Systematic upper and lower bounds for the real and imaginary parts of transition amplitudes

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It is proved that the imaginary part of the diagonal matrix element $\langle\Psi|(E-H-i\Gamma)^{-1}|\Psi\rangle$ of the Green's function is the maximum of a variational functional. This provides convenient lower bounds. Upper bounds to the imaginary part are deduced with the aid of Padé approximants. Upper bounds of the real part of the transition amplitude are shown to follow from the unitarity relation. Finally, upper and lower bounds on nondiagonal matrix elements are derived and it is also shown that it is possible to obtain both upper and lower bounds on the real part of the transition amplitude. The negative consequence of employing these bounds is that we must deal with four-body operators.

I. INTRODUCTION

Variational principles represent an important tool in the theory of collisions. Time-independent formalisms of collision processes[1] are more often utilized than time-dependent formalisms,[2] even though they are *a priori* equivalent, because the former avoid the technically cumbersome limits at infinite time which cause considerable difficulty in the latter. The question of strict upper and lower bounds for transition amplitudes, cross sections, or probabilities, however, has been seldom discussed.[3] This is due to the fact that time-independent variational functionals, while they directly provide the transition amplitude, generate complex numbers which correspond to extrema. Time-dependent variational functionals, on the other hand, are often based on an extremum of the action rather than a strict maximum or minimum, and this extremum is not easily related to a bound on the transition probability itself. Since bounds to experimental cross sections or theoretical predictions are of major interest, the present paper is devoted to a derivation of such bounds.

To discuss the bounds on collision amplitudes, we rely on the fact that in a time-independent formalism these bounds can be related to the bounds on the matrix element of the (resolvent) operator $(E-H-i\Gamma)^{-1}$, where H is an A-particle Hamiltonian,

$$H=\mathscr{T}+\mathscr{V}=\sum_{i=1}^{A} t_i-t_{\text{c.m.}}+\sum_{i>j=1}^{A} v_{ij} \ . \tag{1.1}$$

We shall take the imaginary part of the energy, Γ, to be finite in the discussion and the on-shell limit will be only formally defined. The collision amplitudes discussed in this paper are thus to be interpreted as *energy-averaged amplitudes*. If one introduces real, square-integrable wave packets $|\Psi\rangle=V|\chi\rangle$ and $|\Psi'\rangle=V'|\chi'\rangle$, where $|\chi\rangle$ and $|\chi'\rangle$ are, respectively, the initial and final channel wave functions, all the transition amplitudes needed can be expressed in terms of diagonal matrix elements of the symmetric resolvent operator,[4] $\langle\Psi|G|\Psi\rangle$, $\langle\Psi'|G|\Psi'\rangle$, and $\langle(\Psi\pm\Psi')|G|(\Psi\pm\Psi')\rangle$. This is convenient because H is usually a real-symmetric operator and $|\Psi\rangle$ and $|\Psi'\rangle$ can often be chosen to be real[5] so that one can first investigate easily the bounds on a diagonal matrix element.

The crux of the argument lies in the consideration of the diagonal amplitude

$$\Delta T\equiv\langle\Psi|(E-H-i\Gamma)^{-1}|\Psi\rangle \ , \tag{1.2}$$

where ΔT represents the correction to the Born amplitude. The imaginary part of ΔT is defined as ΓY where

$$Y\equiv\langle\Psi|[(E-H)^2+\Gamma^2]^{-1}|\Psi\rangle \ . \tag{1.3}$$

We show in Sec. II the condition under which Y is a maximum of a variational functional. In Sec. III, we show that this condition is indeed realized so that the variational principle provides the lower bounds on Y. We discuss the Padé approximants of Y, in Sec. IV, which lead to the upper bounds and additional lower bounds. In Sec. V, we discuss the unitarity of the transition amplitude and obtain upper bounds on the real part of the transition amplitude. The case of nondiagonal elements is discussed in Sec. VI, with new bounds obtained for the real part. An illustrative example is provided in Sec. VII. Finally, the physical significance and application of these results is the subject of Sec. VIII, which includes the discussion and concluding remarks.

II. VARIATIONAL PRINCIPLE FOR THE IMAGINARY PART OF THE TRANSITION AMPLITUDE

Let us define an operator Ω by

$$\Omega=(E-H)^2+\Gamma^2 \ . \tag{2.1}$$

The functional

$$F(\Phi)=\frac{\langle\Phi|\Psi\rangle\langle\Psi|\Phi\rangle}{\langle\Phi|\Omega|\Phi\rangle} \tag{2.2}$$

is real when the trial function Φ is a square-integrable A-particle state in the domain of the Hermitian self-conjugate operator Ω. It is understood that Ψ is also square integrable either because it is approximated by a wave packet or because it is the product $V\chi$ of a channel function χ and a rapidly decreasing channel potential V. We shall choose to normalize Ψ by $\langle\Psi|\Psi\rangle=1$ in our subsequent discussions.

It is obvious that F obeys the following inequalities:

$$0\leq F\leq\frac{1}{\Gamma^2}\ . \tag{2.3}$$

The minimum of F is trivially obtained by choosing Φ to be orthogonal to Ψ. To determine another extremum of F, we first note that the Euler-Lagrange conditions

$$(f\Omega-|\Psi\rangle\langle\Psi|)|\Phi\rangle=0\ , \tag{2.4a}$$

$$\langle\Phi|(f\Omega-|\Psi\rangle\langle\Psi|)=0\ , \tag{2.4b}$$

are equivalent because of the Hermiticity of the operator

$$\mathscr{S}=f\Omega-|\Psi\rangle\langle\Psi|\ . \tag{2.5}$$

In Eq. (2.5), f is just the (positive) value taken by F. An extremum is just reached when, according to Eq. (2.4),

$$|\Phi\rangle=\lambda\Omega^{-1}|\Psi\rangle\ , \tag{2.6}$$

where λ is an arbitrary constant. The corresponding stationary value of F is

$$\begin{aligned}F(\Omega^{-1}|\Psi\rangle)&=\langle\Psi|\Omega^{-1}|\Psi\rangle\\&=Y\ .\end{aligned} \tag{2.7}$$

This illustrates that Y does result from a variational principle based on the functional F. It should be even more useful for practical applications to prove that Y is not just an extremum of F, but is the supremum allowed by the inequalities, Eq. (2.3).

Let us consider the difference

$$\delta^2F=\langle\Psi|\Omega^{-1}|\Psi\rangle-\frac{(\langle\Psi|\Omega^{-1}+\langle\Phi'|)|\Psi\rangle\langle\Psi|(\Omega^{-1}|\Psi\rangle+|\Phi'\rangle)}{(\langle\Psi|\Omega^{-1}+\langle\Phi'|)\Omega(|\Phi'\rangle+\Omega^{-1}|\Psi\rangle)}\ , \tag{2.8}$$

where

$$|\Phi'\rangle=|\Phi\rangle-\Omega^{-1}|\Psi\rangle$$

is arbitrary. Explicitly, Eq. (2.8) can be written as

$$\delta^2F=\frac{\langle\Phi'|\Omega|\Phi'\rangle\langle\Psi|\Omega^{-1}|\Psi\rangle-\langle\Phi'|\Psi\rangle\langle\Psi|\Phi'\rangle}{(\langle\Psi|\Omega^{-1}+\langle\Phi'|)\Omega(\Omega^{-1}|\Psi\rangle+|\Phi\rangle)}\ . \tag{2.9}$$

The denominator of Eq. (2.9) being positive definite, it is only the numerator $\mathscr{N}$ which is of interest. It can be written as

$$\begin{aligned}\mathscr{N}&=\langle\Phi'|(Y\Omega-|\Psi\rangle\langle\Psi|)|\Phi'\rangle\\&=\langle\Phi'|\mathscr{S}|\Phi'\rangle\ ,\end{aligned} \tag{2.10}$$

where we have set $f=Y$ in Eq. (2.6), for $\mathscr{S}$.

Thus, Y is a maximum of F if $\mathscr{S}$ can be proved to be a semidefinite positive operator. This is the subject of Sec. III.

III. PROOF OF POSITIVITY OF $\mathscr{S}$

The operator $\mathscr{S}$ is the difference of the positive operator $Y\Omega$ and the projector $|\Psi\rangle\langle\Psi|$. Let the continuous eigenvalue ϵ and a discrete index ν label the complete set of eigenstates $\psi_{\epsilon\nu}$ of Ω. Following the discussions of Ref. 6, two kinds of eigenstates Σ_η of $\mathscr{S}$ can be defined by the diagonalization equation

$$\langle\psi_{\epsilon\nu}|(Y\Omega-|\Psi\rangle\langle\Psi|)|\Sigma_\eta\rangle=\eta\langle\psi_{\epsilon\nu}|\Sigma_\eta\rangle\ , \tag{3.1}$$

namely,

(i) square-integrable eigenstates for which η does not lie in the continuum of Ω, i.e.,

$$\langle\psi_{\epsilon\nu}|\Sigma_\eta\rangle=\frac{\langle\psi_{\epsilon\nu}|\Psi\rangle}{(Y\epsilon-\eta)}\langle\Psi|\Sigma_\eta\rangle \tag{3.2}$$

with the quantization condition

$$1=\sum_\nu\int d\epsilon\frac{|\langle\psi_{\epsilon\nu}|\Psi\rangle|^2}{Y\epsilon-\eta}\ , \tag{3.3}$$

and

(ii) eigenstates for which η lies in the continuum of $Y\Omega$, i.e.,

$$\langle\psi_{\epsilon\nu}|\Sigma_\eta\rangle=\delta(\eta-\epsilon)+\mathscr{P}\frac{\langle\psi_{\epsilon\nu}|\Psi\rangle}{Y\epsilon-\eta}\langle\Psi|\Sigma_\eta\rangle\ , \tag{3.4}$$

where $\mathscr{P}$ denotes the principal part.

[It should be pointed out that discrete eigenstates of H lie in the continuum of Ω which would thus complicate the handling of Eq. (3.4). But this complication is not relevant to the fact that Eq. (3.3) has at most one solution in the domain where η takes on any value between $-\infty$ and the threshold $Y\Gamma^2$ of $Y\Omega$. In this domain, the right-hand side of Eq. (3.3) is a finite, regular, and monotonically increasing function of η with a value equal to zero when η tends to $-\infty$.]

According to Eq. (2.4), the special eigenvalue η actually vanishes. For $\eta=0$, Eq. (3.3) yields

$$Y=\sum_\nu\int d\epsilon\frac{|\langle\psi_{\epsilon\nu}|\Psi\rangle|^2}{\epsilon}\ , \tag{3.5}$$

which is exactly what one would obtain from the definition $Y=\langle\Psi|\Omega^{-1}|\Psi\rangle$. All other eigenvalues of $\mathscr{S}$ are larger than or equal to $Y\Gamma^2$.

Thus $\mathscr{N}$ in Eq. (2.10) and δ^2F in Eq. (2.9) are positive or zero. This proves that Y is the supremum of F, namely, its maximum. It should be stressed that as long as $|\Psi\rangle$ is square integrable, so is $\Omega^{-1}|\Psi\rangle$ since $\Omega^{-1}\leq\Gamma^{-2}$. The stationarity equation, Eq. (2.6), is a supremum of F which remains in the Hilbert space. No singularities need be expected in a practical application of the variational principle.

IV. UPPER BOUNDS AND ADDITIONAL LOWER BOUNDS OF Y

In this section we consider Eq. (1.3) under the form

$$Y=\left\langle\Psi\left|\left[\frac{1}{\Gamma^2+\lambda(E-H)^2}\right]\right|\Psi\right\rangle , \tag{4.1}$$

where λ is an arbitrary constant ($\lambda=1$ for the case of interest). An expansion of Y in powers of λ and a reconstruction of Y by Padé approximants are useful. For a spectral representation of Y in terms of the eigenstates of H is trivial whereby Y is a Stieltjes function of λ for $\lambda>0$. We further note that $(E-H)^2$ is a positive semidefinite operator while both Γ^2 and λ are positive. All these properties lead to the well-known inequalities[7]

$$[N-2/N-1]\leq[N-1/N]\leq\cdots Y\leq\cdots\leq[N/N]$$
$$\leq[N+1/N+1] , \tag{4.2}$$

where we specify, for the sake of clarity, that $N-1$ and N represent the degrees of the numerator and denominator of the $[N-1/N]$ Padé approximant, respectively.

In other words, diagonal Padé approximants make a decreasing, convergent sequence of upper bounds and paradiagonal approximants make an increasing, convergent sequence of lower bounds, respectively. Trivial examples are provided by the [0/0] and the [0/1] approximants, namely,

$$[\Gamma^2+\langle\Psi|(E-H)^2|\Psi\rangle]^{-1}\leq Y\leq\Gamma^{-2} . \tag{4.3}$$

As a matter of fact, these bounds are not independent of the functional F studied in Secs. II and III. As discussed by Baker[7] and Nuttall[7] among others, trial functions which are linear superpositions of Ψ, $(E-H)^2\Psi$, $(E-H)^4\Psi$, etc., provide Padé approximants when they are used in Eq. (2.2) for F. We notice, however, that Padé approximants provide both upper and lower bounds.

V. BOUNDS ON THE REAL PART FROM A SATURATION OF UNITARITY

Let $|n\rangle$ represent a complete set of states and assume $|\Psi\rangle$ to be one of these states, for example $|0\rangle$. Then one obtains

$$\left\langle\Psi\left|\frac{1}{(E-H)^2+\Gamma^2}\right|\Psi\right\rangle$$
$$=\sum_n\left\langle\Psi\left|\frac{1}{E-H-i\Gamma}\right|n\right\rangle\left\langle n\left|\frac{1}{E-H+i\Gamma}\right|\Psi\right\rangle$$
$$\geq\left|\left\langle\Psi\left|\frac{1}{E-H-i\Gamma}\right|\Psi\right\rangle\right|^2 \tag{5.1}$$

or

$$\langle\Psi|\Omega^{-1}|\Psi\rangle\geq\Gamma^2(X^2+Y^2) , \tag{5.2}$$

where Y has been defined by Eq. (1.3), and we have defined the real part of the amplitude by

$$\Gamma X=\left\langle\Psi\left|\frac{(E-H)}{(E-H)^2+\Gamma^2}\right|\Psi\right\rangle . \tag{5.3}$$

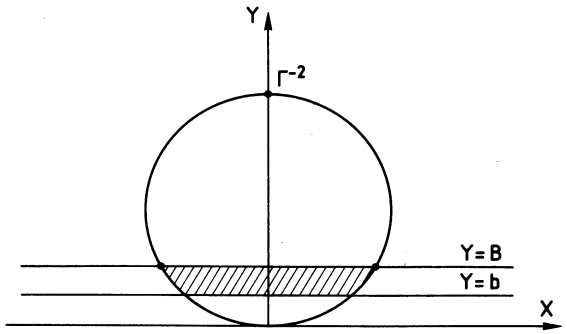

FIG. 1. Figure illustrates the allowed values of X and Y according to the inequality Eq. (5.4). The strip defined by $Y=B$ and $Y=b$ yields the bounds on Y and the cross-hatched region defines the allowed values of X.

As shown in Fig. 1, the physical amplitude $\Delta T=\Gamma(X+iY)$ is thus restricted to the interior or the rim of the disc

$$\Gamma^{-2}Y\geq X^2+Y^2 . \tag{5.4}$$

On the other hand, Secs. III and IV have established that one can calculate two positive numbers b and B such that

$$B\geq Y\geq b . \tag{5.5}$$

It is then trivial to derive from the two inequalities, Eqs. (5.4) and (5.5), that X^2 is bounded above, i.e.,

$$X^2\leq C\equiv\max(\Gamma^{-2}B-B^2,\Gamma^{-2}b-b^2) , \tag{5.6}$$

and

$$-C^{1/2}\leq X\leq C^{1/2} .$$

It should be pointed out that the strip in the complex plane selected by the inequality, Eq. (5.5), may lie close to the real axis or close to the top of the unitarity disk, namely, the point $(0,\Gamma^{-2})$. In the former case, C is determined by B while in the latter case it is determined by b. However, it must be stressed that the best bounds b and B that one may hope to find should behave like Γ^{-1} and not like Γ^{-2}. This is because the limit ΓY is finite when $\Gamma\to0$. The first case, namely, a strip close to the real axis is thus a more likely result of any precise practical calculation. (The value of the bounds on Y in the limit $\Gamma\to0$ are to be defined as[7]

$$b=\lim_{\Gamma\to0}\lim_{N\to\infty}[N-1/N]$$

and

$$B=\lim_{\Gamma\to0}\lim_{N\to\infty}[N/N] ,$$

respectively.) The bound C will thus depend on B rather than on b.

VI. NONDIAGONAL ELEMENTS AND NEW BOUNDS ON THE REAL PART

In many cases both Ψ and H have simultaneously a real representation, while the Green's function $(E-H-i\Gamma)^{-1}$ is a symmetric non-Hermitian operator.

A nondiagonal element $\langle\Psi'|G|\Psi\rangle$, where Ψ' is a real wave packet can be expressed by

$$2\langle\Psi'|G|\Psi\rangle=\langle(\Psi+\Psi')|G|(\Psi+\Psi')\rangle-\langle\Psi|G|\Psi\rangle-\langle\Psi'|G|\Psi'\rangle\ . \tag{6.1}$$

An upper bound to the real part of $\langle\Psi|G|\Psi\rangle$ is then obtained by a subtraction of the lower bounds to the real parts of $\langle\Psi|G|\Psi\rangle$ and $\langle\Psi'|G|\Psi'\rangle$ from an upper bound to the real part of $\langle(\Psi+\Psi')|G|(\Psi+\Psi')\rangle$. Alternatively, one may consider the relation

$$2\langle\Psi'|G|\Psi\rangle=-\langle(\Psi-\Psi')|G|(\Psi-\Psi')\rangle+\langle\Psi|G|\Psi\rangle+\langle\Psi'|G|\Psi'\rangle\ , \tag{6.2}$$

and still obtain an upper bound to the real part of $\langle\Psi'|G|\Psi\rangle$ out of a lower bound to $\mathrm{Re}\langle(\Psi-\Psi')|G|(\Psi-\Psi')\rangle$ and upper bounds to $\mathrm{Re}\langle\Psi|G|\Psi\rangle$ and $\mathrm{Re}\langle\Psi'|G|\Psi'\rangle$.

The same procedure applies equally well to the imaginary parts of off-diagonal elements. Furthermore, when lower bounds of off-diagonal elements are needed, it is trivial to exchange the roles of upper and lower bounds to be subtracted along the rules provided by Eqs. (6.1) and (6.2).

Thus, the set of bounds obtained in the previous sections provide considerable flexibility for the evaluation of bounds on nondiagonal elements. One can equally consider mixtures of states, $\alpha\Psi+\alpha'\Psi'$, to obtain relations

$$2\alpha\alpha'\langle\Psi'|G|\Psi\rangle=\pm\langle(\alpha\Psi\pm\alpha'\Psi')|G|(\alpha\Psi\pm\alpha'\Psi')\rangle\mp\alpha^2\langle\Psi|G|\Psi\rangle\mp\alpha'^2\langle\Psi'|G|\Psi'\rangle \tag{6.3}$$

in order to optimize the bounds under study with respect to the real numbers α and α'.

We want to stress the fact that the real part of the transition amplitude can be interpreted as a nondiagonal element of the imaginary part, i.e.,

$$\left\langle\Psi\left|\frac{(E-H)}{(E-H)^2+\Gamma^2}\right|\Psi\right\rangle=[\langle\Psi|(E-H)]\times\frac{1}{(E-H)^2+\Gamma^2}|\Psi\rangle=\frac{1}{\Gamma}\mathrm{Im}\left\langle\Psi''\left|\frac{1}{E-H-i\Gamma}\right|\Psi\right\rangle\ , \tag{6.4}$$

where

$$\Psi''=(E-H)\Psi\ . \tag{6.5}$$

Thus, in order to calculate $\mathrm{Re}\langle\Psi|G|\Psi\rangle$ one can consider the more general element

$$\mathrm{Im}\langle(\alpha\Psi+\alpha''\Psi'')|G|(\alpha\Psi+\alpha''\Psi'')\rangle=\Gamma\langle\Psi|[\alpha+\alpha''(E-H)]\Omega^{-1}[\alpha+\alpha''(E-H)]|\Psi\rangle\ , \tag{6.6}$$

where full advantage can be taken of the positivity properties of Ω^{-1} and the variational properties discussed in Secs. II to IV.

It is remarkable that this relation between ΔT and $\mathrm{Im}\Delta T$ demands *only one set of calculations at the predetermined energy E.* This is in sharp contrast with the usual relation between ΔT and $\mathrm{Im}\Delta T$ via dispersion relations where one needs to evaluate $\mathrm{Im}\Delta T$ at all energies. As a matter of fact, Eq. (6.6) contains all the information needed for both upper and lower bounds to both the real and imaginary parts of $\langle\Psi|G|\Psi\rangle$.

More generally, all the information needed for both real and imaginary parts of a general nondiagonal element $\langle\Psi'|G|\Psi\rangle$ for arbitrary Ψ and Ψ' are contained in diagonal matrix elements of the positive Hermitian operator Ω^{-1} between suitable admixtures of Ψ, $(E-H)\Psi$, Ψ', and $(E-H)\Psi'$.

VII. AN ILLUSTRATIVE EXAMPLE

The Hamiltonian considered in this section is written in momentum representation as

$$\langle\vec{q}|(\mathscr{T}+\mathscr{V})|\vec{q}\,'\rangle=q^2\delta(\vec{q}-\vec{q}\,')+u(q)u(q')$$

with

$$u(q)=e^{-q^2}\ , \tag{7.1}$$

namely, we consider a one-particle, three-dimensional scattering by a separable potential. For the calculation of ΔT, Eq. (1.2), we assume that the normalization of the wave packet χ which represents the "channel" is such that

$$\langle\vec{q}|\Psi\rangle=\langle\vec{q}|\mathscr{V}|\chi\rangle=u(q)\ . \tag{7.2}$$

The resulting normalization of Ψ is thus not unity, but

$$Y_0=\langle\Psi|\Psi\rangle=(\pi/2)^{3/2}=1.9687\ . \tag{7.3}$$

It is then trivial to show that

$$\Delta T=\frac{D(E)}{1-D(E)}\ \text{with}\ D(E)=\int d\vec{q}\,\frac{u^2(q)}{E-q^2-i\Gamma}\ . \tag{7.4}$$

It is then convenient to define

$$A(E)=\int d\vec{q}\,\frac{u^2(q)}{(E-q^2)^2+\Gamma^2}$$

and

$$B(E)=\int d\vec{q}\,\frac{q^2u^2(q)}{(E-q^2)^2+\Gamma^2} \tag{7.5}$$

and obtain

$$\Delta T=\frac{EA-B+i\Gamma A}{(1-EA+B)+i\Gamma A}\ , \tag{7.6}$$

$$\mathrm{Re}\Delta T=\frac{(EA-B)(1-EA+B)-\Gamma^2A^2}{(1-EA+B)^2+\Gamma^2A^2}\ , \tag{7.7}$$

$$\mathrm{Im}\Delta T=\frac{\Gamma A}{(1-EA+B)^2+\Gamma^2A^2}\ . \tag{7.8}$$

The integrals A and B can be evaluated numerically very easily, hence the exact values of ΔT can be tabulated. These are shown in Table I for various values of E and Γ,

TABLE I. Imaginary and real part of the multistep amplitude for various values of the energy E and the off-shell shift Γ. Padé approximants [0/1] (lower bound) and [1/1] and [0/0] (upper bounds) are given for comparison with the imaginary part.

k ($E=k^2$)	Γ	Γ[0/1]	ImΔT	Γ[1/1]	Γ[0/0]	ReΔT
2	0.1	0.097	0.264	11.013	19.687	1.230
$E=4$	0.2	0.191	0.415	5.535	9.843	1.681
	0.3	0.280	0.542	3.721	6.562	1.597
	0.4	0.362	0.635	2.822	4.922	1.484
	0.5	0.434	0.718	2.289	3.937	1.386
	1	0.653	0.854	1.256	1.969	0.905
	1.5	0.692	0.792	0.924	1.313	0.590
	2.0	0.654	0.702	0.753	0.984	0.407
	2.5	0.595	0.623	0.641	0.788	0.294
4	0.5	0.011	0.011	0.082		0.148
$E=16$	1	0.011	0.011	0.029		
	2	0.011	0.011	0.019		
6	0.5	0.002	0.002	0.013		0.059
$E=36$	1.0	0.002	0.002	0.005		
	2.0	0.002	0.002	0.003		

together with Padé approximants. For the Padé approximants to the imaginary part we consider the expansion

$$Y(\lambda)=\left\langle \Psi \left| \frac{1}{\Gamma^2+\lambda(E-H)^2} \right| \Psi \right\rangle = \frac{Y_0}{\Gamma^2}-\frac{Y_1\lambda}{\Gamma^4}+\frac{Y_2\lambda^2}{\Gamma^6}-\cdots \tag{7.9}$$

with

$$Y_n=\langle \Psi \mid (E-H)^{2n} \mid \Psi \rangle \ . \tag{7.10}$$

A straightforward but slightly tedious calculation leads to

$$Y_1=Y_0(E^2-\tfrac{3}{2}E+\tfrac{15}{16})-Y_0^2(2E-\tfrac{3}{2}+Y_0^3) \ , \tag{7.11}$$

$$Y_2=Y_0(E^4-3E^3+\tfrac{45}{8}E^2-\tfrac{105}{16}E+\tfrac{945}{256}) -Y_0^2(4E^3-9E^2+\tfrac{39}{4}E-\tfrac{75}{16}) +Y_0^3(6E^2-9E+\tfrac{9}{2})-Y_0^4(4E-3)+Y_0^5 \ , \tag{7.12}$$

where one takes advantage of the trivial result

$$\langle \Psi \mid \mathcal{T}^m \mid \Psi \rangle = \frac{(2m+1)!!}{4^m} Y_0 \ . \tag{7.13}$$

One thus obtains readily the approximants

$$[0/0]=\frac{Y_0}{\Gamma^2} \ , \tag{7.14}$$

$$[0/1]=\frac{Y_0^2}{\Gamma^2 Y_0+Y_1} \ , \tag{7.15}$$

$$[1/1]=[0/0]-\frac{Y_1^2}{\Gamma^2(\Gamma^2 Y_1+Y_2)} \ . \tag{7.16}$$

The physical quantity of interest is not Y but ΓY, hence in Table I these Padé approximants have been multiplied by Γ in order to be compared with ImΔT. In the following we refer always to those approximants multiplied by Γ.

Several comments are in order at this stage. It is seen from Table I that the bounds are very satisfactory when Γ is of order E or a moderate fraction of E, say, $\Gamma \sim E/3$. One should expect a fast convergence of the Padé approximants when their order increases. However, when $\Gamma \lesssim E/10$, it is seen that low-order Padé approximants do not provide narrow bounds. The reason for this is clear. On one hand, while ΓY has a finite limit as $\Gamma \to 0$, it is seen that upper bounds such as Γ[0/0], Eq. (7.14) and Γ[1/1], Eq. (7.16), diverge like Γ^{-1}. On the other hand, lower bounds such as Γ[0/1], Eq. (7.15), vanish like Γ. This clearly indicates the need for higher-order Padé approximants and/or a matrix[8] Padé extension of the method. In this matrix method trial functions contain parameters which can be used to push up (down) the lower (upper) bounds.

It is instructive to compare in Fig. 2 the trends of ΓY and the trends of its Padé approximants when $\Gamma \to 0$. As has just been stated, while ΓY has a finite limit, upper bounds tend to diverge like Γ^{-1} and lower bounds to vanish like Γ. The slope of ΓY is of some interest for the understanding of such a pattern. It is given by

$$S=\frac{d}{d\Gamma}(\Gamma Y)=\frac{d}{d\Gamma}\left\langle \Psi \left| \frac{1}{\Gamma+(1/\Gamma)(E-H)^2} \right| \Psi \right\rangle = \Lambda \left\langle \Psi \left| \frac{\Lambda(E-H)^2-1}{[\Lambda(E-H)^2+1]^2} \right| \Psi \right\rangle \ , \tag{7.17}$$

with the notation $\Lambda=\Gamma^{-2}$. [It can be noticed here that the Taylor expansion with respect to λ, Eqs. (4.1) and (7.9), which we used for the derivation of the Padé approximants is as well an expansion in powers of Λ.] Let η label an eigenvalue of $(H-E)$, the spectrum of this operator extending from $-(B_0+E)$ to $+\infty$, where B_0 is

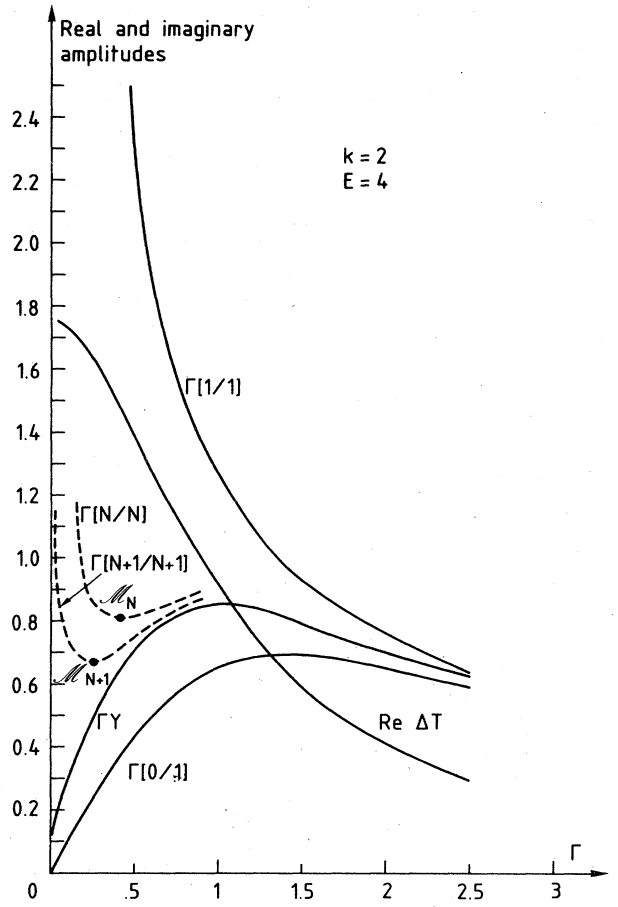

FIG. 2. Imaginary and real part of the multistep amplitude for various values of the off-shell shift Γ. Padé approximants [0/1] (lower bound) and [1/1] and [0/0] (upper bounds) are given for comparison with the imaginary part. Dashed lines are conjectured, showing minima for $\Gamma[N/N]$ and $\Gamma[N+1/N+1]$.

the binding energy of the ground state. If $\rho(\eta)$ is the corresponding spectral density of Ψ, then

$$S=\Lambda\int_{-(B_0+E)}^{\infty}d\eta\,\rho(\eta)\frac{\Lambda\eta^2-1}{(\Lambda\eta^2+1)^2}$$
$$=\Lambda^{1/2}\int_{-\mathscr{B}_0}^{\infty}d\alpha\,\rho\left[\frac{\alpha}{\Lambda^{1/2}}\right]\frac{\alpha^2-1}{(\alpha^2+1)^2} \tag{7.18}$$

with $\alpha=\Lambda^{1/2}\eta$ and $\mathscr{B}_0=\Lambda^{1/2}(B_0+E)$.

Without going into an asymptotic expansion of S about $\Gamma\to 0$ it is seen in Fig. 2 that S seems to be positive and large in the present case. As illustrated qualitatively in Fig. 2 and discussed earlier,[9] this pattern may provide an optimization for the case of an $[N/N]$ Padé approximant. Namely, if a $[N/N]$ approximant multiplied by Γ has a minimum $\mathscr{M}_N$ for a value Γ_N, in the region where S is positive, the following inequalities hold:

$$\lim_{\Gamma\to 0}\Gamma Y<\Gamma_N Y(\Gamma_N)\leq\mathscr{M}_N\ . \tag{7.19}$$

But one also finds the following additional inequalities including the minimum of the next Padé approximant $[N+1/N+1]$ for a value Γ_{N+1} in the same region:

$$\lim_{\Gamma\to 0}\Gamma Y<\Gamma_{N+1}Y(\Gamma_{N+1})$$
$$\leq\mathscr{M}_{N+1}\leq\Gamma_N[N+1/N+1](\Gamma_N)$$
$$\leq\Gamma_N[N/N](\Gamma_N)=\mathscr{M}_N\ . \tag{7.20}$$

Hence the sequence of minima $\mathscr{M}_N$ is the fastest sequence of decreasing upper bounds available from the Padé approximants, and the corresponding values Γ_N are the optimal values of the imaginary parts to be used. It may here be stressed that the use of a finite imaginary part Γ in the present theory is not just an artificial device to avoid the on-shell limit. On the contrary, Γ becomes a variational parameter in order to generate a minimum $\mathscr{M}_N$ for each approximant $[N/N]$ multiplied by Γ.

As discussed at the end of Sec. VI, the case of $\mathrm{Re}\Delta T$ hardly differs from that of $\mathrm{Im}\Delta T$. (There is numerical evidence, however, that the derivative remains finite.) The present illustrative example will just specify, for the sake of completeness, those moments of $(E-H)$ whose calculation would be necessary. According to the definition $\Psi''=(E-H)\Psi$,

$$\left\langle(\Psi+\Psi'')\left|\frac{1}{\Gamma^2+\lambda(E-H)^2}\right|(\Psi+\Psi'')\right\rangle$$
$$=\frac{1}{\Gamma^2}\langle(\Psi+\Psi'')\,|\,(\Psi+\Psi'')\rangle$$
$$-\frac{\lambda}{\Gamma^4}\langle(\Psi+\Psi'')\,|\,(E-H)^2\,|\,(\Psi+\Psi'')\rangle$$
$$+\frac{\lambda^2}{\Gamma^6}\langle(\Psi+\Psi'')\,|\,(E-H)^4\,|\,(\Psi+\Psi'')\rangle-\cdots\ . \tag{7.21}$$

This also reads (with real numbers for all moments)

$$\left\langle(\Psi+\Psi'')\left|\frac{1}{\Gamma^2+\lambda(E-H)^2}\right|(\Psi+\Psi'')\right\rangle$$
$$=\frac{1}{\Gamma^2}(Y_0+2Y_{1/2}+Y_1)-\frac{\lambda}{\Gamma^4}(Y_1+2Y_{3/2}+Y_2)$$
$$+\frac{\lambda^2}{\Gamma^6}(Y_2+2Y_{5/2}+Y_3)-\cdots \tag{7.22}$$

with the obvious notation

$$Y_{(2n+1)/2}=\langle\Psi\,|\,(E-H)^{2n+1}\,|\,\Psi\rangle\ . \tag{7.23}$$

As a trivial case one finds

$$Y_{1/2}=Y_0(E-\tfrac{3}{4})-Y_0^2\ , \tag{7.24}$$

and so on for higher moments.

VIII. APPLICATIONS, DISCUSSION, AND CONCLUSION

The calculation of the functional F, Eq. (2.2), seems *a priori* cumbersome because if H involves two-body operators, Ω involves an algebra of four-body operators. If, however, a set of single orbital products are used as trial

functions Φ, the calculation of F is no longer as formidable. One then generates a Hartree or Hartree-Fock-type approximation[10] to the imaginary part of the transition amplitude. Since Y is the maximum of F, this mean-field approximation (or any other approximate Φ) provides a lower bound to Y. Iterative algorithms are thus expected to converge.

Since the elastic forward amplitudes provide the total cross section through their imaginary part, our result thus provides a systematic lower bound to the total cross section. This result is of interest in practical cases and also in analytic models when a convenient class of analytically calculable trial functions Φ and operators H are available. The other bounds which have been investigated in this paper seem to require slightly more involved practical calculations, for they use moments of the Hamiltonian. This complexity, however, is not worse than that found in traditional shell model calculations.

Finally, it should be pointed out that the bounds on single channel and multichannel scattering amplitudes have been discussed by Blau *et al.*,[3] Sugar and Blankenbecler,[3] and others referred to in these papers. They discuss the scattering problem within the framework of Feshbach-projection-operator[11] formalism and thus consider the bounds on the total transition amplitude. Our formalism considers the bounds on the correction to the Born (or DWBA) amplitude. This correction term in the case of the forward elastic amplitude is the diagonal matrix element of the resolvent operator. If a wave-packet description is made for the channel wave functions, the discussion of bounds on the imaginary part of the amplitude exactly parallels the evaluation of bounds on the strength function. Thus, once again we find a unification of the nuclear structure and nuclear reaction aspects of the problem.

In the present stage of our theory we consider that the goal of reducing transition amplitude calculations to shell model calculations is now within reasonable reach when off-shell amplitudes are concerned. The only major and stimulating question to be met is the on-shell limit. We have stressed several times in this paper that the proper behavior of a bound when $\Gamma \to 0$ should be of order Γ^{-1}. This question is now under investigation. For the time being, we restrict ourselves to finite values of Γ, the physical meaning of which is already of great interest to both the theorist and experimentalist.

A result of some significance seems to appear, namely, that Γ might indeed be a variational parameter for the very estimation of the on-shell limit, as discussed in Fig. 2. If the sign of the derivative of ΓY when $\Gamma \to 0$ turns out to be negative, a variation with respect to Γ will just trade lower limits of upper bounds for upper limits of lower bounds. This opens an interesting line of investigation in the future applications of the theory.

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