

Triton model calculation test of the Bonn W -matrix rank-one approximation

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The rank-one separable part of the W -matrix representation of the t matrix for the Malfliet-Tjon I-III nucleon-nucleon potential has been shown to lead to results for the triton binding energy and low-energy ($E_{\text{lab}} \leq 50$ MeV) nucleon-deuteron scattering that agree well with results for that potential obtained by solving the full local-potential equations. We explore why this prescription appears to work so well for the Malfliet-Tjon I-III model and test it further using the Reid-soft-core spin-singlet interaction, which possesses a very strong short-range repulsion (a stiff core). For this model, a calculation using the rank-one separable part of the W -matrix representation of the two-body t matrix overbinds the triton by 25%.

I. INTRODUCTION

The traditional approach to solving the two-body problem in momentum space has been in terms of the Lippmann-Schwinger equation—a homogeneous equation for the bound state and an inhomogeneous equation for the continuum. Bartnik, Habertzettl, and Sandhas^{1,2} have proposed an alternative formulation. They have outlined a unified description of the bound-state and continuum regimes in terms of a single real, nonsingular inhomogeneous integral equation, the solution of which is the W matrix. One advantage of this prescription is that one can construct an exact representation of the two-body off-shell t matrix in which the bound-state pole and scattering-cut information are contained in a single separable term (a rank-one expansion). The remainder term, which is nonseparable, is a real, nonsingular function that vanishes half on shell.

The hope was expressed in Ref. 1 that the single separable term in the W matrix might, when used as input in exact three-body equations, provide a reasonable approximation to the experimental data. That is, the remainder term in the W -matrix representation of the two-body t matrix might make a negligible contribution. This hope was bolstered by results obtained in Ref. 3 for the triton bound state using the rank-one approximation to the Malfliet-Tjon⁴ model MT I-III (a spin-singlet, spin-triplet interaction that acts only in $l=0$ partial waves) and for neutron-deuteron scattering using that potential and the Alt, Grassberger, and Sandhas⁵ separable-potential formulation of the Faddeev⁶ equations. In the former case, the binding energy obtained using the rank-one separable term in the W matrix had a minimum at $E_t(k) = -8.595$ MeV (as a function of the parameter k in the W -matrix solution at negative two-body energies), which compared very well with the full, local-potential solution⁷ of -8.58 ± 0.1 MeV. Similarly, neutron-deuteron scattering length results for the W matrix ($^4a_{nd} = 6.41$ fm and $^2a_{nd} = 0.86$ fm) compared well with the local-potential

numerical results of Kloet and Tjon⁸ ($^4a_{nd} = 6.35$ fm and $^2a_{nd} = 0.9$ fm).

Our purpose is to apply the W -matrix prescription to a “more realistic potential” (one possessing strong short-range repulsion) and attempt to understand whether this promising rank-one separable-potential approximation to local potentials might be used to make four-body and five-body calculations more tractable. To that end we briefly outline the rank-one W -matrix approximation in Sec. II. We present triton binding energy results for several Malfliet-Tjon models in Sec. III obtained using this W matrix along with full local-potential solutions for the same models. We also explore the three-body bound state for a modified Reid-soft-core⁹ (RSC) spin-singlet potential. Our conclusions are stated in Sec. IV.

II. SUMMARY OF THE BONN W -MATRIX FORMALISM

For completeness we summarize here the elements for the W -matrix representation of the two-body t matrix which we require to carry out our investigation. The off-shell t matrix for partial wave l at energy E is given by

$$t_l(p, p'; E) = W_{kl}(p, k; E) \Delta_{kl}(E^+) W_{kl}(p', k; E) + R_{kl}(p, p'; E), \quad (1)$$

where $E^+ = E + i\epsilon$, $R_{kl}(p, p'; E)$ is the remainder function that vanishes half on shell, and k is a parameter specified below. The function $\Delta_{kl}(E^+)$ in Eq. (1) is given by

$$\Delta_{kl}(E^+) = \frac{k^l}{W_{kl}(k, k; E) \hat{F}_{kl}(E^+)}, \quad (2)$$

where $\hat{F}_{kl}(E^+)$ is defined in terms of a simple integral as

$$\hat{F}_{kl}(E^+) = 1 - \int_0^\infty \frac{q^l W_{kl}(q, k; E)}{E^+ - q^2/m} q^2 dq. \quad (3)$$

The W matrix satisfies the nonsingular integral equation

$$W_{kl}(p, p'; E) = U(p, p') + \int_0^\infty \frac{[U_l(p, q) - U_l(p, k)]}{E - q^2/m} \times q^l W_{kl}(q, p'; E) q^2 dq \quad (4)$$

in which the parameter k satisfies the following constraints:

$$(I) \quad k^2 = mE, \quad E \geq 0 \quad (5a)$$

$$(II) \quad k \text{ arbitrary, } E < 0. \quad (5b)$$

The $U_l(p, q)$ in Eq. (4) is a simple function of the partial wave projection of the potential,

$$U_l(p, q) = q^{-l} V_l(p, q). \quad (6)$$

Here the q^{-l} factor compensates for the q^l behavior of $V_l(p, q)$ as $q \rightarrow 0$ and ensures that $U_l(p, q)$ does not vanish identically at $q=0$. It was demonstrated in Ref. 1 that, at negative energies ($mE = -\alpha^2$), for solutions $W_{kl}(q, k; -\alpha^2/m)$ which satisfy

$$\int_0^\infty \frac{q^l W_{kl}(q, k; -\alpha^2/m)}{-(\alpha^2 + q^2)/m} q^2 dq = 1, \quad (7)$$

$-\alpha^2/m$ is equal to the binding energy E_n (i.e., $-\alpha_n^2/m$) of one of the bound states. The corresponding wave function is given by

$$\psi_{nl} = C_{nl} \frac{W_{kl}(p, k; -\alpha_n^2/m)}{-(\alpha_n^2 + p^2)/m}, \quad (8)$$

where C_{nl} is the normalization constant.

Clearly, the leading term on the right-hand side of Eq. (1) is of a form similar to that arising from a rank-one separable potential such as

$$V(p, p') = g(p) \Lambda g(p'), \quad (9)$$

where Λ is the potential strength and $g(p)$ is the potential form factor. If the remainder $R_{kl}(p, p'; E)$ in Eq. (1), which vanishes half on shell, can be shown to make a negligible contribution in the calculation of three-nucleon observables, then one might utilize such a prescription to simplify few-body calculations with realistic potentials.

To investigate this possibility for models other than that discussed in Refs. 1 and 3, we utilize potentials composed of sums of Yukawa forms

$$V(r) = \sum_i V_i \frac{\exp(-\mu_i r)}{\mu r} \quad (10)$$

$$I_{00}(p, P; E) = \int_{-1}^1 dx \frac{W_{k0} \left[|\mathbf{p} + \frac{1}{2}\mathbf{P}|, k; E - \frac{3P^2}{4m} \right] W_{k0} \left[\frac{1}{2}\mathbf{P} + \mathbf{P}, k; E - \frac{3P^2}{4m} \right]}{(p^2 + P^2 - pPx)/m - E} \quad (17)$$

Equation (16) is the usual separable-potential formulation in which the form factors $g(p)$ in the separable potential of Eq. (9) have been replaced by the W matrix. The gen-

or

$$V(q) = \sum_i \frac{V_i}{2\pi^2} \frac{1}{q^2 + \mu_i^2} \quad (11a)$$

$$= \sum_i V_i(\mathbf{p}, \mathbf{p}'), \quad q^2 = (\mathbf{p} - \mathbf{p}')^2. \quad (11b)$$

The $l=0$ term in the partial wave expansion of Eq. (11b) is

$$V_{i0}(p, p') = \int V_i(\mathbf{p}, \mathbf{p}') d\Omega \\ = \frac{V_i}{2\pi p p'} \ln \frac{(p + p')^2 + \mu_i^2}{(p - p')^2 + \mu_i^2}, \quad (12)$$

and for $l=0$ one has the trivial relation

$$U_0(p, p') = V_0(p, p'). \quad (13)$$

The s -wave separable potential Faddeev equation that determines the three-boson bound state is

$$\psi(\mathbf{p}, \mathbf{P}) = 2G_0 \int d\mathbf{p}' t \left[\mathbf{p}, \mathbf{p}' + \frac{1}{2}\mathbf{P}; E - \frac{3P^2}{4m} \right] \\ \times \psi(\frac{1}{2}\mathbf{p}' + \mathbf{P}, \mathbf{p}'). \quad (14)$$

Expressing the t matrix in terms of the W matrix and neglecting the remainder function, then Eq. (14) is satisfied by the ansatz

$$\psi(\mathbf{p}, \mathbf{P}) = G_0 W_{k0} \left[p, k; E - \frac{3P^2}{4m} \right] u(P). \quad (15)$$

Here G_0 is the free-particle three-nucleon propagator and $u(P)$ is the spectator function describing the dynamics of the third nucleon moving relative to the center of mass of the interaction pair. (Our Jacobi coordinates are \mathbf{p} for the pair and \mathbf{P} for the momentum of the spectator relative to the pair.) After a modest amount of algebra, one can demonstrate that $u(P)$ satisfies the homogeneous integral equation

$$u(P) = 2\Delta_{k0} \left[E - \frac{3P^2}{4m} \right] \int_0^\infty I_{00}(p', P; E) u(p') p'^2 dp', \quad (16)$$

where the kernel is

eralization to include spin and isospin follows the conventional three-nucleon analysis. It is these three-body equations that we solve numerically to explore the utility of

approximating the t matrix by the leading separable term in the W -matrix representation.

III. NUMERICAL RESULTS

In addition to verifying the bound-state results for the MT I-III potential quoted in Ref. 3, we have explored a number of the Malfliet-Tjon⁴ models. The particular parameters used¹⁰ are quoted in Table I. They differ slightly from those quoted originally in Ref. 4. Models I and II correspond to spin singlet, whereas models III and IV correspond to spin triplet. Model V is a spin-averaged interaction. (Note that these potentials possess an implied projection operator and act only in the $l=0$ partial wave.)

Because we are dealing with the bound-state problem, the parameter k in Eq. (4) is arbitrary, as is indicated by the condition expressed in Eq. (5b). As found in Ref. 3, the trinucleon bound-state energy has its minimum as a function of k very close to the value that one obtains solving the configuration-space local-potential Faddeev equation discussed in Ref. 10. We list those triton bound-state energies in Table II, where it is clear that for the MT I-III model the W -matrix prescription duplicates almost exactly the local-potential result. A similar close approximation of the local-potential result by the W -matrix approximation was found for the spin-averaged MT V model.

We were disappointed to discover that the W -matrix prescription did not work nearly as well for the simpler (one term Yukawa) MT II-IV model. In this case the difference between the ^3H binding energies was more than 1 MeV, or some 10%. Combining two term (MT I or MT III) potentials with one term (MT II or MT IV) potentials led to reasonable W -matrix results. However, it was clear from examining the MT II potential (multiplied by a factor of 1.1 to increase the strength of the potential sufficiently to support a three-body bound state with a reasonably large binding energy) and MT IV potentials separately, that neglecting the remainder term $R_{k0}(p, p'; E)$ does not provide a satisfactory representation of the t matrix for a single Yukawa. The fact that the triton bound-state and neutron-deuteron scattering calculations using the W -matrix prescription for the MT I-III model work so well would appear to indicate that a cancellation occurs in that case which makes the contribution of the remainder term negligible.

To test that supposition, we investigated a simple model based upon the RSC spin-singlet interaction. That po-

TABLE II. Triton binding energies obtained by solving the configuration-space Faddeev equations and by solving the W -matrix separable equations for selected Malfliet-Tjon potential models.

Model	E_3 (local) (MeV)	E_3 (W matrix) (MeV)
MT I-III	-8.54	-8.53
MT V	-7.54	-7.50
MT II-IV	-11.8	-10.5
MT II-III	-10.2	-9.9
MT I-IV	-8.5	-8.4
MT II ($\times 1.1$)	-5.6	-4.8
MT IV	-24.9	-21.4

tential alone produces a three-boson bound state ($V^t \equiv V^s$) having about 1 MeV binding. We multiplied the strength of the midrange attraction by a factor of 1.08 to increase the three-body binding energy to about 7 MeV. The potential parameters were

$$V_1 = -10.463 \text{ MeV},$$

$$V_2 = -1815.66 \text{ MeV},$$

$$V_3 = 6484.2 \text{ MeV},$$

with ranges of $\mu (=0.7 \text{ fm}^{-1})$, 4μ , and 7μ . The configuration-space Faddeev equation yields a three-body binding energy of $E_3 \approx -7.1 \text{ MeV}$. The W -matrix prescription yielded a minimum at $E_3(k \approx 0.85) = -9.1 \text{ MeV}$. Apparently the error made in neglecting the remainder due to the very strong (stiff) repulsive short-range Yukawa term overcompensates for that made in neglecting the remainder due to the two longer-range attractive terms. Regardless, the W -matrix prescription fails to reproduce the local-potential result in the region of the parameter k that minimizes the three-body binding energy, in contradiction to the supposition made in Ref. 3.

One comment of a technical nature is in order. Whereas the Malfliet-Tjon models have a sufficiently soft repulsive character at short range that one can solve the W -matrix three-body equations by means of the simple power method, such is not the case for the RSC spin-singlet model. In that case one must resort to a more powerful approach such as the Lanczos procedure described in detail in Ref. 11 or a full eigenvalue solution, in order to avoid the three-body eigenvalue corresponding to the strong short-range repulsion. Spline methods¹² are most efficient in obtaining the W matrix itself.

In attempting to understand why use of just the separable term in the W -matrix representation of the t matrix led to significant underbinding of the triton for the single-term (purely attractive) Yukawa potential model and overbinding for the RSC spin-singlet (strong short-range repulsion) potential model, we examined norms of the remainder term $R_{k0}(p, p'; E)$ for all potential models investigated. (We used a Gaussian weighting about the on-shell momentum to obtain convergence.) However,

TABLE I. Potential parameters for the Malfliet-Tjon models, from Ref. 10.

Model	V_A (MeV fm)	μ_A (fm^{-1})	V_R (MeV fm)	μ_R (fm^{-1})
I	513.968	1.55	1438.720	3.11
II	52.49	0.809	0	
III	626.885	1.55	1438.720	3.11
IV	65.120	0.633	0	
V	570.3316	1.55	1438.4812	3.11

there was no obvious characteristic which would allow us to predict *a priori* which would make a small contribution and whether the triton would be overbound or underbound. This is likely because the separable term in the W matrix does provide a good first order representation of the t matrix (the remainder term vanishes half on shell). [The observed discrepancy in the binding ($\sim 1-2$ MeV) is but a small fraction of the total potential energy of the trinucleon bound state ($\sim 40-50$ MeV).] Thus, in the three-body bound-state calculation the remainder term provides only a small (off-shell) correction to the leading separable term, and it is difficult to know *a priori* what the properties of such an off-shell term will be.

IV. CONCLUSIONS

The Bonn W -matrix representation of the two-body t matrix has two very attractive features: the leading separable term contains the bound-state pole and scattering-cut information, and the nonseparable remainder term vanishes half on shell. This property of the remainder term leads one to hope that corrections from this term in few-body calculations will be small, as was the case for the MT I-III potential. However, the remarkably accurate three-nucleon bound-state results obtained for the MT I-III model using solely the leading separable term of the W -matrix representation are not

found for other potentials of the Yukawa form—the MT II-IV and RSC spin-singlet potential models. The former is purely attractive and the latter has a very stiff, short-range repulsive core. The implication is that the error made in neglecting the W -matrix remainder term for the MT I-III model (which is composed of a long-range attractive term and a shorter-range repulsive term) is small due to cancellations. Furthermore, we do not see in the RSC spin-singlet case the remarkable bounding from below of the local-potential triton energy by the rank-one W -matrix results (for all values of the arbitrary parameter k) that was seen with the MT models. We conclude that, although the leading separable term of the W -matrix representation of the t matrix provides a very good first order approximation, its use alone in few-body bound-state calculations (that is neglecting the nonseparable remainder term) is not justified for all potentials.

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