Stationarity principle for quantum-mechanical resonance states

Donald G. Truhlar and C. Alden Mead
Department of Chemistry, Chemical Physics Program, and Supercomputer Institute, University of Minnesota, 207 Pleasant Street S.E., Minneapolis, Minnesota 55455
(Received 21 March 1990)

We show that the quantum-mechanical time-reversal operator provides a satisfying formulation of the "generalized dilatation transformation" for forming scalar products with partial complex conjugation, and leads to a theoretically justified stationarity principle for finding resonances (i.e., metastable states) in atomic and molecular systems.

I. INTRODUCTION

In recent years, various methods involving complex extensions of the quantum-mechanical eigenvalue problem have been employed to find resonances (i.e., metastable states) in atomic and molecular systems. Formally, these methods lead to complex eigenvalues of the Hamiltonian or generalized forms of it.[1,2] Some of these methods have involved the dilatation transformation of the Hamiltonian,[3,4] while others have been based on redefinition of the scalar product so as to allow complex "expectation values" of the energy.[1,5] While these methods have often been quite successful, the relation between them has not always been clear, nor has it been as clear as one might wish as to why the methods based on redefined scalar products work.

In this paper, we focus on the method used (but not always explicitly formulated) in Ref. 5, which has been named the generalized dilatation transformation or (GDT) by Reinhardt.[2] We will formulate this approach in later sections with some precision; here we just briefly summarize it.

Consider a molecular system in which total angular momentum is conserved, and let $\Psi(c_k;J,M)$ be a trial function with definite angular momentum quantum numbers J and M (standing as usual for total angular momentum and component in a chosen z direction), and depending on parameters c_k, which are allowed to be complex. Reinhardt[2] defines the GDT conjugate $\Psi^{\mathrm{GDT}*}$ as the function obtained from Ψ by complex conjugating only the part depending on angular variables. One then defines a variational function $W(c_k)$ as

$$W(c_k)=\frac{\int \Psi^{\mathrm{GDT}*}(c_k)\hat{H}\Psi(c_k)d\tau}{\int \Psi^{\mathrm{GDT}*}(c_k)\Psi(c_k)d\tau}, \tag{1}$$

where $\hat{H}$ is the Hamiltonian. Evidently, $W(c_k)$ is capable of taking on complex values. In the GDT method, one seeks stationary points of $W(c_k)$, real and complex. The real stationary points of W are then interpreted as bound-state eigenvalues of the Hamiltonian, while the complex ones with negative imaginary parts are interpreted as resonances. (Complex stationary points with positive imaginary parts are normally not of physical interest.)

The GDT method has proven quite successful in locating resonances, but nonetheless there are some unsatisfying features. In the first place, it is not clear how to perform partial complex conjugation with different coordinate systems, phase conventions, or representations. (For example, the distinction between radial and angular variables in Jacobi or heliocentric coordinates is not preserved under a transformation to hyperspherical coordinates.) Moreover, the relation to more rigorously established approaches, such as dilatation of the Hamiltonian or the location of poles of the resolvent operator, is unclear, leaving unanswered the question of *why* the GDT method leads to good results.

The purpose of the present paper is to put the GDT approach on a more nearly rigorous basis, by showing how to define it more precisely and generally, and then demonstrating that it leads to a true stationarity principle for locating poles of the resolvent operator. [From now on, when we speak of a resonance, we will always mean a pole of the resolvent operator located in the lower half energy plane.] In Sec. II, we discuss the precise formulation of GDT conjugation, and show that, when precisely formulated, it is simply related to time reversal, leading to a definition of GDT conjugation which is independent of coordinate system, phase convention, and representation, and which is applicable in the presence of spin. Section III presents the general theory of the stationarity principle, and proves the main result that stationary points of W as defined by the more precise form of Eq. (1) correspond to poles of the resolvent operator. In Sec. IV, we illustrate the approach by means of a calculation on a simple model. There is some further discussions in Sec. V and a brief summary in Sec. VI. Some mathematical points are discussed in the Appendixes. Our treatment is not mathematically rigorous in all respects: most importantly, we will frequently assume that expressions involving operators, and products of operators, which are functions of complex variables can be analytically continued. When such expressions are written out in terms of matrix elements, this amounts to assuming that an infinite sum of analytic functions is itself analytic. Nevertheless, we feel that we have put the GDT approach on a sounder basis then heretofore, and that we have taken a

worthwhile step—though not the last step—toward a truly rigorous theory.

II. RELATION BETWEEN GDT AND TIME REVERSAL

This section will be divided into two subsections. In Sec. II A, we discuss in some detail the formulation of the GDT method, so that the ambiguities in the usual definition[2] become apparent, as do the required properties of the phase convention which will lead to a useful definition. In Sec. II B, it is shown how this definition of GDT conjugation is expressible in terms of an antiunitary operator simply related to time reversal.

A. Usual formulation of GDT conjugation

To motivate our development, it is convenient to carry out GDT conjugation in two steps. Suppose that Ψ is written as a sum of the form

$$\Psi(c_k;J,M)=\sum_\alpha \Psi_\alpha(c_k,J,M;\rho)\chi_\alpha(M;\Omega) , \tag{2}$$

where the Ψ_α depend on scalar variables ρ, and the χ_α are spherical harmonics, or products of them, depending on angular variables Ω, each with total z component of angular momentum M. In order for Ψ as defined in (2) to have the specified value of the total angular momentum, one must have

$$\sum_\beta \langle \chi_\alpha|\hat{J}^2|\chi_\beta\rangle \Psi_\beta = J(J+1)\Psi_\alpha . \tag{3}$$

We now define a function Ψ^{GDT}, without the asterisk, whose complex conjugate will be $\Psi^{\mathrm{GDT}*}$. It is related to Ψ as follows:

$$\Psi^{\mathrm{GDT}}=\sum_\alpha \Psi_\alpha^* \chi_\alpha . \tag{4}$$

Ψ^{GDT} will still be an eigenfunction of $\hat{J}^2$ with the same eigenvalue if the matrix elements appearing in (3) are real, and we assume that the phase convention for the χ_α has been chosen so that this is the case:

$$\mathrm{Im}\langle \chi_\alpha|\hat{J}^2|\chi_\beta\rangle = 0 . \tag{5}$$

As we will see in Sec. II B, it is always easy to guarantee that Eq. (5) is satisfied. The "GDT conjugate" is now defined as the complex conjugate to Ψ^{GDT}

$$\Psi^{\mathrm{GDT}*}=\sum_\alpha \Psi_\alpha \chi_\alpha^* . \tag{6}$$

This is consistent with the definition of Ref. 2, according to which GDT conjugation consists of applying complex conjugation only to the angular part of the trial function. Note that the phase convention for the functions χ_α must be at least partially specified in order for this definition of GDT conjugation to be unambiguous. For example, if we multiply each Ψ_α in (2) by a phase factor $e^{i\gamma_\alpha}$ and each χ_α by $e^{-i\gamma_\alpha}$, there is no change in Ψ, but Ψ^{GDT} would acquire significantly different properties.

Once $\Psi^{\mathrm{GDT}*}$ is defined, one can define $W(c_k)$ as in (1) and look for stationary points of it. It is worthwhile to point out that, in cases of interest, W will be an analytic function of the parameters c_k, but will of course have singularities, including branch points, at certain values of the variables c_k. There may therefore be two or more Riemann sheets for W, and different stationary points may be on different sheets. The method, however, does not restrict itself to a single Riemann sheet: all stationary points on all sheets (for which Im $W \le 0$) can be associated with resonances. It is also worth noting that, if ordinary complex conjugation were used instead of GDT conjugation, it would not longer be possible to consider W an analytic function of the parameters, with ordinary conjugation, W would be real for all values of the parameters, real or complex, and thus could not be an analytic function.

B. GDT conjugation in terms of time reversal

The time-reversal operator $\hat{T}$, which has the property of reversing all momenta and spin, is an example of an antiunitary operator. The properties of antiunitary in general, and of $\hat{T}$ in particular, have been discussed extensively in the literature.[6-8] Here we briefly review a few fundamental properties which will be needed in what follows.

For any antiunitary operator $\hat{\Theta}$, any two kets $|\Psi\rangle$ and $|\phi\rangle$, and any two complex constants a and b, one has[8]

$$\langle \hat{\Theta}\Psi|\hat{\Theta}\phi\rangle = \langle \Psi|\phi\rangle^* , \tag{7}$$

$$\hat{\Theta}(a|\Psi\rangle + b|\phi\rangle) = a^*\hat{\Theta}|\Psi\rangle + b^*\hat{\Theta}|\phi\rangle . \tag{8}$$

Although Eq. (8) as written applies to constant a and b, it is shown in Appendix A that it implies complex conjugation of the Ψ in expressions such as (2) as well.

The time reversal operator $\hat{T}$ is antiunitary, satisfying (7) and (8), and also has the property of being involutional:[6] If $\hat{T}$ is applied twice, the result is the same state as before, except perhaps for a phase factor. It can be shown[6-8] that this phase factor is always $+1$, and that the plus sign applies if the overall spin of the system is integer, the minus sign if it is half odd integer:

$$\hat{T}^2 = 1 \quad \text{for integer spin} , \tag{9a}$$

$$\hat{T}^2 = -1 \quad \text{for odd integer spin} . \tag{9b}$$

Of more direct use to use than $\hat{T}$ itself is the related antiunitary operator $\hat{C}$, defined[8] by

$$\hat{C} = \hat{R}_x \hat{T} , \tag{10}$$

where $\hat{R}_x$ is the unitary operator for rotation through π about an axis perpendicular to the quantization axis. $\hat{C}$ is evidently antiunitary and involutional, and it can be shown[8] that, regardless of spin,

$$\hat{C}^2 = 1 . \tag{11}$$

Now consider the operation of $\hat{C}$ on one of the angular functions χ_α of Eq. (2). Application of $\hat{T}$ reverses the angular momentum component, but then $\hat{R}_x$ restores it to its original value, so the result is the same function as before, except perhaps for a phase factor:

$$\hat{C}\chi_\alpha(M;\Omega)=e^{i\lambda}\chi_\alpha(M:\Omega)\ . \tag{12}$$

Notice, however, that if we write $\chi'_\alpha=e^{i\lambda/2}\chi_\alpha$, then we find, making use of (8) and (12),

$$\hat{C}\chi'_\alpha=\hat{C}e^{i\lambda/2}\chi_\alpha=e^{-i\lambda/2}\hat{C}\chi_\alpha=e^{i\lambda/2}\chi_\alpha=\chi'_\alpha\ . \tag{13}$$

Thus, by an appropriate choice of phase convention, we can assure that,

$$\hat{C}\chi_\alpha=\chi_\alpha\ . \tag{14}$$

Moreover, the phase convention that guarantees (14) is also the one that guarantees (5). To see this, notice that $\hat{C}$ leaves $\hat{J}^2$ invariant; in other words,

$$[\hat{C},\hat{J}^2]=0\ . \tag{15}$$

If (14) is satisfied, we can make use of (7), (14), (15), and the Hermitian property of $\hat{J}^2$ to obtain

$$\begin{aligned}\langle\chi_\alpha|\hat{J}^2|\chi_\beta\rangle^*=\langle\chi_\beta|\hat{J}^2|\chi_\alpha\rangle&=\langle\hat{C}\chi_\beta|\hat{C}\hat{J}^2\chi_\alpha\rangle^*\\&=\langle\hat{C}\chi_\beta|\hat{J}^2|\chi_\alpha\rangle^*\\&=\langle\chi_\beta|\hat{J}^2|\chi_\alpha\rangle^*\\&=\langle\chi_\alpha|\hat{J}^2|\chi_\beta\rangle\ ,\end{aligned} \tag{16}$$

which is the same as (5).

Now, applying $\hat{C}$ to the trial function Ψ defined by (2), making use of (8) and (14), and comparing with (3), we find

$$\hat{C}\Psi=\sum_\alpha\Psi^*_\alpha\chi_\alpha=\Psi^{\mathrm{GDT}}\ . \tag{17}$$

(For a discussion of the validity of applying complex conjugation to the functions Ψ_α, see Appendix A.) Moreover, $\hat{C}\Psi$ possesses none of the ambiguities of the original definition involving partial complex conjugation. It is well defined regardless of coordinate system, phase convention, or representation. The presence of spin also causes no problems. From now on, we will drop the GDT notation and will work with $\hat{C}$.

With this definition, we can now rewrite (1) as

$$W=\frac{\langle\hat{C}\Psi|\hat{H}|\Psi\rangle}{\langle\hat{C}\Psi|\Psi\rangle}\ , \tag{18}$$

where the use of bra-ket notation is justified by the invariance under change of representation of all quantities appearing in (18). The stationary problem may now be solved in the usual way by means of the requirement

$$\delta(\langle\hat{C}\Psi|H|\Psi\rangle-\lambda\langle\hat{C}\Psi|\Psi\rangle=0\ , \tag{19}$$

where δ denotes a variation with respect to the parameters c_κ, and λ is a Lagrange multiplier.

Since $\hat{C}$ commutes with the Hamiltonian and satisfies (11), the eigenkets $|\Phi\rangle$ of the Hamiltonian can be chosen[7,8] such that $\hat{C}|\Phi\rangle=|\Phi\rangle$. For, if $|\Phi\rangle$ is an eigenket of $\hat{H}$ with eigenvalue E, so is $\hat{C}|\Phi\rangle$. If $\hat{C}|\Phi\rangle$ is already just a phase factor times $|\Phi\rangle$, we can use the procedure of (13) to rephase $|\Phi\rangle$ so it is unchanged by $\hat{C}$. If $\hat{C}|\Phi\rangle$ is linearly independent of $|\Phi\rangle$, we can define the kets

$$|\Phi_a\rangle=|\Phi\rangle+\hat{C}|\Phi\rangle \tag{20a}$$

and

$$|\Phi_b\rangle=i(|\Phi\rangle-\hat{C}|\Phi\rangle)\ , \tag{20b}$$

and it follows immediately from (8) and (11) that both are left unchanged by $\hat{C}$. Thus (19) reduces to the ordinary stationarity principle for the eigenvalue problem if one restricts oneself to trial functions invariant under $\hat{C}$. By considering the more general case, we will obtain solutions corresponding to resonances. In Sec. III, the general theory is examined more closely.

Notice that the functionals in (18), unlike those in (1), are defined in unambiguous in all cases. This is the central result of the present section.

III. GENERAL THEORY

The goal of this section is to prove that stationary points of W, as defined by (18), correspond to poles of the resolvent operator. In order to prove this however, we must first lay some groundwork, which is done in Sec. III A–III D. Once this is done, the proof of the stationarity principle is quite simple, and this is done in Sec. III E.

A. Preliminaries: Hamiltonian, basis set, trial function

We consider a Hamiltonian $\hat{H}$ possessing certain symmetries, such as commuting with angular momentum, so that the problem of determining its spectrum can be split *a priori* into blocks such as JM blocks, and we can confine our attention to a single such block. In the problems we consider, moreover, there exists an antiunitary operator $\hat{C}$ which satisfies (11), commutes with $\hat{H}$, and does not couple different JM blocks.

As discussed in Sec. II B, we construct a complete set of basis kets $|j\rangle$ for our block, all of which are invariant under $\hat{C}$, i.e., all of which satisfy

$$\hat{C}|j\rangle=|j\rangle\ . \tag{21}$$

This is called[9] a $\hat{C}$-adapted basis.

Our Hamiltonian commutes with $\hat{C}$ by hypothesis, but we will need a generalization of this to operators that need not be Hermitian. Accordingly, consider an operator $\hat{G}$, not necessarily Hermitian, which satisfies

$$\hat{C}\hat{G}=\hat{G}^\dagger\hat{C},\quad \hat{G}\hat{C}=\hat{C}\hat{G}^\dagger\ , \tag{22}$$

where the second relation follows from the first after multiplying on both sides by $\hat{C}$ and using (11). The relation (22) is independent of representation, as shown in Appendix B.

The matrix for an operator satisfying (22) with respect to a basis obeying (21) is symmetric; for, if (21) and (22) are satisfied, we can use these relations in addition to (7) and (11) to obtain

$$\begin{aligned}\langle k|\hat{G}|j\rangle=\langle j|\hat{G}^\dagger|k\rangle^*&=\langle\hat{C}j|\hat{C}\hat{G}^\dagger|k\rangle\\&=\langle\hat{C}j|\hat{G}|\hat{C}k\rangle=\langle j|\hat{G}|k\rangle\ .\end{aligned} \tag{23}$$

Conversely, if $\hat{G}$ is symmetric in such a basis, it follows that (22) is satisfied. For any ket $|F\rangle$, we find, using (8),

(21), and (23),

$$\hat{C}\hat{G}|F\rangle=\hat{C}\hat{G}\sum_j|j\rangle\langle j|F\rangle=\hat{C}\sum_{j,k}|k\rangle\langle k|\hat{G}|j\rangle\langle j|F\rangle$$
$$=\sum_{j,k}|k\rangle\langle k|\hat{G}|j\rangle^*\langle j|F\rangle^*$$
$$=\sum_{j,k}|k\rangle\langle k|\hat{G}^\dagger|j\rangle\langle j|F\rangle^*$$
$$=\hat{G}^\dagger\hat{C}|F\rangle\ . \tag{24}$$

B. Eigenvalue problem

Now consider a variational problem analogous to (19) for an operator satisfying (22):

$$\delta\langle\hat{C}\Psi|\hat{G}|\Psi\rangle-\lambda\langle\hat{C}\Psi\Psi\rangle)=0\ . \tag{25}$$

Because of (8), we see that

$$\delta|\hat{C}\Psi\rangle=\hat{C}|\delta\Psi\rangle\ , \tag{26}$$

so (25) becomes

$$\langle\hat{C}\delta\Psi|\hat{G}|\Psi\rangle+\langle\hat{C}\Psi|\hat{G}|\delta\Psi\rangle-\lambda\langle\hat{C}\delta\Psi|\Psi\rangle$$
$$-\lambda\langle\hat{C}\Psi|\delta\Psi\rangle=0\ . \tag{27}$$

Using (7), (11), and (22), we can rearrange the second term on the left-hand side of (27) as

$$\langle\hat{C}\Psi|\hat{G}|\delta\Psi\rangle=\langle\delta\Psi|\hat{G}^\dagger|\hat{C}\Psi\rangle^*=\langle C\delta\Psi|\hat{C}\hat{G}^\dagger\hat{C}|\Psi\rangle$$
$$=\langle\hat{C}\delta\Psi|\hat{G}|\Psi\rangle\ . \tag{28}$$

Similarly, the fourth term becomes

$$\langle\hat{C}\Psi|\delta\Psi\rangle=\langle\delta\Psi|\hat{C}\Psi\rangle^*=\langle\hat{C}\delta\Psi|\hat{C}^2\Psi\rangle=\langle\hat{C}\delta\Psi|\Psi\rangle\ . \tag{29}$$

Inserting (28) and (29) into (27), and making use of the fact that $\langle\hat{C}\delta\Psi|$ is arbitrary, we see that (27) reduces to

$$(\hat{G}-\lambda)|\Psi\rangle=0\ . \tag{30}$$

Thus the variational problem (25) is equivalent to an eigenvalue problem, just like the more familiar variational principle. Unlike the usual variational problem, however, (25) lends itself to analytic continuation.

C. Analytic continuation

Consider a trial function $|\Psi(c_k)\rangle$, depending analytically on the parameters c_k in such a way that, for all of our basis vectors, $\langle j|\Psi(c_k)\rangle$ is an analytic function of the parameters. Now, since

$$\langle\hat{C}\Psi|j\rangle=\langle j|\hat{C}\Psi\rangle^*=\langle\hat{C}j|\hat{C}^2\Psi\rangle=\langle j|\Psi\rangle\ , \tag{31}$$

it follows that all the $\langle\hat{C}\Psi|j\rangle$ are also analytic functions of the parameters. From this, we can conclude that, under suitable convergence criteria which we will assume are fulfilled (as discussed at the end of the Introduction), both

$$\langle\hat{C}\Psi|\hat{H}|\Psi\rangle=\sum_{j,k}\langle\hat{C}\Psi|j\rangle\langle j|\hat{H}|k\rangle\langle k|\Psi\rangle \tag{32a}$$

and

$$\langle\hat{C}\Psi|\Psi\rangle=\sum_j\langle\hat{C}\Psi|j\rangle\langle j|\Psi\rangle \tag{32b}$$

are also analytic functions of the parameters; from this, it follows further that W, defined in (18), is also an analytic function of the c_k. Note that the usual variational average energy $W_0=\langle\Psi|\hat{H}|\Psi\rangle/\langle\Psi|\Psi\rangle$ is *not* an analytic function of the parameters, because of the complex conjugation. The variational principle using W reduces to the usual one for W_0 if one restricts oneself to trial functions left invariant by $\hat{C}$ (which includes all actual eigenfunctions of $\hat{H}$); W, however, unlike W_0, can be analytically continued.

To get an idea of what can occur, assume that $\hat{H}$ has discrete eigenvalues ω_α, and a continuous spectrum ranging from ω_0 to infinity. W will then have the form

$$W(c_k)=\sum_\alpha\omega_\alpha\rho_\alpha(c_k)+\int_{\omega_0}^{\infty}\omega\rho(\omega,c_k)d\omega\ . \tag{33}$$

The function $\rho(\omega,c_k)$ will in general be an analytic function of ω and c_k except perhaps for certain singularities. Suppose, for example, that ρ, considered as a function of ω for fixed c_k, has a pole at $\omega=\nu(c_k)$, so that the location of the pole will change with the c_k. As the c_k vary so that $\nu(c_k)$ passes through the real axis at a point beyond ω_0. W will experience an abrupt change. Thus W considered for simplicity as a function of one of the c_k with the others fixed, will have a branch point where $\nu(c_k)=\omega_0$, with a cut along the curve $\nu(c_k)=x$, $\omega_0<x<\infty$. As is the case with any analytic function, the location of the branch *point* is determined by the structure of the function, but the direction in which one draws the branch *cut* is a matter of choice, corresponding to a choice of Riemann sheet. We expect, therefore, that W will often possess more than one Riemann sheet, and that analytic extensions of W may lead to complex stationary points on one or more of these. We will call the sheet obtained by taking the branch cuts along the real axis the *principal sheet;* sheets obtained by distorting one or more of the cuts into the lower half-plane will be called *continuation sheets.*

D. Resolvent and projection operators

The resolvent operator[10] $\hat{R}(w)$, a function of the complex variable w, is formally the inverse of $(w-\hat{H})$, satisfying

$$\hat{R}(w)(w-\hat{H})=(w-\hat{H})(\hat{R}(\omega)=1\ . \tag{34}$$

$\hat{R}(w)$, or strictly speaking each matrix element of it, is an analytic function of w, with a pole at each discrete eigenvalue ω_α of $\hat{H}$ and a branch cut along the real axis corresponding to the continuous spectrum of $\hat{H}$, with a branch point at each continuum threshold.

The product of resolvents for two different values of w, $\hat{Z}(w_1,w_2)=\hat{R}(w_1)\hat{R}(w_2)$, satisfies

$$(w_1-\hat{H})\hat{Z}(w_1,w_2)(w_2-\hat{H})=1\ , \tag{35}$$

which is solved by

$$\hat{Z}(w_1,w_2)=\frac{1}{w_1-w_2}[\hat{R}(w_1)-\hat{R}(w_2)] . \tag{36}$$

We will find this result to by useful later in this section.

The resolvent, like any analytic function, obeys the Cauchy integral formula, which can be conveniently expressed as

$$\hat{R}(w)=\frac{1}{2\pi i}\oint_C \frac{\hat{R}(\omega)d\omega}{w-\omega} , \tag{37}$$

where the contour C is the *clockwise* path shown in Fig. 1(a), for a Hamiltonian with discrete negative eigenvalues and a continuous spectrum of positive energies. Equations such as (37) are always understood to apply to each matrix element of the operator(s) concerned, with each side of the expression to be constructed, in principle, one matrix element at a time. Accordingly, since any particular matrix element of $\hat{R}(\omega)$ becomes small for large ω, the circle at infinity can be omitted and the path distorted to that shown in Fig. 1(b)

From the form of the contour in Fig. 1(b), we see that the resolvent can be expressed as

$$\hat{R}(w)=\sum_\alpha \frac{\hat{g}_\alpha}{w-\omega_\alpha}+\int \frac{\hat{g}(\omega)d\omega}{w-\omega} , \tag{38}$$

where the $\hat{g}_\alpha$ are residues at the poles, the integral goes in the outward direction along the branch cut, and

$$\hat{g}(\omega)=\frac{1}{2\pi i}[\hat{R}_-(\omega)-\hat{R}_+(\omega)] , \tag{39}$$

where $\hat{R}_-(\omega)$ and $\hat{R}_+(\omega)$ are the functions obtained by continuing from the left half-plane below and above the cut, respectively.

For multichannel continua, there are two or more thresholds ω_σ, each with its own branch point, and $\hat{g}(\omega)$ has contributions from more than one channel. In that case, Eq. (38) becomes

$$\hat{R}(w)=\sum_\alpha \frac{\hat{g}_\alpha}{w-\omega_\alpha}+\sum_\sigma \int_{\omega_\sigma}^{\infty} \frac{\hat{g}_\sigma(\omega)d\omega}{w-\omega} , \tag{40}$$

a well-known[2] result. Evidently, if $\hat{H}$ commutes with the antiunitary operator $\hat{C}$, then $\hat{R}(w)$, $\hat{g}_\alpha$, and $\hat{g}_\sigma(\omega)$ are symmetric in a basis satisfying (21).

The locations of the branch points are consequences of the structure of the Hamiltonian, and through it, of the analytic structure of matrix elements of $\hat{R}(w)$. By changing the direction of a branch cut, however, we can obtain analytic continuations of $\hat{R}(\omega)$ onto other Riemann sheets. In particular, we may distort one or more of the cuts into the lower half-plane, as shown in Fig. 2(a). The distorted cut beginning at threshold ω_σ will be called S_σ. Figure 2(b) shows where $\hat{R}_+$ and $\hat{R}_-$ contribute to the integral along one of the cuts. Although $\hat{R}_-(w)$ has no poles in the lower half-plane, $\hat{R}_+(w)$ may have poles there, and in that case the distortion of the cut leads to more residue terms in the continued form of $\hat{R}(w)$, as indicated in parts (c) and (d) of Fig. 2. The expression (40) for $\hat{R}(w)$ remains formally unchanged, but the sum over α may now include complex values, and the integrals need not be along the real axis.

The Hamiltonian itself may be expressed in terms of the resolvent as an integral over a circle at infinity which reduces to contributions from the spectrum as follows:

$$\hat{H}=\frac{1}{2\pi i}\oint w\hat{R}(w)dw=\sum_\alpha \omega_\alpha \hat{g}_\alpha+\sum_\sigma \int_{\omega_\sigma}^{\infty}\omega\hat{g}_\sigma(\omega)d\omega . \tag{41a}$$

A matrix element of (41a) has the form

$$\langle u|\hat{H}|v\rangle=\sum_\alpha \omega_\alpha\langle u|\hat{g}_\alpha|v\rangle+\sum_\sigma \int_{\omega_\sigma}^{\infty}\omega\langle u|\hat{g}(\omega)|v\rangle d\omega . \tag{41b}$$

If the direction of each branch cut σ is distorted in the direction S_σ, (41a) becomes (the subscript in braces denotes the direction of distortion of the branch cut)

$$\hat{H}_{\{S_\sigma\}}=\sum_\alpha \omega_\alpha\hat{g}_\alpha+\sum_\sigma \int_{S_\sigma}\omega\hat{g}_\sigma(\omega)d\omega , \tag{42a}$$

a matrix element of which is

$$\langle u|\hat{H}_{\{S_\sigma\}}|v\rangle=\sum_\alpha \omega_\alpha\langle u|\hat{g}_\alpha|v\rangle+\sum_\sigma \int_{S_\sigma}\omega\langle u|\hat{g}_\sigma(\omega)|v\rangle d\omega . \tag{42b}$$

For fixed $\langle u|$ and $|v\rangle$, the integrands in (42b) are ana-

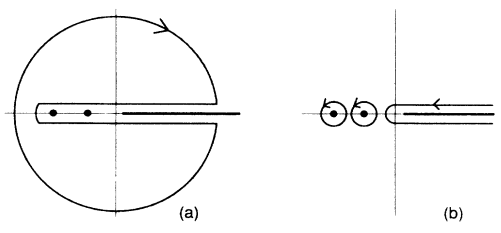

FIG. 1. Contours for resolvent in Eq. (37). The points on the negative real axis represent discrete eigenvalues of the Hamiltonian, and the heavy line along the positive real axis represents the continuous spectrum.

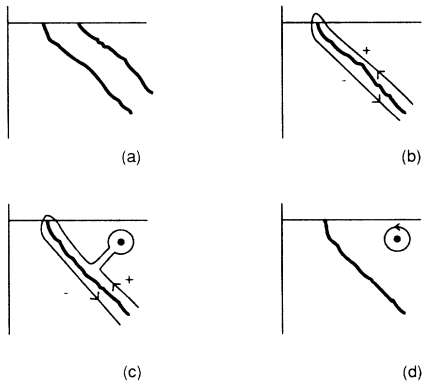

FIG. 2. (a) Distortion of two branch cuts into lower half-plane. (b) Contribution of (+) and (−) branches of resolvent to one of the cuts of (a). (c) Appearance of a pole of the (+) branch of the resolvent. (d) Distorted cut of (c) with contribution of the pole isolated.

lytic continuations of those in (42a). As illustrated in Fig. 2, the sum over α in (42a) and (42b) may contain terms not included in the corresponding sums in (41a) and (41b).

The matrix element $\langle u|\hat{H}_{\{S_\sigma\}}|v\rangle$ will be unaffected by the change of direction of the cuts if the elements $\langle u|\hat{g}_\sigma(\omega)|v\rangle$, considered as function so ω, have no singularities in the lower half-plane. In general, however, analogously to the discussion following Eq. (33), $\hat{H}_{\{S_\sigma\}}$ must be considered as a different operator from $\hat{H}$, not necessarily Hermitian, leading to continuation sheets of the functions $\langle u|\hat{g}_\sigma(\omega)|v\rangle$. If $u|$ and/or $|v\rangle$ depend on parameters, (42b) gives analytic continuations of the matrix element as function of the parameters onto continuation sheets.

Given a particular choice for the branch cuts of $\hat{R}(w)$, we can define for any closed curve C in the complex w plane a pseudoprojection operator $\hat{\mathcal{P}}(C)$ as

$$\hat{\mathcal{P}}(C)=\frac{1}{2\pi i}\oint_C \hat{R}(w)dw \ . \tag{43}$$

As illustrated in Fig. 3, $\hat{\mathcal{P}}(C)$ consists of residues $\hat{g}_\alpha$ at all poles contained within C, and the integral of $\hat{g}_\sigma(\omega)$ along any portion of a cut σ contained within C, as expressed by the relation

$$\hat{\mathcal{P}}(C)=\sum_{\alpha(C)}\hat{g}_\alpha+\sum_\sigma\int_{S_\sigma(c)}\hat{g}_\sigma(\omega)d\omega \ . \tag{44}$$

To evaluate the product of two such pseudoprojection operators, we can use (36), which applies by analytic continuation to any continued version of $\hat{R}(w)$, as follows:

$$\begin{aligned}\hat{\mathcal{P}}(C_1)\hat{\mathcal{P}}(C_2)&=\frac{1}{(2\pi i)^2}\oint_{C_1}dw_1\oint_{C_2}dw_2\hat{R}(w_1)\hat{R}(w_2)\\&=\frac{1}{(2\pi i)^2}\oint_{C_1}dw_1\oint_{C_2}dw_2\left[\frac{1}{w_1-w_2}\right]\\&\quad\times[\hat{R}(w_2)-\hat{R}(w_2)\\&\quad-\hat{R}(w_2)] \ ,\end{aligned} \tag{45}$$

where the last equality comes from (36). Integrating the first term over w_1 and the second one over w_2, and using the residue theorem both times, we see that we are left with the portion of C_1 contained in C_2 and the portion of C_2 contained in C_1, so that the result is the projection for C_{12}, the curve made up of these two portions and enclosing the portion of the plane enclosed by *both* C_1 and C_2. The result for the product is thus

$$\hat{\mathcal{P}}(C_1)\hat{\mathcal{P}}(C_2)=\hat{\mathcal{P}}(C_{12}) \ . \tag{46}$$

The situation is illustrated in Fig. 4.

By making various choices of the curves C_1 and C_2 so as to enclose only a single pole, a portion of a cut but no pole, etc., one easily obtains the following properties of the $\hat{g}$ operators:

$$\hat{g}_\alpha\hat{g}_\beta=\hat{g}_\alpha\delta_{\alpha\beta} \ , \tag{47a}$$

$$\hat{g}_\alpha\hat{g}_\sigma(\omega)=\hat{g}_\sigma(\omega)\hat{g}_\alpha=0 \ , \tag{47b}$$

$$\int_{K_\sigma}d\omega_\sigma\int_{K_\tau}d\omega_\tau\hat{g}_\sigma(\omega_\sigma)\hat{g}_\tau(\omega_\tau)=\delta_{\sigma\tau}\int_{K_{\sigma\tau}}\hat{g}_\sigma(\omega)d\omega \ , \tag{47c}$$

where in (47c) the curves K_σ and K_τ are portions of S_σ and S_τ, and $K_{\sigma\tau}$ is the segment, if any, where K_σ and K_τ coincide. If there are two or more continua whose cuts coincide for all or part of their length, one can obtain (47c) by imagining the cuts infinitesimally distorted so as to become nonoverlapping.

The properties (47a)–(47c) correspond to the properties of projection operators onto orthogonal spaces, with the $\hat{g}_\alpha$ projecting onto discrete subspaces and an integral along a curve of $\hat{g}_\sigma(\omega)$ onto a portion of the continuum; however, for distorted versions of $\hat{R}(w)$, the $\hat{g}_\alpha$ and $\hat{g}_\sigma(\omega)$ are not necessarily Hermitian, which distinguishes them from ordinary projection operators. Hence we use the term pseudoprojection operator.

E. Stationarity principle

Given a trial function $|\Psi\rangle$, depending analytically on parameters c_k, we now seek solutions to the variational problem (19) and its analytic continuations. As discussed in the treatment of Eqs. (33), (41), and (42), one can obtain an analytic continuation of (19) by distorting each cut σ into the direction S_σ, giving the analytically continued variational principle

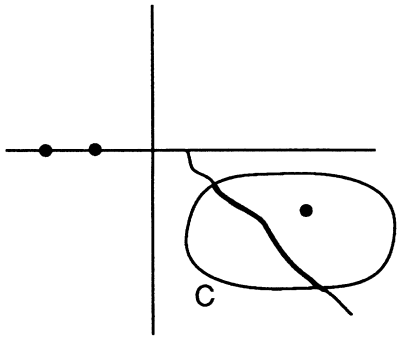

FIG. 3. Portion of a branch cut and pole selected by the pseudoprojection operator of curve C.

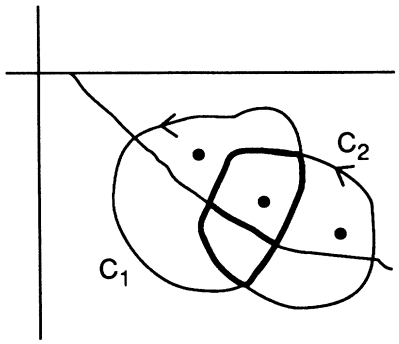

FIG. 4. Product of two pseudoprojection operators, as expressed by Eqs. (45) and (46). The intersection curve and the portion of the cut contained within it are emphasized.

$$\delta(\langle \hat{C}\Psi|\hat{H}_{\{S_\sigma\}}|\Psi\rangle-\lambda\langle \hat{C}\Psi|\Psi\rangle)=0\ , \tag{48}$$

where the operator $\hat{H}_{\{S_\sigma\}}$ is given by (42). Now, the operators $\hat{g}_\sigma(\omega)$ are symmetric in representations satisfying (21); this property, just expressing the equality of two functions

$$\langle j|\hat{g}_\sigma(\omega)|k\rangle=\langle k|\hat{g}_\sigma(\omega)|j\rangle \tag{49}$$

is not lost in analytic continuation. It therefore follows from the work of Sec. III A that $\hat{H}_{\{S_\sigma\}}$ satisfies (22). The treatment of Sec. III B is therefore applicable to (48), which, according to (30), reduces to

$$\hat{H}_{\{S_\sigma\}}|\Psi\rangle=\left[\sum_\alpha \omega_\alpha\hat{g}_\alpha+\sum_\sigma\int_{S_\sigma}\omega\hat{g}_\sigma(\omega)d\omega\right]|\Psi\rangle$$
$$=\lambda|\Psi\rangle\ . \tag{50}$$

Now let $|Y\rangle$ be an arbitrary ket, and try $|\Psi\rangle=\hat{g}_\beta|Y\rangle$, where $\hat{g}_\beta$ is any one of the pole residue operators, real or complex. Making use of (47a) and (47b), we easily find

$$\hat{H}_{\{S_\sigma\}}|\Psi\rangle=\left[\sum_\alpha \omega_\alpha\hat{g}_\alpha\hat{g}_\beta+\sum_\sigma\int_{S_\sigma}\omega\hat{g}_\sigma(\omega)\hat{g}_\beta\right]|Y\rangle$$
$$=\omega_\beta\hat{g}_\beta|Y\rangle=\omega_\beta|\Psi\rangle\ . \tag{51}$$

In other words, Eq. (50) is satisfied by our trial function, so there is a solution of the variational problem for every pole of $\hat{H}_{\{S_\sigma\}}$. Equation (51) thus establishes our variational principle, and it is the main result of this paper.

IV. EXAMPLE: CALCULATIONS WITH A SIMPLE MODEL

A. Definitions and resolvent

The model we use in this section is of a type that has been studied extensively in the literature, going back at least to the classic work by Weisskopf and Wigner.[11] Our model consists of a free particle moving in one dimension, or in three dimensions with zero angular momentum, which can be annihilated and recreated (or which can be trapped in a metastable state and reemitted). There are thus two types of zero-order basis states: a state with no particle present (bound state), denoted by $|q\rangle$, with zero-order energy ε, and a continuum of states $|\omega\rangle$, in which a free particle is present with zero-order energy ω, $0<\omega<\infty$. There is also coupling between the states, which may have the effect of replacing the bound state $|q\rangle$ by a resonance. In detail, the model is defined by the relations

$$\langle q|q\rangle=1,\quad \langle q|\omega\rangle=0,\quad \langle\omega|\omega'\rangle=\delta(\omega-\omega')\ ; \tag{52}$$

$$\hat{H}|q\rangle=|q\rangle\varepsilon+\int_0^\infty|\omega\rangle f(\omega)d\omega\ ; \tag{53}$$

$$\hat{H}|\omega\rangle=|\omega\rangle\omega+|q\rangle f(\omega)\ . \tag{54}$$

The function $f(\omega)$ is taken to be real; thus the antiunitary operator $\hat{C}$ in this representation can be taken as simple complex conjugation of all coefficients. In other words, for any ket

$$|F\rangle=|q\rangle a+\int_0^\infty|\omega\rangle g(\omega)d\omega\ , \tag{55}$$

we have

$$\hat{C}|F\rangle=|q\rangle a^*+\int_0^\infty|\omega\rangle g^*(\omega)d\omega\ . \tag{56}$$

It is clear that $\hat{C}$ commutes with $\hat{H}$ and satisfies (11). It then also follows from (34) that the resolvent in this representation is symmetric.

To find the resolvent operator, we use (34) and (52)–(54) as follows:

$$\langle\omega|w-\hat{H}|q\rangle\langle q|\hat{R}(w)|q\rangle$$
$$+\int_0^\infty\langle\omega|w-\hat{H}|\omega'\rangle d\omega'\langle\omega'|\hat{R}(w)|q\rangle$$
$$=-f(\omega)\langle q|\hat{R}(w)|q\rangle+(w-\omega)\langle\omega|\hat{R}(w)q\rangle=0\ , \tag{57}$$

$$\langle\omega|\hat{R}(w)|q\rangle=\frac{f(\omega)\langle q|\hat{R}(w)|q\rangle}{w-\omega}\ . \tag{58}$$

For the diagonal matrix elment $\langle q|\hat{R}(w)|q\rangle$, we again use (24) and (52)–(54), and find

$$\langle q|w-\hat{H}|q\rangle\langle q|\hat{R}(w)|q\rangle$$
$$+\int_0^\infty\langle q|w-\hat{H}|\omega\rangle d\omega\langle\omega\hat{R}(\omega)|q\rangle$$
$$=(w-\varepsilon)\langle q|\hat{R}(w)|q\rangle$$
$$-\int_0^\infty f(\omega)d\omega\langle\omega|\hat{R}(w)|q\rangle=1\ . \tag{59}$$

Combining (58) and (59), we now have

$$\langle q|\hat{R}(w)|q\rangle=\frac{1}{w-\varepsilon-\zeta(w)}\ , \tag{60}$$

$$\langle\omega|\hat{R}(w)|q\rangle=\frac{f(\omega)}{(w-\omega)[w-\varepsilon-\zeta(w)]}\ , \tag{61}$$

where

$$\zeta(w)=\int_0^\infty\frac{f^2(\omega)d\omega}{w-\omega}\ . \tag{62}$$

To obtain resolvent matrix elements between two continuum states, we use (34), (52)–(54), (61), and the symmetry of $\hat{R}(w)$ to obtain

$$\langle\omega|\hat{R}(w)|q\rangle\langle q|w-\hat{H}|\omega'\rangle$$
$$+\int_0^\infty\langle\omega|\hat{R}(w)|\omega''\rangle d\omega''\langle\omega''|w-\hat{H}|\omega'\rangle$$
$$=-\frac{f(\omega)f(\omega')}{(w-\omega)[w-\varepsilon-\zeta(w)]}$$
$$+(w-\omega')\langle\omega|\hat{R}(w)|\omega'\rangle=\delta(\omega-\omega')\ , \tag{63}$$

so that

$$\langle\omega|\hat{R}(w)|\omega'\rangle=\frac{\delta(\omega-\omega')}{w-\omega}$$
$$+\frac{f(\omega)f(\omega')}{[w-\varepsilon-\zeta(w)](w-\omega)(w-\omega')}\ . \tag{64}$$

The results (60), (61), and (64) can be summarized as

$$\hat{R}(w)=\int_0^\infty \frac{|\omega\rangle d\omega\langle\omega|}{w-\omega} + \frac{1}{w-\varepsilon-\zeta(w)}\left[|q\rangle+\int_0^\infty \frac{|\omega\rangle d\omega f(\omega)}{w-\omega}\right] \times\left[\langle q|+\int_0^\infty \frac{f(\omega')d\omega'\langle\omega'|}{w-\omega'}\right] . \quad (65)$$

We see from (65) that the resolvent $\hat{R}(w)$ will have a pole at any point for which $w=\varepsilon+\zeta(w)$. This can happen on the negative real axis if the properties of $f(\omega)$ are such that $\varepsilon+\zeta(0)<0$, which we assume not be the case. If the integral in (62) is taken along the real axis, there can be no poles for complex values of w, since Imw and Im$\zeta(w)$ always have opposite signs. Thus there are no poles on the principal sheet. However, $\zeta(w)$ as defined in (62) has a branch point at $w=0$, and we get a continuation sheet by taking the cut below the real axis. On this sheet, there may be poles.

B. Trial function and variational calculation

To illustrate the variational procedure as applied to our model, we consider a trial function of the form

$$|\Psi\rangle+|q\rangle+\int_0^\infty|\omega\rangle g(\omega)d\omega , \quad (66)$$

where $g(\omega)$ is a function to be determined. Using (56), we find

$$\hat{C}|\Psi\rangle=|q\rangle+\int_0^\infty|\omega\rangle g^*(\omega)d\omega . \quad (67)$$

Now, using (52)–(54), (66), and (67), we find

$$\langle\hat{C}\Psi|\hat{H}|\Psi\rangle=\varepsilon+2\int_0^\infty f(\omega)g(\omega)d\omega \quad (68)$$

and

$$\langle\hat{C}\Psi|\Psi\rangle=1+\int_0^\infty g^2(\omega)d\omega . \quad (69)$$

Inserting (68) and (69) into the expression (18) for W, we find

$$W=\frac{\varepsilon+2\int_0^\infty f(\omega)g(\omega)d\omega+\int_0^\infty \omega g^2(\omega)d\omega}{1+\int_0^\infty g^2(\omega)d\omega} . \quad (70)$$

The variational problem consists of setting the variational derivative of W with respect to $g(\omega)$ equal to zero. Taking the variational derivative and setting it equal to zero, we find

$$\frac{\delta W}{\delta g(\omega)}=2\left[1+\int_0^\infty g^2(\nu)d\nu\right]^{-2}\left[[f(\omega)+g(\omega)]\left[1+\int_0^\infty g^2(\nu)d\nu\right]-g(\omega)\left[\varepsilon+2\int_0^\infty f(\nu)g(\nu)d\nu+\int_0^\infty \nu g^2(\nu)d\nu\right]\right]=0 . \quad (71)$$

Setting the quantity in large square brackets in (71) equal to zero and solving, we easily obtain

$$g(\omega)=\frac{f(\omega)}{Z-\omega} , \quad (72)$$

with

$$Z=\frac{\varepsilon+2\int_0^\infty f(\nu)g(\nu)d\nu+\int_0^\infty \nu g^2(\nu)d\nu}{1+\int_0^\infty g^2(\nu)d\nu} . \quad (73)$$

We notice that $g(\omega)$ as given by (72) has a pole at $\omega=Z$, and that Z is itself a functional of $g(\omega)$. It will not be surprising, therefore, if more than one sheet appears.

We have a solution to our problem if (72) is consistent with (73). Inserting (72) into (73), we find

$$Z=\frac{\varepsilon+2\int_0^\infty \frac{f^2(\nu)d\nu}{Z-\nu}+\int_0^\infty \frac{\nu f^2(\nu)d\nu}{(Z-\nu)^2}}{1+\int_0^\infty \frac{f^2(\nu)d\nu}{(Z-\nu)^2}} . \quad (74)$$

Equation (74) can be simplified by using the definition (62) of the function $\zeta(Z)$, and by noticing that

$$\zeta'(Z)=\frac{d\zeta(Z)}{dZ}=-\int_0^\infty \frac{f^2(\nu)d\nu}{(Z-\nu)^2} . \quad (75)$$

Using (62) and (75), we can transform (74) into the form

$$Z=\frac{\varepsilon+\zeta(Z)-Z\zeta'(Z)}{1-\zeta'(Z)} , \quad (76)$$

or simply

$$Z=\varepsilon+\zeta(Z) . \quad (77)$$

Comparing (77) with the discussion following (65), we see that solutions of (77), which are solutions of our variational problem, coincide precisely with poles of the resolvent operator. As noted earlier, however, these will not occur on the principal sheet.

Finally, having found a solution of (77), it is a straightforward matter to substitute (72) and (77) back into (70) to obtain

$$W_{\text{stationary}}=Z . \quad (78)$$

The calculations of this subsection confirm directly that our variational principle locates poles of the resolvent for this simple model.

V. DISCUSSION

The method used here depends on the existence of an antiunitary operator that commutes with the Hamiltonian and satisfies (11). In principle, such an operator exists for any Hamiltonian. To see this, let $|\Phi_\alpha\rangle$ be the eigenkets of $\hat{H}$, and expand an arbitrary ket $|\Psi\rangle$ as

$$|\Psi\rangle=\sum_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|\Psi\rangle , \quad (79)$$

where the sum formally includes an integral over the continuum. Now we define the antiunitary operator $\hat{\Theta}$ by

$$\hat{\Theta}|\Psi\rangle=\sum_{\alpha}|\Phi_{\alpha}\rangle\langle\Phi_{\alpha}|\Psi\rangle^{*} . \tag{80}$$

In other words, $\hat{\Theta}$ is just complex conjugation in the representation of the eigenkets of the Hamiltonian. The operator $\hat{\Theta}$ evidently commutes with $\hat{H}$ and satisfies (11), so it can be used in the same way that $\hat{C}$ has been used in this paper.

In the absence of time reversal invariance, however, it will normally be difficult to find an appropriate antiunitary operator without first diagonalizing the Hamiltonian. In practice, therefore, the method is limited to systems with time reversal invariance, i.e., to systems without external magnetic fields.

The method of complex dilatation[3,4] is *different* from our method, although both are capable of revealing resonances. In the complex dilatation method the Hamiltonian

$$\hat{H}=\hat{T}+\hat{V} \tag{81}$$

is replaced by

$$\hat{H}_{\theta}=\hat{T}e^{-2i\theta}+\hat{V}e^{-i\theta} , \tag{82}$$

an operator which is not the same as our $\hat{H}_{|S_{\sigma}|}$. The Hamiltonian defined by (82) becomes non-Hermitian even for matrix elements involving no singularities in the complex plane, and its matrix elements are not necessarily analytic continuations of matrix elements of $\hat{H}$. It is easy to convince oneself, however, that the operator defined by (82) satisfies (22), so it eigenvalues can also be found by seeking stationary points of

$$W_{\theta}=\frac{\langle\hat{C}\Psi|\hat{H}_{\theta}|\Psi\rangle}{\langle\hat{C}\Psi|\Psi\rangle} . \tag{83}$$

We have established a genuine stationarity principle for resonances, but a stationarity principle for a function of complex variables is not the same as a minimum principle, for which one can always be sure that allowing greater flexibility in a trial function will bring one closer to the correct answer. Indeed, a trial function depending on a small number of parameters may lead to spurious stationary points: points that are stationary with respect to a limited set of variations, but which are not approximations to true stationary points.

VI. SUMMARY

We have defined a functional (18) involving the antiunitary operator (10) defined in terms of time reversal. This functional has real and complex stationary values, and the latter may be associated with resonances. In particular we have shown that every pole of the resolvent operator is associated with a stationary value of (18). Equation (18) is defined in all representations, and it provides a theoretical justification of the empirically successful method of generalized dilatation transformations for calculating complex resonance energies.

ACKNOWLEDGMENTS

This work has been supported by the National Science Foundation through Grants Nos. CHE-8662825, CHE-8713564, and CHE-8920520.

APPENDIX A: VALIDITY OF EQ. (17)

In arriving at (17), it was taken for granted that Eq. (8) could be applied to the functions Ψ_{α} as if they were constants. That this is so can be seen by making use of the existence, established by Eq. (21), of a complete basis set of functions left invariant by $\hat{C}$. If each Ψ_{α} is expanded in these, and (8) applied, the result follows immediately.

APPENDIX B: PROOF THAT EQ. (22) IS INDEPENDENT OF REPRESENTATION

As has been shown in the literature,[6-8] any antiunitary operator such as $\hat{C}$ can be represented as

$$\hat{C}=\tilde{\beta}K , \tag{B1}$$

where K stands for complex conjugation and $\tilde{\beta}$ is unitary. We use a tilde instead of a caret to designate $\tilde{\beta}$ because its transformation properties are different.[8] For a change of representation characterized by a unitary operator $\hat{U}$, such that an ordinary operator $\hat{G}$ is replaced by

$$\hat{G}'=\hat{U}\hat{G}\hat{U}^{\dagger} , \tag{B2}$$

$\tilde{\beta}$ becomes[11]

$$\tilde{\beta}'=\hat{U}\tilde{\beta}\hat{U}^{T} , \tag{B3}$$

where T denotes the transpose.

Using (A1), we can rewrite (22) as

$$\tilde{\beta}\hat{G}^{*}=\hat{G}^{\dagger}\tilde{\beta} . \tag{B4}$$

In the primed representation we have

$$\begin{aligned}\tilde{\beta}'\hat{G}^{*\prime}&=\hat{U}\tilde{\beta}\hat{U}^{T}\hat{U}^{*}\hat{G}^{*}\hat{U}^{T}=\hat{U}\tilde{\beta}\hat{G}^{*}\hat{U}^{T}\\&=\hat{U}\hat{G}^{\dagger}\beta\hat{U}^{T}=\hat{U}\hat{G}^{\dagger}\hat{U}^{\dagger}\hat{U}\tilde{\beta}\hat{U}^{T}\\&=\hat{G}^{\dagger\prime}\tilde{\beta}' ,\end{aligned} \tag{B5}$$

which completes the proof.

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