Variational scattering theory with functionals of fractional form

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The recently proposed functional of Takatsuka and McKoy, derived from the Schwinger-type Newton functional, is shown to follow from the usual Hulthén-Kohn variational principle. A generalization of their method becomes obvious in this approach and its better convergence is demonstrated on a simple example.

In a recent paper[1] Takatsuka and McKoy use the Lippmann-Schwinger equation

$$\psi = S + G_0 V \psi \tag{1}$$

to obtain the stationary functional of fractional form,

$$F_1 = \frac{\langle \tilde{C}|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle \tilde{C}|\hat{H}|\tilde{C}\rangle} \ , \tag{2}$$

from the Schwinger-type stationary functional

$$F_0 = \frac{\langle \psi|VG_0V|S\rangle\langle S|VG_0V|\psi\rangle}{\langle \psi|VG_0V - VG_0VG_0V|\psi\rangle} \ . \tag{3}$$

In the above, as elsewhere in our Comment, we use the notation of Takatsuka and McKoy and consider, initially, the single-channel problem. Thus $\hat{H} = E - H$, where $H = H_0 + V$ is the Hamiltonian and E the total energy of the system, S is the regular solution of $H_0 u = Eu$ such that

$$S \sim (\mu/k)^{1/2}\sin(kr - \tfrac{1}{2}l\pi) \ ,$$

G_0 is the Green's function associated with H_0, while $\tilde{C} = G_0 V\psi = \psi - S$. In a companion paper[2] Takatsuka and McKoy apply the many-channel generalization of (2), viz.,

$$F_{mn} = \frac{\langle \tilde{C}_m|V|S_n\rangle\langle S_m|V|\tilde{C}_n\rangle}{\langle \tilde{C}_m|\hat{H}|\tilde{C}_n\rangle} \ , \tag{4}$$

to a coupled–square-well example. In (4),

$$V = \sum_{m\neq n} |\chi_m\rangle V_{mn}\langle\chi_n| \ ,$$

where

$$\langle\chi_m|\chi_n\rangle = \delta_{mn} \ ,$$

and

$$\hat{H}|\tilde{C}_m\rangle = V|S_m\rangle \ ,$$

with

$$S_m \sim |\chi_m\rangle(\mu_m/k_m)^{1/2}\sin(k_m r - \tfrac{1}{2}l_m\pi) \ . \tag{5}$$

We wish to point out that the functional F_1 follows simply from the standard Hulthén-Kato identity,[3–5]

$$\tfrac{1}{2}\lambda = \tfrac{1}{2}\lambda_1 + \langle\psi_1|\hat{H}|\psi_1\rangle - \langle\psi_1 - \psi|\hat{H}|\psi_1 - \psi\rangle \ , \tag{6}$$

where ψ is the desired exact solution of $\hat{H}\psi = 0$ with $\psi \sim S + \lambda C$, where

$$C \sim (\mu/k)^{1/2}\cos(kr - \tfrac{1}{2}l\pi)$$

and $\lambda = \tan\eta$. ψ_1 is a comparison function such that

$$\psi_1 \sim S + \lambda_1 C \ . \tag{7}$$

If we write

$$\psi_1 = S + a\phi_1 \ , \tag{8}$$

where a is an adjustable parameter, then the stationary Hulthén functional

$$\tfrac{1}{2}\lambda[\psi_1] = \tfrac{1}{2}\lambda_1 + \langle\psi_1|\hat{H}|\psi_1\rangle \tag{9}$$

becomes

$$\begin{aligned}\tfrac{1}{2}\lambda[\psi_1] &= \tfrac{1}{2}\lambda_1 + \langle S|\hat{H}|S\rangle + a[\langle S|\hat{H}|\phi_1\rangle \\ &\quad + \langle\phi_1|\hat{H}|S\rangle] + a^2\langle\phi_1|\hat{H}|\phi_1\rangle \\ &= -\langle S|V|S\rangle - 2a\langle\phi_1|V|S\rangle + a^2\langle\phi_1|\hat{H}|\phi_1\rangle \ .\end{aligned}$$

Extremizing this stationary functional with respect to the linear parameter a gives

$$\tfrac{1}{2}[\psi_1] = -\langle S|V|S\rangle - \frac{\langle\phi_1|V|S\rangle\langle S|V|\phi_1\rangle}{\langle\phi_1|\hat{H}|\phi_1\rangle} \ . \tag{10}$$

If we now identify $a\phi_1$ with $\tilde{C}$, then (10) is just the result of Takatsuka and McKoy[1] [cf. their Eq. (4.11)], since the functional on the right of (10) is just their functional F_1 [cf. their Eq. (2.15)]. $\lambda[\psi_1]$, as given in (10), is of course stationary with respect to further variation of ψ_1, i.e., of ϕ_1. Also, it is obvious from (8) that there is no restriction on the asymptotic form of ϕ_1 (i.e., $\phi_1 \sim \lambda_1 C$, but λ_1 can be taken to be zero). The functional in (10) is evidently of fractional form, i.e., independent of the normalization of ϕ_1, (or, equivalently, $\tilde{C}$) since an optimization with respect to the linear normalization parame-

ter a has been carried out (note that the optimal value of a is just $\langle\phi_1|V|S\rangle/\langle\phi_1|\hat{H}|\phi_1\rangle$).

The method of Takatsuka and McKoy is thus just the usual variational method in which an optimization with respect to a linear parameter (the normalization of $\tilde{C}=\psi-S$) has been carried out. Any difference between the standard and the Takatsuka-McKoy methods must, therefore, be due to differences in the trial function ψ_1 (i.e., ϕ_1) used. It may, nevertheless, be useful in some applications to do the variation (optimization) of the adjustable features of different parts of a trial function independently. Thus one could write the trial function in the form

$$\psi_1=\bar{\psi}+a\phi_1 \ . \tag{11}$$

Then, instead of (10) one obtains

$$\tfrac{1}{2}\lambda[\psi_1]=\tfrac{1}{2}\lambda[\bar{\psi}]-\frac{\langle\phi_1|\Delta V|\bar{\psi}\rangle\langle\bar{\psi}|\Delta V|\psi_1\rangle}{\langle\phi_1|\hat{H}|\phi_1\rangle} \ , \tag{12}$$

corresponding to the optimized value

$$a=\langle\phi_1|\Delta V|\bar{\psi}\rangle/\langle\phi_1|\hat{H}|\phi_1\rangle \ ,$$

where ΔV is defined by $\hat{H}\bar{\psi}=\Delta V\bar{\psi}$.

The functionals in (12) are stationary with respect to independent variations of $\bar{\psi}$ and ϕ_1 and, again, ϕ_1 can but need not have the asymptotic form $\lambda_1 C$, i.e., ϕ_1 can be an L^2 function. Thus, if one has already obtained an approximate solution $\bar{\psi}$ to ψ ($\bar{\psi}$ can, of course, be variationally obtained, or by any other method), then a variation correction ϕ_1 to $\bar{\psi}$ [cf. Eq. (11)] can be obtained by extremizing (12) with respect to ϕ_1, for the given $\bar{\psi}$.

In order to demonstrate that the use of the functional (12) will lead to better convergence than the functional of Takatsuka and McKoy [Eq. (2)], that is, if $\bar{\psi}$ is chosen to be a better approximation to ψ than the Born approximation, we consider zero energy scattering by a square well as an illustrative example: The exact result for the scattering length (in units of the well width) is $a=1-\tan K_0/K_0$, where $K_0^2=2mV_0R^2/\hbar^2$, and where V_0 and R are the well depth and well width, respectively. We take for $\bar{\psi}$ the simple form

$$\bar{\psi}=r-\bar{a}(1-e^{-\beta r}) \ , \tag{13}$$

where $\bar{a}$ and β are determined variationally. For this given $\bar{\psi}$ we take

$$\phi_1=\sum_{n=1}^{N}\alpha_n r^n e^{-\gamma r} \ , \tag{14}$$

and determine the parameters γ and α_n by extremizing (12).

Figures 1 and 2 show the results for two different well strengths, namely, $K_0=1$ and 2, which are, respectively, below and above the first "resonance" in the exact scattering length (which has vertical asymptotes at $K_0=\pi/2, 3\pi/2, 5\pi/2$, etc.) Note that the Born approximation $-\frac{1}{3}K_0^2$ gives a reasonable value at $K_0=1$ but is of the wrong sign at $K_0=2$. The figures illustrate the convergence of the approximate value of the scattering length obtained from the functional (12) with the number of short-range terms in (14), using the $\bar{\psi}$ as given in (13), as well as for

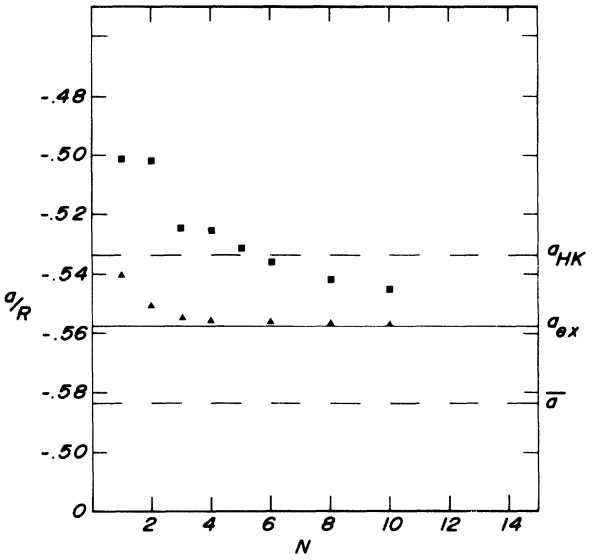

FIG. 1. Square-well scattering length for $2mR^2V_0/\hbar^2=1$. a_{ex}: exact result: a_{HK}: Hulthén-Kohn value using the trial function (13) with trial value $\bar{a}$. Triangles: present results with ϕ_1 as in Eq. (14). Squares: the same calculation, but with $\bar{\psi}=r$ only.

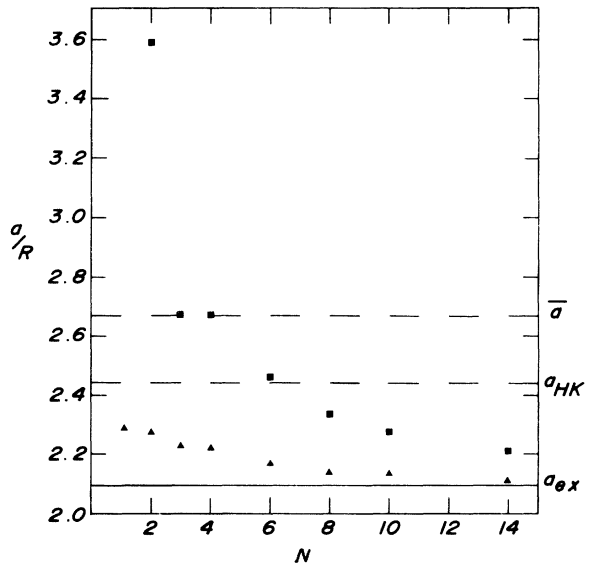

FIG. 2. Square-well scattering length for $2mR^2V_0/\hbar^2=4$. The legend is as in Fig. 1.

$\bar{\psi} = r$, for which (12) reduces to the method of Takatsuka and McKoy (2). It is clear that the convergence improves substantially with the more realistic $\bar{\psi}$.

For actual physical applications we note that the functional (12) offers the opportunity to improve upon a given elaborate calculation by simply adding to it appropriate correction terms ϕ_1 that are then independently varied. For example, for the description of inelastic many-particle processes, $\bar{\psi}$ might be a close-coupling expansion over the open channels while ϕ_1 could be taken to be an L^2 algebraic expansion, including correlation terms.

For the many-channel case, the Hulthén stationary functional for the K matrix is

$$\tfrac{1}{2}K_{ij}^{H}[\psi^{T}] = \tfrac{1}{2}K_{ij}^{T} + \langle \psi_i^{T} | \hat{H} \psi_j^{T} \rangle \quad , \tag{15}$$

where the trial solutions $\psi^{T} \sim S + CK^{T}$, with

$$S = S_i \delta_{ij}, \quad K^{T} = [K_{ij}^{T}] \quad ,$$

etc. If the trial solutions are written in two parts,

$$\psi_i^{T} = \bar{\psi}_i + a_i \phi_i \quad , \tag{16}$$

then extremization of (15) with respect to the linear parameters a_i yields

$$\tfrac{1}{2}K_{ij}^{H}[\psi^{T}] = \tfrac{1}{2}K_{ij}^{H}[\bar{\psi}] - \langle \phi_i | \hat{H} \bar{\psi}_i \rangle \langle \hat{H} \bar{\psi}_i | \phi_i \rangle / \langle \phi_i | \hat{H} \phi_j \rangle \quad . \tag{17}$$

If $\bar{\psi}_i$ are taken to be simply the undistorted waves (5), then the functional on the right-hand side of (17) is identical with Takatsuka and McKoy's functional F_{ij} [Eq. (4)]. Clearly any difference between the standard variational methods based on the Hulthén functional (15) and those based on the functional (4) can come only from differences in the trial functions that are used, since (4) is just (15) after optimization with respect to one linear parameter for each channel trial function has been done.

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