following manner. First, by setting $E=E_a$ in Eq. (49), we obtain

$$\langle A'|\tilde{\mathcal{R}}(E_a)|A\rangle=\langle A'|V|A\rangle+\sum_B \langle A'|\mathcal{R}(E_b)|B\rangle \frac{1}{E_a-E_b} \times\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle. \tag{50}$$

Second, by changing indices as $A\leftrightarrow A'$ in Eq. (50) and taking the complex conjugate, we have

$$\langle A'|\tilde{\mathcal{R}}(E_{a'})|A\rangle=\langle A'|V|A\rangle+\sum_B \langle A'|\mathcal{R}(E_b)|B\rangle \times\frac{1}{E_{a'}-E_b}\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle. \tag{51}$$

Here we have used

$$\sum_B \langle A'|\tilde{\mathcal{R}}(E_b)|B\rangle \frac{1}{E_{a'}-E_b}\langle B|\mathcal{R}(E_b)|A\rangle =\sum_B \langle A'|\mathcal{R}(E_b)|B\rangle \frac{1}{E_{a'}-E_b}\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle,$$

which we can show by using Eqs. (41) and (45). Subtracting Eq. (51) from Eq. (50), we eliminate V to obtain

$$\langle A'|\tilde{\mathcal{R}}(E_a)|A\rangle-\langle A'|\tilde{\mathcal{R}}(E_{a'})|A\rangle =\sum_B \langle A'|\mathcal{R}(E_b)|B\rangle\left(\frac{1}{E_a-E_b}-\frac{1}{E_{a'}-E_b}\right)\langle B|\tilde{\mathcal{R}}(E_b)|A\rangle. \tag{52}$$

This is a system of self-consistent nonlinear equations for the half-on-shell matrix elements of $\tilde{\mathcal{R}}(E)$ [or of $\mathcal{R}(E)$, because of Eq. (41)]. We note that Eq. (52) is obviously the R-matrix version of the Low equation [1,4]. In fact, by starting from Eq. (16) and following the same way as in the above, we can obtain the original Low equation in the T-matrix theory as

$$\langle A'|\mathcal{T}(E_a)|A\rangle-\langle A'|\mathcal{T}^{\dagger}(E_{a'})|A\rangle =\sum_B \langle A'|\mathcal{T}(E_b)|B\rangle\left(\frac{1}{E_a-E_b+i\eta}-\frac{1}{E_{a'}-E_b-i\eta}\right) \times\langle B|\mathcal{T}^{\dagger}(E_b)|A\rangle. \tag{53}$$

It should be stressed here that the Low equation does not explicitly depend on the potential V, and therefore that its applicability may exceed the domain of potential scattering. This important feature of the Low equation warrants its numerical as well as analytical investigations.

Now we compare Eqs. (52) and (53). It is known that Eq. (53) in the T-matrix theory is very difficult to solve [6], and has not been used in actual calculations. One of the main difficulties is that one must solve Eq. (53) with the unitarity constraint of Eq. (12), which itself is a complicated nonlinear equation. In the R-matrix version (52), on the other hand, the only constraint is that $\tilde{\mathcal{R}}(E)$ [and therefore $\mathcal{R}(E)$] be Hermitian. Let us explain the above situation in a different way. Because of Eq. (43), we can regard Eq. (52) as a closed system of equations for only the Hermitian part of $\mathcal{T}(E)$. On the other hand, Eq. (53) [along with Eq. (12)] is a system of coupled equations for the Hermitian and anti-Hermitian parts of $\mathcal{T}(E)$. The above observation shows clearly that the R-matrix version (52) is much more tractable than the original T-matrix version (53). We believe that the Low equation, in its standing wave representation (52), is now ready for numerical studies as well as for analytical investigations.

The Low equation is a good example where the R-matrix description is truly more convenient than the T-matrix description, while both theories ultimately lead to the same results. This shows clearly that the R-matrix theory, in its present formulation, can claim its due place in the description of scattering phenomena in addition to the standard T-matrix theory.

VI. SUMMARY

Let us summarize the present work. The R-matrix theory describes scattering phenomena in terms of the scattering operator $\mathcal{R}(E)$ and the standing wave state $|Ea\rangle_P$. To date, the R-matrix theory has lacked the biorthogonal complement of $|Ea\rangle_P$, and the corresponding scattering operator, and the proper completeness relation. In this situation, we have presented the following results. First, we have shown that the scattering operator $\widetilde{\mathcal{R}}(E)$ of Eq. (27) and the corresponding scattering state $\widetilde{|Ea\rangle}_P$ of Eq. (28) are related to $\mathcal{R}(E)$ and $|Ea\rangle_P$ in the R-matrix theory by Eqs. (38) and (45), respectively. Second, and most important, we have proven that $\widetilde{|Ea\rangle}_P$ is biorthogonal to $|Ea\rangle_P$. We have then obtained the completeness relation (32) in terms of the standing wave states, that has long been missing in the R-matrix theory. Finally, in order to show the importance of the above completeness relation, we have derived the spectral representation (49) of $\widetilde{\mathcal{R}}(E)$, and the Low equation (52) in the R-matrix theory. In particular, we have shown that the Low equation in its R-matrix version is much more controllable than its original T-matrix version. Having solved the long-standing problem of the completeness relation in the R-matrix theory, we believe that the present work has made the R-matrix description as complete as and in some cases even more useful than the T-matrix description of scattering phenomena.

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