Appearance of anomalies in the Takatsuka-McKoy variational method: An illustrative example

M. A. Abdel-Raouf*
Physics Department, York University, Toronto, Ontario, Canada M3J 1P3

(Received 4 November 1983; revised manuscript received 23 April 1984)

It is demonstrated that the method of the fractional functional proposed by Takatsuka and McKoy, and the variational method of Moe and Saxon and of Kolsrud are identical. In particular, we show that the method is, contrary to Takatsuka and McKoy's claim, not free of anomalies; it implies the incorporation of the boundary conditions, it does not satisfy a minimum principle, and suffers from inconsistency. In order to illustrate the validity of our arguments, we investigate the s-wave scattering of electrons by Yukawa potentials.

Recently, Takatsuka and McKoy[1,2] (we refer henceforth to the authors and the first reference as TM), Takatsuka, Lucchese, and McKoy,[3] Lucchese, Takatsuka, Watson, and McKoy,[4] and Mu-Tao, Takatsuka, and McKoy[5] (see also Gross and Runge[6] and Lucchese and McKoy[7]) have published a series of papers in which they proposed what they claim to be new variational techniques for treating scattering problems. In analogy to Schwinger's variational method (SVM), the functionals proposed by these authors have fractional forms. One of these functionals, however, does not contain any Green's integral operator. TM stated that the trial functions employed in this case need not satisfy the boundary conditions appropriate to the scattering problem (that is, they can be square integrable) and that the method is free of anomalies. (The first claim has been restressed in the work of Gross and Runge.[6]) Thus they claim that this particular method (henceforth to be referred to as TMVM) has many of the advantages of the SVM, while at the same time, it is as easy to apply as the standard Hulthén-Kohn variational method.

In this work, the novelty of the techniques of the above mentioned authors is questioned. In particular, we show that the TMVM is, in fact, equivalent to one of the methods suggested some years ago by Moe and Saxon[8] and by Kolsrud,[9] which are versions of the usual Hulthén-Kohn method and, therefore, require the knowledge of the boundary conditions of the scattering problem under consideration. We also indicate that the other variational techniques by McKoy and collaborators are based on well-known variational functionals which are derivatives of the fundamental functional used in SVM. These functionals were deduced by Kolsrud[9] and rederived by several nuclear physicists using the separable approximation. We also point out that the Euler equations of the functional used in TMVM and its inverse [F_1^t and $(F_1^t)^{-1}$ in their notations] are not identical with Schrödinger's equation unless t, the arbitrary parameter involved in their functional for suppressing the spurious singularities, is restricted to a certain value. We consider this fact as a source of inconsistency in TMVM. Next, we demonstrate theoretically that the TMVM is not free of spurious singularities and cannot be used for characterizing true resonances. In order to illuminate this point, we investigate the scattering of electrons by a Yukawa potential ($2e^{-2r}/r$). We believe that the numerical results obtained validate our objections to the TM method. (For simplicity, we confine ourselves to the discussion of single channel problems. The extension to multichannel processes is straightforward.)

Finally, we disprove the claims of TM that the functional in TMVM can be adjusted to fulfill a minimum principle.

Before going to the main point of this Comment, let us first clarify the connection between SVM and the Moe-Saxon method, and recall some of their important properties. For this purpose, it is convenient to formulate a generalized variational functional which incorporates all Schwinger-type methods (see Abdel-Raouf[10]). Indeed, this can be readily done by using the separable approximation, which is discussed in the works of Zubarev[11-13] and Belyaev, Podkopayev, Wrzecionko, and Zubarev.[14] Thus, we consider the functional (the notation is the same as in TM),

$$F=\frac{\langle\xi^2|(VG)^{m_2}V|S\rangle\langle S|V(GV)^{m_1}|\xi^1\rangle}{\langle\xi^2|[(VG)^{m_2}V-(VG)^{m_2}V(GV)^{m_1}]|\xi^1\rangle}\;, \qquad (1)$$

where

$$|\xi^1\rangle=\sum_{i=1}^{n}a_i|\xi_i^1\rangle,\quad |\xi^2\rangle=\sum_{j=1}^{n}a_j|\xi_j^2\rangle\;,$$

$\{|\xi_i^1\rangle\}$, and $\{|\xi_j^2\rangle\}$ are two sets of separating functions; m_1 and m_2 are integers; and $|S\rangle$, V, and G are defined in TM. The stationarity of F, with respect to a_i's, leaves us with

$$F=\sum_{i,j=1}^{n}\langle S|V(GV)^{m_1}|\xi_i^1\rangle A_{ij}^{(n)}\langle\xi_j^2|(VG)^{m_2}V|S\rangle\;, \qquad (2a)$$

where

$$(\underline{A}^{-1})_{ji}=\langle\xi_j^2|[(VG)^{m_2}V-(VG)^{m_2}V(GV)^{m_1}]|\xi_i^1\rangle\;. \qquad (2b)$$

Therefore, for all values of m_1 and m_2, the Euler equation associated with F and F^{-1} is expressed by

$$(VG)^{m_2}\{(V-VGV)|\psi\rangle-V|S\rangle\}=|0\rangle\;, \qquad (3)$$

where, for the exact solution, we have

$$|\psi\rangle=\sum_{i=1}^{\infty}a_i(GV)^{m_1-1}|\xi_i^1\rangle\;. \qquad (4)$$

Equation (3) implies that the brackets $\{\}$ should vanish for all $m_1>0$ and $m_2\geq 0$ which leads to the well-known Lippmann-Schwinger equation. It is clear from Eqs. (2a) and (2b) that this is true, independently, of the form of $|\xi_i^2\rangle$ and that, to different choices of m_1 and m_2, one obtains a hierarchy of Schwinger-type variational methods, the first element of which is SVM. [Recall that $F = K_{11} = \tan(\eta^{(n)})$, $\eta^{(n)}$ is the approximate phase shift and that these methods are absolutely free of anomalies; see, e.g., Sloan and Brady.[15]] Of particular interest is to set $m_1 = m_2 = 1$ and expand two functions $|\tilde{C}\rangle$ and $|\omega\rangle$ from the following elements, respectively,

$$|\tilde{C}_i\rangle = GV|\xi_i^1\rangle, \quad |\omega_j\rangle = GV|\xi_j^2\rangle, \quad i,j = 1,2,\ldots,n \ . \tag{5}$$

Substitution into (1) and (2a) and (2b) provides us with

$$F = \frac{\langle\omega|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle\omega|\hat{H}|\tilde{C}\rangle} \tag{6}$$

and

$$F = \sum_{i,j=1}^{n} \langle S|V|\tilde{C}_i\rangle A_{ij}^{(n)} \langle\omega_j|V|S\rangle \ , \tag{7a}$$

where

$$(\underline{A}^{-1})_{ji} = \langle\omega_j|\hat{H}|\tilde{C}_i\rangle \tag{7b}$$

and

$$\hat{H} = E - H \ .$$

Setting $|\omega\rangle = |\tilde{C}\rangle$, reduces Eqs. (6) and (7a) and (7b) to the forms

$$F_1 = \frac{\langle\tilde{C}|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle\tilde{C}|\hat{H}|\tilde{C}\rangle} \tag{8}$$

and

$$F_1 = \sum_{i,j=1}^{n} \langle S|V|\tilde{C}_i\rangle A_{ij}^{(n)} \langle\tilde{C}_j|V|S\rangle \ , \tag{9a}$$

where

$$(\underline{A}^{-1})_{ji} = \langle\tilde{C}_j|\hat{H}|\tilde{C}_i\rangle \ . \tag{9b}$$

The Euler equation characteristic of the functionals F and F_i, Eqs. (6) and (8), as well as their inverses, is given by

$$\{(E-H)|\tilde{C}\rangle - V|S\rangle\} = |0\rangle$$

or

$$\hat{H}|\tilde{C}\rangle = V|S\rangle \ , \tag{10}$$

where

$$|\tilde{C}\rangle = \sum_{i=1}^{\infty} a_i|\tilde{C}_i\rangle \ . \tag{11}$$

Therefore, Eq. (10) leads to Schrödinger's equation

$$(E-H)|\psi\rangle = |0\rangle \ , \tag{12}$$

if and only if,

$$|\tilde{C}\rangle = |\psi\rangle - |S\rangle \ . \tag{13}$$

In other words, the functional F_1 provides us with two possibilities of constructing the trial wave function $|\tilde{C}\rangle$, namely, (a) $|\tilde{C}\rangle = \sum_{i=1}^{n} a_i GV|\xi_i^1\rangle$, where $|\xi_i^1\rangle$'s are appropriate to the form of V, e.g., if V is such that $\int_0^\infty |V| dr < \infty$, then $|\xi_i^1\rangle$ can be expressed in terms of square-integrable functions. In this case the Euler equation of (6) and (8) is the Lippmann-Schwinger equation. (b) $|\tilde{C}\rangle$ is independent of Green's operators but, because of Eq. (13), it has to satisfy the boundary conditions. For example, $|\tilde{C}\rangle$ is expanded by

$$|\tilde{C}\rangle = \tan(\eta_t^{(n)})|C\rangle + \sum_{i=1}^{n} a_i|\chi_i\rangle \ , \tag{14}$$

where $\eta_t^{(n)}$ is the trial phase shift, $|C\rangle$ is the irregular part of the asymptotic form of $|\psi\rangle$, and $|\chi_i\rangle$ is a square-integrable function.

The variational methods characterized by the functionals F and F_1, Eqs. (6) and (8), were first introduced by Moe and Saxon[8] [their Eqs. (37) and (25), respectively] within the framework of the choice (b), while the method based on F_1 was given [in addition to the case $m_1 = m_2 = 1,2$ under the choice (a)] nearly at the same time by Kolsrud[9] [his Eqs. (6) and (7)].

Moe and Saxon referred to F_1 as an amplitude- (or normalization-) independent Kohn's functional. Indeed, the authors showed that F_1 is related to Kohn's variational functional, $[\tan(\eta^{(n)})]_{\text{Kohn}}$, by

$$-\tfrac{1}{2}[\tan(\eta^{(n)})]_{\text{Kohn}} = \langle S|V|S\rangle + F_1 = \langle S|V|S\rangle + \frac{\langle\tilde{C}|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle\tilde{C}|\hat{H}|\tilde{C}\rangle} \ , \tag{15}$$

where $\langle S|V|S\rangle$ represents the Born approximation of the tangent of the phase shift. From Eq. (15), it is obvious that the stationarities of $[\tan(\eta^{(n)})]_{\text{Kohn}}$ and F_1 are equivalent, and the phase shifts calculated by both methods are identical, if the same trial functions are used (see also Darewych and Horbatsch[16]).

In their attempts to reduce F_1 (or F) to functionals independent of the boundary conditions, Moe and Saxon pointed out that all cases [see Eq. (30) in their work] lead to complex phase shifts, which means that probability is not preserved and the symmetry of the reactance maxtrix is violated. Contrary to Schwinger-type variational methods, the main disadvantage of using the Moe-Saxon methods is the appearance of spurious singularities, which are adherant to Hulthén-Kohn methods. Actually, if $|\tilde{C}\rangle$ is expanded as in Eq. (14), one can show that the possible vanishing of the determinant of $(\underline{A}^{-1})$, Eq. (9b), is exactly the reason for anomalies in Kohn's method as analyzed by Nesbet[17] (see also Abdel-Raouf and Dubé[18] and Abdel-Raouf[10,19]). (The absence and appearance of anomalies in both types of methods are investigated in the work of Schwartz.[20])

In light of the above comments, we now consider the Takatsuka-McKoy variational method. TM have investigated the functional F_1, Eq. (8), and realized that it is not free of spurious singularities. [Note that the other fractional functionals given by TM and their group (e.g., Lee *et al.*[5]) were deduced by several previous authors (see, e.g., Sloan and Adhikari,[21,22] Zubarev,[11-13] and Belyaev *et al.*[14]), and can be developed from Eq. (1) by considering different values for m_1 and m_2 as well as various forms of the separating functions $|\xi^1\rangle$ and $|\xi^2\rangle$.]

In order to avoid the anomalous singularities in F_1, TM proposed, instead, the following functional [Eq. (4.1) in TM]:

$$F_1^t = \frac{\langle \tilde{C}_t | V | S \rangle \langle S | V | \tilde{C}_t \rangle}{\langle \tilde{C}_t | (\hat{H} - tX) | \tilde{C}_t \rangle} , \quad (16)$$

where $X = V|S\rangle\langle S|V$ and t is arbitrary parameter different than zero. If we take $|\tilde{C}_t\rangle = \sum_{i=1}^{n} a_i |\tilde{C}_{ti}\rangle$, the stationarity of F_1^t gives, as pointed out by TM [their Eqs. (4.8) and (4.9)], the following relations:

$$F_1^t = \sum_{i,j=1}^{n} \langle S | V | \tilde{C}_{ti} \rangle \underline{A}_{ij}^{(n)} \langle \tilde{C}_{tj} | V | S \rangle , \quad (17)$$

where

$$(\underline{A}^{-1})_{ji} = \langle \tilde{C}_{tj} | (\hat{H} - tX) | \tilde{C}_{ti} \rangle . \quad (18)$$

Takatsuka and McKoy indicated that $\delta F_1^t = 0$ leads to the (Euler) equation

$$(\hat{H} - tX)|\tilde{C}_t\rangle = V|S\rangle$$

or

$$\hat{H}|\tilde{C}_t\rangle = (1 + t\langle S | V | \tilde{C}_t \rangle) V|S\rangle , \quad (19)$$

where now

$$|\tilde{C}_t\rangle = \sum_{i=1}^{\infty} a_i |\tilde{C}_{ti}\rangle . \quad (20)$$

The authors have correctly stated that X is a positive definite operator and, therefore, t can be always adjusted to guarantee that F_1^t is free of poles, that is to say $(\underline{A}^{-1})$ of Eq. (18), is nonsingular. Thus, assuming a given form for $|\tilde{C}_t\rangle$ at which $\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle$ has a spurious singularity, tX can be used for shifting this singularity, leaving us with a nonsingular F_1^t. However, F_1^t does not give the scattering parameters directly. In order to calculate these parameters, one uses the equations [see Eq. (4.11) in TM]

$$-\tfrac{1}{2}[\tan(\eta^{(n)})]_{\rm TM} = \langle S | V | S \rangle + \frac{F_1^t}{1 + tF_1^t} . \quad (21)$$

Considering Eqs. (17), (19), and (21), TM deduced the following conclusions: (i) All elements of $\{|\tilde{C}_{ti}\rangle\}$ can be square integrable functions. (ii) $[\tan(\eta^{(n)})]_{\rm TM}$ is free of anomalies, since F_1^t is already forced to be free of poles. (iii) The true resonances are characterized by [TM, Eq. (4.13)] the equation

$$F_1^t = -1/t \ \text{ or } (F_1^t)^{-1} = -t . \quad (22)$$

We now provide the basis for our objections, mentioned at the beginning of this work, to points (i)–(iii).

(I) Comparing Eqs. (10) and (19), we see that the Euler equation of F_1^t leads to Schrödinger's equation (12), if and only if,

$$|\tilde{C}\rangle = \frac{1}{1 + t\langle S | V | \tilde{C}_t \rangle} |\tilde{C}_t\rangle = x_t |\tilde{C}_t\rangle , \quad (23)$$

where x_t is a number depends on t. Thus, $|\tilde{C}_t\rangle$ has to satisfy the boundary conditions. On the other hand, the weak point of Eq. (19) is the arbitrariness due to the parameter t. This can be removed if t is confined to additional (physical) restrictions, which contradicts with the role of t as discussed by TM and represents, according to our opinion, a source of inconsistency in TMVM. Furthermore, by using the identity

$$\langle \tilde{C}_t | V | S \rangle \langle S | V | \tilde{C}_t \rangle = \langle \tilde{C}_t | X | \tilde{C}_t \rangle , \quad (24)$$

we can express the inverse of F_1^t as

$$(F_1^t)^{-1} = -t + \frac{\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle}{\langle \tilde{C}_t | X | \tilde{C}_t \rangle} , \quad (25)$$

which yields the Euler equation

$$\hat{H}|\tilde{C}_t\rangle = X|\tilde{C}_t\rangle = \langle S | V | \tilde{C}_t \rangle V|S\rangle . \quad (26)$$

Again, comparing Eq. (26) with Eq. (10), we find

$$|\tilde{C}\rangle = \frac{1}{\langle S | V | \tilde{C}_t \rangle} |\tilde{C}_t\rangle = y_t |\tilde{C}_t\rangle . \quad (27)$$

In other words, F_1^t and $(F_1^t)^{-1}$ provides two different Euler equations, the first contains t explicitly and the other does not. This peculiar characteristic of Takatsuka and McKoy's functional does not show up in any of Schwinger-type methods.

(II) By using the identity (24), one can easily write F_1^t as

$$F_1^t = \frac{\langle \tilde{C}_t | X | \tilde{C}_t \rangle}{\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle - t\langle \tilde{C}_t | X | \tilde{C}_t \rangle} . \quad (28)$$

Substitution into Eq. (21) yields

$$-\tfrac{1}{2}[\tan(\eta^{(n)})]_{\rm TM} = \langle S | V | S \rangle + \frac{\langle \tilde{C}_t | V | S \rangle \langle S | V | \tilde{C}_t \rangle}{\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle} . \quad (29)$$

Comparing Eqs. (15) and (29) we remark that (A) $[\tan(\eta^{(n)})]_{\rm TM}$ is identical with $[\tan(\eta^{(n)})]_{\rm Kohn}$ as long as $|\tilde{C}\rangle$ and $|\tilde{C}_t\rangle$ are developed from the same basis set, since, as it is also indicated by TM, $F_1(|\tilde{C}\rangle)$ is invariant with respect to the exchange of $|\tilde{C}_t\rangle$ and $|\tilde{C}\rangle$. (Note that both functions are now distinguished through their linear parameters.) (B) $[\tan(\eta^{(n)})]_{\rm TM}$ is independent of t. (C) Considering F_1^t, Eqs. (16)–(18), we notice that if the nonlinear parameters involved in $|\tilde{C}_t\rangle$ are changed such that F_1^t is stationary and it happens that $\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle^{-1}$ is singular, any value of t ($t \neq 0$) can be used for shifting this singularity. Clearly the resultant F_1^t is nonsingular. However, because of remark (B), the spurious singularity of $[\tan(\eta^{(n)})]_{\rm TM}$ cannot be removed. It is obvious that if we employ these components of $|\tilde{C}_t\rangle$ for developing $|\tilde{C}\rangle$ in Kohn's method, Eq. (15), we again obtain the same sort of anomalies. Equivalently, if $[\tan(\eta^{(n)})]_{\rm Kohn}$ is singular for a given form of components of $|\tilde{C}\rangle$, $[\tan(\eta^{(n)})]_{\rm TM}$ will be singular if these components are used for constructing $|\tilde{C}_t\rangle$. This fact makes it seem, at least to us, that spurious singularities appear in TMVM as frequently as in Kohn's method.

(III) From Eq. (25), we deduce that the relation

$$(F_1^t)^{-1} = -t \quad (30)$$

is satisfied at all zeros of $\langle \tilde{C}_t | \hat{H} | \tilde{C}_t \rangle$, which is the condition of both true and spurious resonances of $[\tan(\eta^{(n)})]_{\rm TM}$. Since Eqs. (22) and (30) are identical, we conclude that TMVM cannot be used for specifying the correct resonance.

Although the above theoretical arguments are sufficiently rigorous, we now present our illustrative example for testing

TABLE I. Variation of F_1^t and $[\tan(\eta_0^{(n')})]_{TM}$ with α and t at $k=1.0$ and $n=3$.

t	α	F_1^t	$[\tan(\eta_0^{(n')})]_{TM}$
0	0.5	−0.068 992 730 8	0.484 559 052
	1.5	−1.035 920 30	0.553 757 651
	2.5	−1.076 476 81	0.561 868 952
1	0.5	−0.064 539 943 9	0.484 559 052
	1.5	−0.093 868 048 6	0.553 757 651
	2.5	−0.097 184 494	0.561 868 952
2	0.5	−0.060 627 075 8	0.484 559 052
	1.5	−0.085 812 954	0.553 757 651
	2.5	−0.088 577 381 3	0.561 868 952

their validity, namely, the application of TMVM to the scattering of electrons by Yukawa's potential ($2e^{-2r}/r$). In this case, the operator $E-H$ is given (only s-wave is considered and atomic units are used) by

$$E-H=k^2+\frac{d^2}{dr^2}+2e^{-2r}/r \ , \tag{31}$$

where k^2 is the energy of the incident electrons and $V=-2e^{-2r}/r$ is the scattering potential. The trial wave function is chosen to be

$$|\psi^{(n)}\rangle=|S\rangle+|\tilde{C}_t\rangle \ , \tag{32}$$

where

$$S=(8\pi k)^{-1/2}\sin(kr) \ , \tag{33a}$$

$$\tilde{C}_t=(8\pi)^{-1/2}\tan(\eta^{(n)})(1-e^{-\alpha r})\frac{\cos(kr)}{k^{1/2}}+\sum_{i=1}^{n}a_i\chi_i \ , \tag{33b}$$

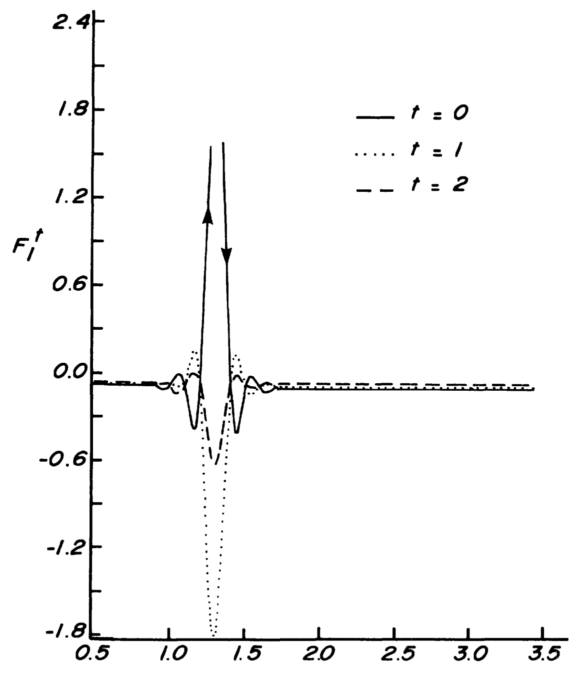

FIG. 1. Variation of F_1^t with α at $k=0.5$ a.u. and $n=7$.

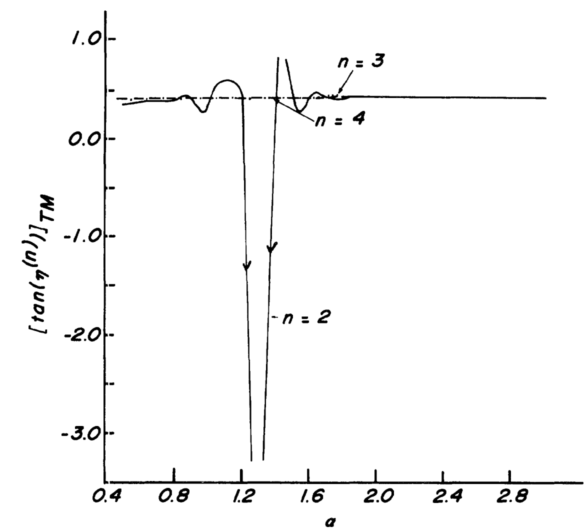

FIG. 2. Variation of $[\tan(\eta_0^{(n')})]_{TM}$ with α at $t=2$ and $k=0.5$ a.u.

and

$$\chi_i=r^ie^{-\alpha r} \ . \tag{33c}$$

α is a free parameter and $\tan(\eta^{(n)})$ and a_i's are variational parameters.

In Table I, we give the values of F_1^t and $[\tan(\eta_0^{(n')})]_{TM}$ calculated using Eqs. (17) and (21), respectively, when $t=0$, i.e., when $F_1^t=F_1$ [see Eqs. (16) and (8)] at $k=1.0$ a.u., $n=3$, and several values of α. The same table involves F_1^t and $[\tan(\eta_0^{(n')})]_{TM}$ for $t=1$ and $t=2$. It is clear that while F_1^t depends on t, $[\tan(\eta_0^{(n')})]_{TM}$ is, as we deduced above, totally independent of this parameter.

In Fig. 1, we plot F_1^t as a function of α at $n=2$, $k=0.5$ a.u. and $t=0$, 1, and 2. Obviously, F_1^0 possesses a pole at $\alpha\simeq 1.3$ which has been shifted at $t=1$ and $t=2$. Figure 2, on the other hand, illustrates the variation of $[\tan(\eta_0^{(n')})]_{TM}$, at $k=0.5$ a.u., $t=2$ and $n=2$, 3, and 4, with the free parameter α. From this figure we notice that $[\tan(\eta_0^{(n')})]_{TM}$ has a singularity at $n=2$ and $\alpha\simeq 1.3$, i.e., the same value of α at which F_1^0 is singular. Considering the exact solution of this scattering problem (see Abdel-Raouf[23]), we conclude that this singularity is a spurious one and that TMVM cannot avoid its occurrence. (A comparison between the best phase shifts obtained by TMVM and the exact ones is given in Table II.)

Finally, we would like to comment on Takatsuka and McKoy's claim about the formulation of bounds for the true value of $(F_1^t)^{-1}$ [or $(G_{\alpha\alpha}^t)^{-1}$, Eq. (6.2) in TM]. In order

TABLE II. Comparison between the exact phase shifts (in radians) and the variational ones obtained by TMVM and the least-squares method (Ref. 23).

k (a.u.)	η_0 exact	η_0 TM	η_0 LSM
0.5	0.412 287 75	0.412 29	0.412 28
1.0	0.512 014 16	0.511 97	0.512 01

that $(F_1^t)^{-1}$ satisfies a minimum principle, it is essential (see Kato[24]) that $\hat{H}-tX+cX>0$ (c is a constant) or $\hat{H}+(c-t)X>0$, i.e., $\hat{H}+\gamma X>0$ for certain constant γ. However, X is a positive definite operator and $\hat{H}$ is, for arbitrary V a discrete nondegenerate operator of indifinite sign, i.e., $\hat{H}$ has an infinite number of eigenvalues ranging from $-\infty$ to $+\infty$ (see Abdel-Raouf[10]). In other words, there is no $\gamma(\neq\pm\infty)$ for which the previous inequality holds. If such a γ were existing, one would be able to find a solution for Kato's auxiliary eigenvalue problem (for arbitrary V) and, consequently, it would be easy to find bounds for K_{11} using Kato's inequality (see also Hahn, O'Malley, and Spruch,[25] Kolker[26] and Abdel-Raouf[10]). Indeed, the fact that $\hat{H}$ possesses infinite number of negative and positive eigenvalues makes it impossible, at least to us, to find the γ for which the preceding inequality always holds, even if $\hat{H}$ is a bounded operator and $\hat{H}-tX$ is free of poles.

I am extremely indebted to Professor J. W. Darewych, Professor R. P. McEachran, and Professor A. D. Stauffer for fruitful discussions as well as their invaluable help and hospitality during my stay at York University.

---

*Present address: Faculty of Engineering Ain Shams University, Abbassia, Cairo, Egypt.

[1] K. Takatsuka and V. McKoy, Phys. Rev. A **23**, 2352 (1981).
[2] K. Takatsuka and V. McKoy, Phys. Rev. A **23**, 2359 (1981).
[3] K. Takatsuka, R. R. Lucchese, and V. McKoy, Phys. Rev. A **24**, 1812 (1981).
[4] R. R. Lucchese, K. Takatsuka, D. K. Watson, and V. McKoy, in *Proceedings of the Symposium on Electron-Atom and Molecule Collisions, Bielefeld, 1982,* edited by J. Hinze (Plenum, New York, 1983).
[5] Lee Mu-Tao, K. Takatsuka, and V. McKoy, J. Phys. B **14**, 4115 (1981).
[6] E. K. U. Gross and E. Runge, Phys. Rev. A **26**, 3004 (1982).
[7] R. R. Lucchese and V. McKoy, Phys. Rev. A **28**, 1382 (1983).
[8] D. Moe and D. Saxon, Phys. Rev. **111**, 950 (1958).
[9] M. Kolsrud, Phys. Rev. **112**, 1436 (1958).
[10] M. A. Abdel-Raouf, Phys. Rep. **108**, 1–164 (1984).
[11] A. L. Zubarev, Yad. Fiz. **23**, 77 (1976) [Sov. J. Nucl. Phys. **23**, 40 (1976)].
[12] A. L. Zubarev, Fiz. Elem. Chastits At. Yadra **7**, 553 (1976) [Sov. J. Part. Nucl. **7**, 215 (1976)].
[13] A. L. Zubarev, Theor. Math. Phys. **30**, 45 (1977).
[14] V. B. Belyaev, A. P. Podkopayev, J. Wrzecionko, and A. L. Zubarev, J. Phys. B **12**, 1225 (1979).
[15] I. H. Sloan and T. J. Brady, Phys. Rev. **6**, 701 (1972).
[16] J. W. Darewych and M. Horbatsch, Phys. Rev. A **27**, 2245 (1983).
[17] R. K. Nesbet, Phys. Rev. A **175**, 134 (1968).
[18] M. A. Abdel-Raouf and L. J. Dubé, Phys. Rev. A **27**, 1704 (1983).
[19] M. A. Abdel-Raouf, Phys. Rep. **84**, 163 (1982).
[20] C. Schwartz, Phys. Rev. **141**, 1468 (1966).
[21] I. H. Sloan and S. K. Adhikari, Nucl. Phys. **A241**, 429 (1975).
[22] S. K. Adhikari and I. H. Sloan, Nucl. Phys. **A241**, 429 (1975).
[23] M. A. Abdel-Raouf, Acta. Phys. Acad. Sci. Hung. **48**, 31 (1980).
[24] T. Kato, Prog. Theor. Phys. **6**, 295 (1951).
[25] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **130**, 381 (1963).
[26] H. J. Kolker, J. Chem. Phys. **58**, 2288 (1973).