Accuracy of the unitary pole approximation at positive energies for local potentials containing a hard core

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The accuracy of the unitary pole approximation (UPA) to the two-body t matrix at positive energies has been examined for the case of a local potential with a hard core. To this effect the S-wave phase shifts and the half-shell functions (Baranger, Giraud, Mukhopadhyaya, and Sauer) have been calculated for the Herzfeld potential as well as for its UPA. The agreement between the two sets, though satisfactory, is not as good as reported by Levinger and O'Donoghue, who did similar calculations for various singlet potentials. This result may be attributed to the existence of a bound-state pole in t matrix in the negative energy region in the case of the Herzfeld potential.

NUCLEAR STRUCTURE Unitary pole approximation, hard core potential, positive energies.

In recent years several separable expansions and approximations to the two-body t matrix have been proposed.¹ Amongst these the unitary pole expansion of Harms² and its one term version, the unitary pole approximation (UPA),³ have been extensively studied at both negative and positive energies. The accuracy of the UPA has been tested through two- and three-body calculations 4 and it has proved to be quite useful (for criticism, see Refs. 5 and 6). As the UPA is based on the concept of pole dominance, it should, in general, be a good approximation at negative energies close to the bound state pole. The interesting feature, however, is that the UPA has also been found⁴ to be good at positive energies for the potentials without hard cores. Apart from the calculations of Brady et al.⁴ for Tabakin's rank-two separable potential containing hard shell repulsion, no direct calculations have been reported at positive energies in the case of local potentials containing hard cores. Since we had already tested the UPA at negative energies for hard core potentials,⁷ we have now carried through the calculation for positive energies also and report the results here. Another motivation to do the present calculations is that these results are also required as input parameters in a scheme we are pursuing in connection with off-shell continuation of the two-body t matrix with bound states.

Since one can go uniquely from the half-off-shell t matrix to full-off-shell t matrix through the subtracted Low equation,⁸ we compare the half-shell functions defined by Baranger *et al.* (BGMS)⁹ and the phase shifts rather than the full-off-shell tmatrix elements at positive energies.

For our calculations, we have chosen the Herz-

feld potential (hard core with square well outside)¹⁰:

$$V(r) = +\infty , \quad r \le a$$

= - V₀ , $a < r \le b$ (1)
= 0 , $r > b$

with parameters $V_0 = 1.54$ fm⁻², a = 0.4 fm, b = 1.737 fm and where the potential binds the deuteron with energy B = 0.435 MeV. From Laughlin and Scott,¹¹ we know that the half-off-shell (S-wave) t matrix element for energy $S = k^2 + i0$ is given by

$$2\pi^{2}t_{0}(k', k; k^{2} + i0) = \frac{\sin k'a}{k'}u'(a+) + \int_{a}^{\infty} dr \frac{\sin k'r}{k'}V(r)u(r) ,$$
(2)

where terms have meanings as given by Laughlin and Scott.¹¹ For the Herzfeld potential Eq. (2) can be written as

$$2\pi^{2}t_{0}(k', k; k^{2} + i0) = \frac{\sin k'a}{k'}u_{1}'(a+)$$
$$-V_{0}\int_{a}^{b}dr\frac{\sin k'r}{k'}u_{1}(r) , \qquad (3)$$

where $u_1(r)$ is now the solution of the Lippman-Schwinger equation in the range r = a to r = b with appropriate boundary conditions and is given by¹²

$$u_1(r) = C \sin\beta(r - a) \quad , \tag{4}$$

where C is a constant and $\beta^2 = k^2 + V_0$. This solu-

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tion ensures that $u_1(r)$ vanishes at hard core radius *a*. To determine *C*, we note that the form of the wave function outside r = b is given by $(8 = k^2 + i0)$:

$$u_2(r) = \frac{\sin kr}{k} - Ae^{ikr} \quad . \tag{5}$$

Matching the functions at boundary r = b, and separating out the magnitude and phase, we get

$$C = \frac{1}{R} e^{i(\theta - kb)}, \qquad (6)$$

where

$$R^{2} = \beta^{2} \cos^{2}\beta(b-a) + k^{2} \sin^{2}\beta(b-a)$$
(7)

$$\theta = \tan^{-1} \left[\frac{k}{\beta} \tan\beta(b-a) \right] . \tag{8}$$

Using (4) and (6) in (3), we get

$$2\pi^{2}t_{0}(k', k; k^{2}+i0) = \left(\beta \frac{\sin k'a}{k'} - \frac{V_{0}I}{k'}\right) \frac{1}{R} e^{i(\theta - kb)} , \qquad (9)$$

where

$$I = \frac{\sin[\beta(a-b) + k'b]}{2(k'-\beta)} + \frac{\sin[\beta(a-b) - k'b]}{2(k'+\beta)} - \frac{\sin k'a}{2(k'-\beta)} + \frac{\sin k'a}{2(k'+\beta)} .$$
(10)



FIG. 1. Exact (solid line) and UPA (dashed line) phase shifts $\delta(k)$ for the Herzfeld potential.

Now following the definition of half-shell function $\varphi(k, k')$ from Baranger *et al.* (BGMS)⁹

$$t_0(k', k; k^2 + i0) = \varphi_{\text{exact}}(k, k')e^{i\delta_0(k)} , \qquad (11)$$

a straightforward comparison gives

$$\varphi_{\text{exact}}(k,k') = \frac{1}{2\pi^2 R} \left(\frac{\beta \sin k'a}{k'} - \frac{V_0 I}{k'} \right)$$
(12)

and exact phase shifts $\delta_0(k)$ as

$$\delta_0(k) = \theta - kb \quad . \tag{13}$$

It may be verified that expressions (12) and (13) are consistent because by putting k' = k in (12) and using (13) and (11) we arrive at the definition of on-shell t matrix¹¹

$$t_0(k, k; k^2 + i0) = -\frac{1}{2\pi^2 k} \sin \delta_0(k) e^{i\delta_0(k)} \quad . \tag{14}$$

Also, the expression for the exact phase shifts (13) can be independently arrived at from the definition of the S matrix.¹⁰

Having thus determined the exact half-shell function and phase shifts, we now proceed to de-



FIG. 2. Exact (solid line) and UPA (dashed line) halfshell functions $\varphi(k, k')$ at different values of k for low values of momentum k' for the Herzfeld potential. $\varphi_{\text{exact}}(0.072, k')$ overlaps $\varphi_{\text{UPA}}(0.0053, k')$ by mere coincidence.

termine the same quantities in the UPA. In the UPA, the half-off-shell t matrix element is given by^{2,7,10,12}

$$2\pi^{2}t_{\text{UPA}}(k', k; k^{2} + i0)$$

= $\frac{\pi}{2}\psi(k', -B)\Delta(k^{2} + i0)\psi(k, -B)$, (15)

where

$$-\left[\Delta(k^{2}+i0)\right]^{-1}=1+\int_{0}^{\infty}\frac{\psi^{2}(q,-B)}{k^{2}-q^{2}+i0}q^{2}dq\quad(16)$$

and $\psi(q, -B)$ are the form factors for the potential under consideration and are given by (for Herzfeld potential)^{10,12}

$$q\psi(q, -B) = \left(\frac{2}{\pi}\right)^{1/2} \left\{ DK \sin qa - \frac{V_0 D}{K^2 - q^2} \times \left[K \sin qa + \sin K(b - a)q \cos qb - K \cos K(b - a) \sin qb \right] \right\}, \quad (17)$$

where

$$K^2 = V_0 - B \tag{18}$$



FIG. 3. Exact (solid line) and UPA (dashed line) halfshell functions $\varphi(k, k')$ at low values of k for high values of momentum k' for the Herzfeld potential. $\varphi_{\text{exact}}(0.072, k')$ overlaps $\varphi_{\text{UPA}}(0.0053, k')$ by mere coincidence.

and the constant

$$D^{2} = \frac{2}{V_{0}} \left[(b-a) - \frac{\sin 2K(b-a)}{2K} \right]^{-1} .$$
 (19)

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Using the relation

$$\frac{1}{k^2 - q^2 + i0} = \mathcal{O}\frac{1}{k^2 - q^2} - \frac{i\pi}{2k}\,\delta(k - q) \quad , \tag{20}$$

the definition of UPA half-shell function $\varphi_{\rm UPA}(k,k')$ and UPA phase shifts $\delta_{\rm UPA}(k)$

$$t_{\rm UPA}(k', k; k^2 + i0) = \varphi_{\rm UPA}(k, k') e^{i\delta_{\rm UPA}(k)} , \qquad (21)$$

separating the right hand side of (15) into its magnitude and phase and comparing Eqs. (21) and (15), we get

$$\varphi_{\rm UPA}(k,k') = -\frac{1}{4\pi} \frac{\psi(k',-B)\psi(k,-B)}{[A^2(k)+B^2(k)]^{1/2}}$$
(22)

and

$$\delta_{\rm UPA}(k) = \tan^{-1} \frac{B(k)}{A(k)} , \qquad (23)$$

where

$$A(k) = 1 + \mathcal{P} \int_{0}^{\infty} q^{2} dq \frac{\psi^{2}(q, -B)}{k^{2} - q^{2}}$$
(24)



FIG. 4. Exact (solid line) and UPA (dashed line) half-shell functions $\varphi(k, k')$ at high values of both k and k' for the Herzfeld potential.



FIG. 5. Fractional error plot against momentum k' for phase shift and half-shell functions at different values of k.

and

$$B(k) = \frac{\pi k}{2} \psi^2(k, -B) \quad . \tag{25}$$

It may be noted that Eqs. (22) to (25) are valid for UPA for any potential. For Herzfeld potential, we have substituted (17) wherever required. It can also be easily verified that (22) and (23) are consistent because for the case k' = k, we again get the definition (14) with δ_0 replaced by δ_{UPA} . For calculation of the principal value integral, we have followed the method suggested by BGMS.⁹

We have calculated the values of φ_{exact} , φ_{UPA} , δ_{0} , and δ_{UPA} for various values of k and k'. In Fig. 1 are plotted the curves for the phase shifts. The UPA phase shifts are seen to differ from exact phase shifts by no more than about 10° over a large range of momenta. However, while the exact phase shift is found to change sign at about $k=1.6 \text{ fm}^{-1}$, i.e. $k^2=2.56 \text{ fm}^{-2}$, the UPA phase shift does not. This is to be expected since the UPA is equivalent to using rank-one separable potentials. The effective range parameters for the UPA to the Herzfeld potential are found to be r_0 (effective range) = 1.35 fm and C_0 (scattering length) = 10.49 fm which compare favorably with the exact value for this potential viz. r_0 = 1.95 fm and C_0 = 10.8 fm.

For use in a many-body problem, a comparison of exact and UPA half-shell functions is more meaningful. In Fig. 2, we have shown the halfshell functions for low values of k' for different choices of k (change in k effectively means change in energy). At low values of k' as well as k, the agreement is not very encouraging. However, at medium and high values of k the agreement appears to be better. In Figs. 3 and 4 are shown the halfshell functions for high values of k' and different values of k. Because at medium values of k it was difficult to make a proper comparison on the scale of Fig. 3, the scale in Fig. 4 has been suitably enlarged. It can be seen that at high values of k', the agreement between exact and UPA halfshell functions is again better. These results are not quite the same as those of Levinger and O'Donoghue⁴ who find the UPA quite good at low momenta for singlet potentials. This can be understood by noting that since Levinger and others

use singlet potentials, they are not far from the antibound state pole at low values of momenta and should expect the UPA to be fairly good. On the other hand, for the Herzfeld potential, which has a bound state pole at -0.435 MeV, the UPA would not be as good at positive energies for low momenta because of the position of the bound state pole. However, the surprising feature of our results is that at high momenta, the behavior of the UPA appears to be much better in regard to half-shell functions.

After plotting fractional errors for phase shifts and half-shell functions in Fig. 5, however, it is seen that the "better" agreement of the UPA at high energies is only apparent since the fractional error remains nearly constant over a very large momentum range (except in the region where phase shift changes sign). So one can conclude that the UPA is a workable approximation up to energies equal to 3.0 fm^{-2} for potentials with hard cores, beyond which an at least two term UPE must be used.¹³ In this context it may be mentioned that the conclusions of Srivastava and Sirohi,⁴ that the UPA to hard core potentials at positive energies is altogether a failure, is not exactly consistent with our findings.

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