Nonsingular integral equation for two-body scattering and applications in two and three dimensions

H. T. C. Stoof, L. P. H. de Goey, W. M. H. M. Rovers, P. S. M. Kop Jansen, and B. J. Verhaar
Department of Physics, Eindhoven University of Technology, NL-5600 MB Eindhoven, The Netherlands
(Received 14 December 1987)

We introduce a new nonsingular scattering integral equation, which is suitable for the investigation of the total (also off-shell) transition matrix in arbitrary dimension $n \geq 2$. In particular, the low-energy properties are derived and lead, in connection with spin-polarized atomic hydrogen H↓, to the low-temperature behavior of two- and three-body surface processes. In addition, for three dimensions the method leads in a natural way to a separable approximation to the T matrix for all energies, with the possibility of formulating a procedure for optimizing this approximation. To show the practicability of the equation we also present numerical results for both $n=2$ and $n=3$.

I. INTRODUCTION

In the last decade the preparation and study of two-dimensional systems has attracted a great deal of attention. Surface physics with its development of new sensitive detection techniques such as the scanning tunneling microscope, two-dimensional electron gases exhibiting the integral and fractional quantum Hall effect, and high-T_c superconductors, in which the layer structure of the lattice may play an important role in the pairing mechanism, are just a few example of the increasing interest in this field of physics.

Another experimentally accessible two-dimensional system is low-temperature spin-polarized atomic hydrogen (H↓) that is adsorbed at a surface of liquid helium.[1] The two-dimensional gas plays a vital role in connection with experiments aiming at Bose-Einstein condensation: At temperatures below about 0.3 K the density of the adsorbed gas is so high that the stability of the gas sample as a whole is mainly determined by two-dimensional relaxation and recombination processes. Indeed, the three-body recombination on the helium surface is the main cause of the inability of the conventional compression experiments to achieve the Bose-Einstein transition in the H↓ gas.[2] To circumvent this dominant decay process, it is important to understand the physical mechanism through which the recombination proceeds and hence to be able to predict the magnetic field and low-temperature behavior of the surface recombination rate constant L_s. However, formulating a Faddeev formalism for this three-body problem in two dimensions, as was done in the volume case,[3] leads to substantial problems caused by the logarithmic energy dependence of the two-dimensional two-body T (transition) operator.

As a first step in solving the above-mentioned problems and arriving at a three-body effective-range theory, we introduce in Sec. II a new method to study the complete T matrix and in particular its energy dependence. The most important results, needed for subsequent applications, are given in Eqs. (4) and (7). We formulate the method in arbitrary dimension and apply it to two and three dimensions. Sections III and IV are devoted to two-dimensional scattering and we here discuss the complete agreement of our method with the effective-range theory formulated previously[4] and derive some preliminary results on the low-temperature behavior of the three-body decay rate L_s. After that we turn in Sec. V to the three-dimensional case and derive a separable approximation to the T matrix for both positive and negative energies. This approximation may be of some use in connection with the solution of Faddeev or Alt-Grassberger-Sandhas (AGS) equations[5] in, for example, nuclear physics, where a one-term separable expansion is already highly accurate.

II. τ MATRIX

The T matrix in dimension $n \geq 2$ and for a (integer-valued) partial wave l obeys a Lippmann-Schwinger equation[5] that in the momentum representation takes the form

$$T_l(p,p',E)=V_l(p,p')+\int_0^\infty dp''(p'')^{n-1}V_l(p,p'')\times\frac{1}{E^+-(p'')^2/2\mu}\times T_l(p'',p',E)\ . \tag{1}$$

Here μ is the reduced mass of the two colliding particles, E is the total energy available, and the angular momentum associated with the partial wave l is $\sqrt{l(l+n-2)}\hbar$. We assume the interaction to be local and rotationally invariant, in which case all partial waves are decoupled from one another and the (real) momentum representation of the potential $V(r)$ turns out to be

$$V_l(p,p')=\frac{4}{\Gamma^2(\frac{1}{2}n)(2\hbar)^n}\int_0^\infty dr\, r^{n-1}j_{l,n}(pr/\hbar)V(r)\times j_{l,n}(p'r/\hbar)\ . \tag{2}$$

The functions $j_{l,n}(z)$ play an important role in a generalization of quantum-mechanical scattering theory to arbitrary dimension. They are the solution of a radial Schrödinger equation with the centrifugal barrier

$$\frac{\hbar^2}{2\mu r^2}[(l+\tfrac{1}{2}n-1)^2-\tfrac{1}{4}]$$

and are related to Bessel functions of the first kind $J_\nu(z)$ by

$$j_{l,n}(z)\equiv\Gamma(\tfrac{1}{2}n)\left[\frac{2}{z}\right]^{(1/2)n-1}J_{l+(1/2)n-1}(z)\ . \tag{3}$$

The coefficient is chosen such that $j_{0,n}(0)=1$. Furthermore, with this choice these functions reduce in three dimensions to the conventional[5] spherical Bessel functions $j_l(z)$. For general n relations (1) and (2) imply the symmetry of $V_l(p,p')$ and $T_l(p,p',E)$ in the momentum variables. For convenience we use from now on units such that $\hbar=2\mu=1$ and in addition suppress the subscript l.

In the case of positive energies $E\geq 0$ the notation $E^+=E+i0$ used in Eq. (1) specifies the usual integration contour around the singularity associated with the energy denominator. However, this singularity can be avoided by introducing a real and symmetrical τ^Λ matrix by the equation

$$\tau^\Lambda(p,p',E)=V(p,p')+\int_0^\infty dp''\frac{(p'')^{n-1}}{E-(p'')^2}[V(p,p'')\tau^\Lambda(p'',p',E)-\Theta(\Lambda-p'')V(p,k)\tau^\Lambda(k,p',E)]\ . \tag{4}$$

We denote the on-shell momentum by $k=\sqrt{E}$ and the Heaviside unit-step function by $\Theta(x)$. Note that at $p''=k$, where the denominator vanishes, the quantity in square brackets also vanishes. Moreover, the cutoff parameter $\Lambda>k$ is needed to obtain a convergent integral and will turn out to have an additional advantage in Sec. V for the purpose of optimizing a separable approximation. The relation between the T and τ^Λ matrices is easily found by subtracting and adding

$$V(p,k)T(k,p',E)I_\Lambda(E)\equiv V(p,k)T(k,p',E)\int_0^\Lambda dp''\frac{(p'')^{n-1}}{E^+-(p'')^2} \tag{5}$$

to the right-hand side of the Lippmann-Schwinger equation (1), which leads to

$$T(p,p',E)=V(p,p')+V(p,k)I_\Lambda(E)T(k,p',E)+\int_0^\infty dp''\frac{(p'')^{n-1}}{E-(p'')^2}[V(p,p'')T(p'',p')-\Theta(\Lambda-p'')V(p,k)T(k,p',E]\ .$$

This equation for the T matrix is identical to that satisfied by

$$\tau^\Lambda(p,p',E)+\tau^\Lambda(p,k,E)I_\Lambda(E)T(k,p',E)\ ,$$

which can be obtained by using Eq. (4) once with p' replaced by k and once with p' itself. We thus find the relation

$$T(p,p',E)=\tau^\Lambda(p,p',E)+\tau^\Lambda(p,k,E)I_\Lambda(E)T(k,p',E)\ . \tag{6}$$

From the right-hand side we can eliminate $T(k,p',E)$ by applying the same equation for the special choice $p=k$. The result of the manipulations is

$$T(p,p',E)=\tau^\Lambda(p,p',E)-\frac{\tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)}{\tau^\Lambda(k,k,E)}+\frac{\tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)}{[\tau^\Lambda(k,k,E)]^2}\times\frac{1}{[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)}\ . \tag{7}$$

Note that the T matrix is complex only via the function $I_\Lambda(E)$.

To see that the right-hand side of Eq. (7) is indeed independent of the cutoff parameter Λ, we rewrite the defining equation for $\tau^\Lambda(p,p',E)$ as

$$\tau^\Lambda(p,p',E)=V(p,p')+V(p,k)\tau^\Lambda(k,p',E)[I_{\Lambda'}(E)-I_\Lambda(E)]+\int_0^\infty dp''\frac{(p'')^{n-1}}{E-(p'')^2}[V(p,p'')\tau^\Lambda(p'',p',E)-\Theta(\Lambda'-p'')V(p,k)\tau^\Lambda(k,p',E)]\ , \tag{8}$$

and, similarly to the derivation of Eq. (6), we obtain a relation between the τ matrices with different cutoffs

$$\tau^\Lambda(p,p',E)=\tau^{\Lambda'}(p,p',E)+\tau^{\Lambda'}(p,k,E)\tau^\Lambda(k,p',E)\times[I_{\Lambda'}(E)-I_\Lambda(E)]\ . \tag{9}$$

This result implies the Λ independence of the expressions

$$\tau^\Lambda(p,p',E)-\tau^\Lambda(p,k,E)\tau^\Lambda(k,p',E)/\tau^\Lambda(k,k,E)\ ,$$

$$\tau^\Lambda(p,k,E)/\tau^\Lambda(k,k,E)\ ,$$

$$[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)\ .$$

Hence we have also proven the Λ independence of Eq. (7).

In connection with effective-range theory it is of interest to note that we expect $\tau_l^{\Lambda}(p,p',E)$ to be well behaved as a function of its arguments and to possess an expansion in p,p', and E close to $p=p'=E=0$, with only even (odd) powers of p and p', if l is even (odd). We are led to this because the integral equation for the τ matrix is nonsingular and the interaction $V_l(p,p')$ has a similar Taylor expansion around $p=p'=0$. For a rigorous proof of this conjecture in the most important case of two dimensions we refer to the Appendix, but in addition our numerical results presented in Sec. III confirm the expectations mentioned. Together with Eq. (7) this property indicates that the singular energy dependence of the T matrix in even dimensions is given by the function $I_{\Lambda}(E)$, which can be calculated analytically. In two dimensions this leads to a logarithmic behavior of various kinds of scattering quantities, such as the phase shift and the wave function itself.

Finally, we note that the connection (7) between the T and τ matrices reduces to the single expression

$$T(k,k,E)=\frac{1}{[1/\tau^{\Lambda}(k,k,E)]-I_{\Lambda}(E)} \tag{10}$$

for the on-shell T matrix. Comparing with the more familiar expression for $T(k,k,E)$ in terms of the phase shift for n-dimensional scattering, i.e.,

$$T(k,k,E)=\frac{1}{\frac{\pi i k^{n-1}}{2}-\frac{\pi k^{n-2}}{2}\cot\delta(k)}\ , \tag{11}$$

following from the relation

$$S(k,k,E)=1-\pi i k^{n-2}T(k,k,E)$$

between the S and T matrix elements, we are able to relate $\cot\delta(k)$ to the smoothly behaving τ matrix and the simple function $I_{\Lambda}(E)$. In Sec. III we will study this relation for two-dimensional scattering to derive the effective-range formula of Ref. 4.

III. LOW-ENERGY SCATTERING: ON-SHELL T MATRIX

We now apply the formalism discussed in Sec. II to low-energy scattering. To this end we calculate the function $I_{\Lambda}(E)$ to be

$$I_{\Lambda}(E)=-\frac{\pi i k^{n-2}}{2}-\frac{\Lambda^{n-2}}{n-2}-k^2\frac{\Lambda^{n-4}}{n-4}+\cdots+\cdots-\begin{cases}\dfrac{k^{n-2}}{2}\ln\left[\dfrac{\Lambda-k}{\Lambda+k}\right], & n=\text{odd}\\ \dfrac{k^{n-2}}{2}\ln\left[\dfrac{\Lambda^2-k^2}{k^2}\right], & n=\text{even}\end{cases} \tag{12}$$

where the last term included before the curly bracket is $-k^{n-3}\Lambda$ ($n=$odd) or $-k^{n-4}\Lambda^2$ ($n=$even). For odd dimensions this yields an analytical behavior near $k=0$, with

$$\ln\left[\frac{\Lambda-K}{\Lambda+k}\right]=-2\frac{k}{\Lambda}-\frac{2}{3}\frac{k^3}{\Lambda^3}+\cdots\ ,$$

while for even dimensions a logarithmic dependence results,

$$\ln\left[\frac{\Lambda^2-k^2}{k^2}\right]=-2\ln\left[\frac{k}{\Lambda}\right]-\frac{k^2}{\Lambda^2}-\frac{1}{2}\frac{k^4}{\Lambda^4}+\cdots\ .$$

Restricting ourselves to the lowest partial wave, we also expand $1/\tau^{\Lambda}(k,k,E)$ in k,

$$1/\tau^{\Lambda}(k,k,E)=a_0(\Lambda)+a_2(\Lambda)k^2+a_4(\Lambda)k^4+\cdots\ .$$

Equation (10) then leads to

$$1/T(k,k,E)=\frac{\pi i k^{n-2}}{2}+c_0+c_2k^2+\cdots+\cdots+\begin{cases}c_{n-1}k^{n-1}+\cdots, & n=\text{odd}\\ k^{n-2}\ln(c_{n-1}k)+c_nk^n+\cdots, & n=\text{even}\end{cases} \tag{13}$$

where the last term before the curly bracket is $c_{n-3}k^{n-3}$ ($n=$odd) or $c_{n-4}k^{n-4}$ ($n=$even). This agrees completely with the k dependence of $\cot\delta(k)$ found in Refs. 4 and 6. For $n=2$, in particular, Eq. (13) may be cast into the form

$$1/T(k,k,E)=\frac{\pi i}{2}-\gamma-\ln(ka/2)-\tfrac{1}{4}r_e^2k^2+\cdots\ , \tag{14}$$

with a the scattering length, r_e the effective range, and $\gamma=0.577\,215\,665\ldots$ Euler's constant. The values of a and r_e can be calculated from the on-shell τ matrix via the equations

$$\begin{aligned}&\ln(ka/2)=-\gamma-a_0(\Lambda)+\ln(k/\Lambda)\ ,\\ &r_e^2=-4a_2(\Lambda)+2/\Lambda^2\ .\end{aligned} \tag{15}$$

The numerical results to be presented here and in the following for $n=2$ are all associated with hydrogen b atoms (having both electron and proton spins down with respect to an external magnetic field) adsorbed on a

superfluid helium surface, in which case the $2\frac{1}{2}$-dimensional model is commonly used to find the interaction potential of the H atoms.[7] This potential is shown in Fig. 1 and is calculated by assuming a Mantz-Edwards[8] interaction potential between the hydrogen atoms and the helium film. We find $a=2.4a_0$ and $r_e=13a_0$, in agreement with the values found by integrating the Schrödinger equation and examining[9] the phase shifts $\delta(k)$. We conclude that the τ method leads to a low-energy dependence of the on-shell T matrix that is in accordance with effective-range theory and can also be used to find accurate results for the expansion parameters.

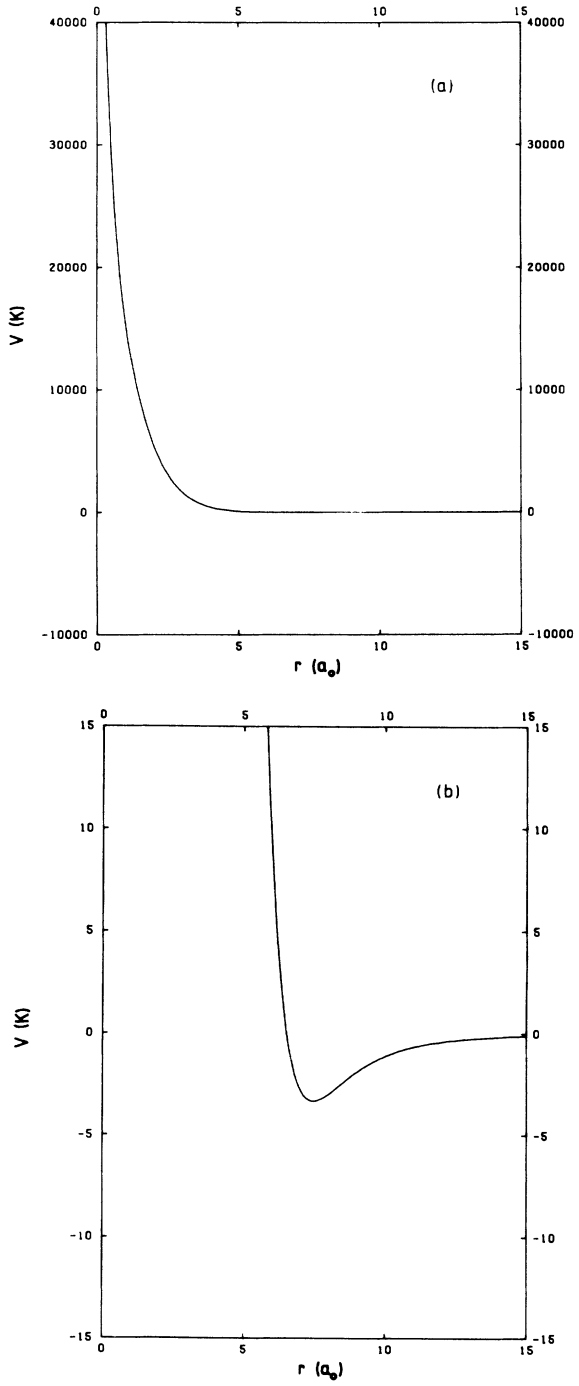

FIG. 1. (a) Potential ($2\frac{1}{2}$-dimensional model) among two hydrogen atoms in the $|b\rangle$ state and adsorbed on the superfluid helium surface. (b) Modified version with expanded vertical scale showing the shallow potential well due to the van der Waals interaction.

Also for all other dimensions Eq. (13) may be rewritten in the standard form of the low-energy expansion introduced in Ref. 4. It is of interest to recall that the expansion parameters occurring in this elegant standard form all have the dimension of length; each of them is defined as the radius of an equivalent hard sphere giving rise to this same specific term in the expansion. Adhikari *et al.* point out in a recent publication[10] that such a definition has the disadvantage in the special case of dimension $n=2$ that a varies between 0 and $+\infty$ when the potential is changed. This contrasts with $n=3$ where a is known to vary between $-\infty$ and $+\infty$, its sign reflecting the repulsiveness or attractiveness of the potential. The latter connection thus being lost for $n=2$, Adhikari *et al.* introduce an alternative scattering length parameter a_{AGL} related to a by $a_{\mathrm{AGL}}=-\ln(a/R_c)$, where R_c is the "range" of the potential. Apart from the vagueness implied by the arbitrariness in the choice of R_c, especially for interactions decaying slowly with r, it is of interest to note that the positive definiteness of a for $n=2$ is not as difficult to understand from the physical point of view as Ref. 10 suggests; $n=2$ is the only integer dimension for which the lowest partial wave $l=0$ has a negative centrifugal "barrier" extending over a long range.

Also the sign of the phase shift is an aspect in which $n=2$ differs. For any weak potential, whether predominantly attractive or repulsive, δ is always negative. Further smooth changes of the potential to arbitrary strength cause δ to change continuously, taking negative values only.

Another point of view illustrating the fundamental difference between two- and three-dimensional concepts of scattering length is the following. In varying the depth of a potential well $V(r)$ for $n=2$ a bound level enters the well precisely at the same potential depth where the phase shift vanishes. In three dimensions this happens at different well depths. This difference is naturally reflected in the different behavior of the corresponding quantity a; the two a values 0 and $-\infty$ for $n=3$ merge into a single value 0 when the dimension changes to 2. The quantity a_{AGL}, however, goes through zero for a well depth without a clear-cut physical significance.

IV. LOW-ENERGY SCATTERING: HALF-SHELL T MATRIX

After the treatment of the on-the-energy-shell quantities, we turn to the half-shell T matrix. As is well known the half-shell T matrix determines completely the two-body scattering wave function $\Psi_E^{(+)}(\mathbf{r})$. The latter in turn determines, for instance, the probability for relaxation induced by magnetic dipole interactions in adsorbed H↓, via its role as an initial or final state in a distorted-wave Born integral. With that application in mind we specialize in this section to $n=2$. In the restricted portion of

space contributing effectively to the Born integral and for the relevant low collision energies $\Psi_E^{(+)}(\mathbf{r})$ is to a very good approximation rotationally symmetric and given by

$$\Psi_E^{(+)}(\mathbf{r})=\frac{1}{\sqrt{2\pi}}\int_0^\infty dp\, pJ_0(pr) \times\left[\frac{\delta(p-k)}{p}+\frac{1}{E^+-p^2}T(p,k,E)\right], \tag{16}$$

in terms of the half-shell T matrix for the lowest partial wave.

Our purpose in this section is to describe the E dependence of $\Psi_E^{(+)}(\mathbf{r})$ by means of one overall factor, which offers a definite advantage in predicting the temperature dependence of the rate of decay of H↓ due to surface dipolar relaxation.

To that end we start from Eq. (16), subtract and add $I_\Lambda(E)J_0(kr)T(k,k,E)$ and express the half-shell T matrix in τ-matrix elements by means of

$$T(p,k,E)=\frac{\tau^\Lambda(p,k,E)}{\tau^\Lambda(k,k,E)}\frac{1}{[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)}. \tag{17}$$

The result is

$$\Psi_E^{(+)}(\mathbf{r})=\frac{1}{\sqrt{2\pi}}\frac{1}{[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)}\left[\frac{J_0(kr)}{\tau^\Lambda(k,k,E)}+\int_0^\infty dp\frac{p}{E-p^2}\left[\frac{\tau^\Lambda(p,k,E)}{\tau^\Lambda(k,k,E)}J_0(pr)-\Theta(\Lambda-p)J_0(kr)\right]\right]. \tag{18}$$

We then take the limit $E,k\to 0$ in the expression between square brackets, which is possible because it is a smooth function of these variables. (See Sec. II.) Hence in the domain $E\ll 1/r_0^2$ (for radii $r<r_0$ $V(r)$ is significantly different from zero) and $r\ll 1/\sqrt{E}$ the wave function is well described by

$$\Psi_E^{(+)}(\mathbf{r})=\frac{1}{[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)}\frac{\psi(r)}{\sqrt{2\pi}}, \tag{19}$$

in which the energy-independent function $\psi(r)$ is given by

$$\psi(r)=\frac{1}{\tau^\Lambda(0,0,0)}-\int_0^\infty\frac{dp}{p}\left[\frac{\tau^\Lambda(p,0,0)}{\tau^\Lambda(0,0,0)}J_0(pr)-\Theta(\Lambda-p)\right]. \tag{20}$$

In Fig. 2 the function $\psi(r)$ in the case of two colliding b atoms is presented. Equation (19) is in agreement with a result obtained earlier,[9] i.e., for small E the energy dependence is given by a simple factor

$$[\pi i/2-\ln(ka/2)-\gamma+O(k^2)]^{-1}.$$

The explicit expression (20) for $\psi(r)$ is an extension with respect to the $\ln(r/a)$ dependence outside the range of the interaction ($r>r_0$), which was found in Ref. 9.

As mentioned before, the E dependence (19) of the two-body wave function may be used to calculate the temperature dependence of magnetic dipole relaxation rates in adsorbed H↓. Suppose that the energy released in the reaction is large. In that case the E dependence of the final state may be neglected at the low temperature considered. Then the temperature behavior of these two-body decay rates is governed by the factor

$$C_s(T)=\left\langle\left|\frac{1}{[1/\tau^\Lambda(k,k,E)]-I_\Lambda(E)}\right|^2\right\rangle_{\rm th}=\left\langle\frac{1}{\pi^2/4+[\ln(ka/2)+\gamma+O(k^2)]^2}\right\rangle_{\rm th}, \tag{21}$$

in which the thermal average is over the relative energy E of the colliding particles. If, on the contrary, the amount of energy released is small, such as for the process $bb\to ab$, the $l=0\to l=0$ contribution (usually denoted by $m=0\to m=0$) to the rate dominates and the final-state wave function also has a significant logarithmic energy dependence. Therefore the thermal average in Eq. (21) should be replaced by one over the product of two factors, both for the initial and final channels, to obtain more accurate results. Again this agrees with the conclusions of Verhaar *et al.*[9]

Another application is the recombination of three $|b\rangle$-state hydrogen atoms adsorbed on the helium surface. In analogy to two-body scattering we can show that the exact symmetrical initial state $\Psi_E^{(+)}(\mathbf{r},\mathbf{R})$ takes the form

$$\Psi_E^{(+)}(\mathbf{r}_1,\mathbf{R}_1)=\sum_{i=1}^{3}\frac{\chi(\mathbf{r}_1,\mathbf{R}_1;\mathbf{p}_i,\mathbf{q}_i)}{[1/\tau^\Lambda(p_i,p_i,p_i^2)]-I_\Lambda(p_i^2)}, \tag{22}$$

where $\{\mathbf{p}_i,\mathbf{q}_i\}$ are the Jacobi momenta of the incoming

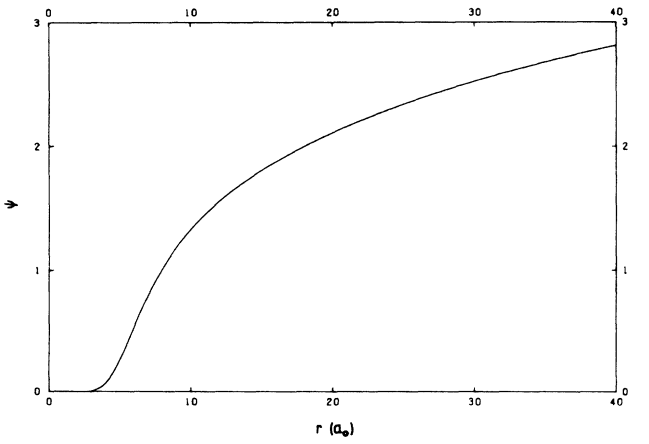

FIG. 2. The energy-independent part $\psi(r)$ of the scattering wave function of two b atoms at low energies [Eqs. (19) and (20)].

particles obeying the on-shell condition $E=p_i^2+3q_i^2/4$ and $\{r_1,\mathbf{R}_1\}$ stands for one of the three particular choices of Jacobi coordinates.[5] Unfortunately the precise behavior of $\chi(\mathbf{r},\mathbf{R};\mathbf{p}_i,\mathbf{q}_i)$ as a function of $\mathbf{p}_i$ and $\mathbf{q}_i$ is difficult to analyze, because the kernel of the Faddeev equations contains singularities due to the free propagator

$$1/(E^+-p^2-3q^2/4)$$

that are not damped out by phase-space factors in the limit $E\to 0$, in contrast with the three-dimensional situation.[3] Furthermore, the T matrix with its logarithmic energy dependence is also involved in the kernel and may induce a strong $\mathbf{p}_i$ and $\mathbf{q}_i$ dependence. In view of these difficulties, it does not seem possible at present to make general statements concerning the properties of χ for small $\mathbf{p}_i$ and $\mathbf{q}_i$ on the basis of the Faddeev formalism.

However, such statements are possible in the context of a simple Jastrow-type ansatz for $\Psi_E^{(+)}(\mathbf{r}_1,\mathbf{R}_1)$, which has proved to be excellent for $E=0$ in three dimensions.[11] Including also the center-of-mass wave function $\exp(i\mathbf{K}\cdot\mathbf{R})$ and denoting the position and momentum of particle j by $\mathbf{x}_j$ and $\mathbf{k}_j$, respectively, it reads

$$e^{i\mathbf{K}\cdot\mathbf{R}}\Psi_E^{(+)}(\mathbf{r}_1,\mathbf{R}_1)=\sum_{\mathcal{P}}\mathcal{P}e^{i\mathbf{k}_1\cdot\mathbf{x}_1}e^{i\mathbf{k}_2\cdot\mathbf{x}_2}e^{i\mathbf{k}_3\cdot\mathbf{x}_3}\times F_{\mathbf{p}_1}(\mathbf{r}_1)F_{\mathbf{p}_2}(\mathbf{r}_2)F_{\mathbf{p}_3}(\mathbf{r}_3)\ , \tag{23}$$

where the summation is over all possible permutations of the three particles. Note that the variables $\mathbf{r}_i$ and $\mathbf{p}_i$ in Eq. (23), contrary to $\mathbf{x}_i$ and $\mathbf{k}_i$, are numbered according to the spectator-index notation. The Jastrow factors $F_{\mathbf{p}}(\mathbf{r})$ tend to 1 for large separations and depend on the asymptotic relative momenta among the particles. They are of such a form that the $\mathbf{r}_i$ part of $\Psi_E^{(+)}$, i.e.,

$$e^{i\mathbf{p}_i\cdot\mathbf{r}_i}F_{\mathbf{p}_i}(\mathbf{r}_i)\equiv G_{\mathbf{p}_i}(\mathbf{r}_i)$$

is identical to a two-body scattering state. Applying this same idea in two dimensions we have [cf. Eq. (19)]

$$G_{\mathbf{p}}(\mathbf{r})=\frac{1}{[1/\tau^{\Lambda}(p,p,p^2)]-I_{\Lambda}(p^2)}\frac{\psi(r)}{\sqrt{2\pi}}\ . \tag{24}$$

Thus the wave function (23) becomes a product of three G functions multiplied by an exponential. In the low-temperature limit the latter can be replaced by 1, the dominant energy dependence being contained in the product

$$\prod_{i=1}^{3}\frac{1}{[1/\tau^{\Lambda}(p_i,p_i,p_i^2)]-I_{\Lambda}(p_i^2)}\ .$$

The behavior at low temperatures of, for instance, a three-body recombination decay rate is therefore given by a Boltzmann average of this quantity, which can be evaluated readily without detailed knowledge of the wave function $\Psi_E^{(+)}(\mathbf{r}_1,\mathbf{R}_1)$.

V. SEPARABLE APPROXIMATION TO THE T MATRIX

In this section we will only consider three dimensions, although the discussions can immediately be generalized to arbitrary dimension. In the context of three-body calculations it is favorable to dispose of separable expressions for the two-body T matrix. As is well known the Faddeev equations then reduce to a two-body problem. Our aim is to find such a separable approximation by neglecting the $\tau^{\Lambda}(p,p',E)$ term in the right-hand side of Eq. (7) that contains Λ as a free parameter. Minimizing this term, in a certain sense, as a function of Λ, one might hope that the separable part

$$T^{\mathrm{SA}}(p,p',E)=\frac{\tau^{\Lambda}(p,k,E)\tau^{\Lambda}(k,p',E)}{\tau^{\Lambda}(k,k,E)}\times\left[\frac{1}{1-I_{\Lambda}(E)\tau^{\Lambda}(k,k,E)}-1\right] \tag{25}$$

of the right-hand side constitutes an accurate approximation to the T matrix. Neglecting the -1 term one would be led to the separable expression obtained by using the Noyes-Kowalski method.[12] As is well known this term has unphysical poles whenever the on-shell T-matrix element $T(k,k,E)$, or equivalently $\tau^{\Lambda}(k,k,E)$, is equal to zero. In our case they are canceled by including the -1 term. Actually, it was already shown by Osborn[13] that such a pole could be avoided by adding an additional separable term to the approximation. Because his method involves the eigenfunctions of the Noyes-Kowalski kernel, it is rather laborious in contrast with our method, where only the τ^{Λ} matrix is needed. A second advantage of our approach is connected with the possibility of applying it to negative energies, which are unavoidable in three-body calculations; Eq. (25) can be used for both signs of E if we define for example $k^2=|E|$. Actually, if $E<0$ any k can be used, because in this case the integrant of Eq. (4) contains no singularities. We thus do not need to solve integral equations as in the Noyes-Kowalski method, where the V matrix for complex momenta is required with all associated complications in the case of long-range potentials (like the van der Waals interaction decaying as $1/r^6$).

It is also possible to find a connection with the W matrix of Bartnik *et al.*[14] The W matrix too has the important disadvantage that it does not contain a free parameter, making it impossible to optimize the separable approximation. One is therefore completely dependent on the specific features of the potential which should make the remaining nonseparable part sufficiently small.

One way to optimize our separable approximation would be by minimizing the norm squared of the neglected τ term,

$$\|\tau\|^2=\int d\mu(p)\int d\mu(p')\,\tau^2(p,p',E)\equiv(\tau,\tau) \tag{26}$$

using some measure $\mu(p)$ to evaluate the integrals involved. For example, the measure $\mu(p)=p^n/n$ results in the usual Hilbert-Schmidt norm, since the τ matrix is real and symmetric in the momentum variables. Actually, the choice of $\mu(p)$ is a second degree of freedom in addition to the value of Λ, to optimize the separable approximation; it can be used to emphasize specific regions of the (p,p') plane where the approximation should be accurate. To find an algorithm for actual calculations that accomplishes the minimalization, we recall that the matrices

$$A(p,p',E)=\frac{\tau^{\Lambda}(p,k,E)\tau^{\Lambda}(k,p',E)}{[\tau^{\Lambda}(k,k,E)]^2},$$
$$B(p,p',E)=\tau^{\Lambda}(p,p',E)-A(p,p',E)\tau^{\Lambda}(k,k,E) \quad (27)$$

are independent of Λ. Expressing $\tau^{\Lambda}(p,p',E)$ in terms of $A(p,p',E)$, $B(p,p',E)$, and the matrix element $\tau^{\Lambda}(k,k,E)$, the condition $\partial\|\tau^{\Lambda}\|^2/\partial\Lambda=0$ amounts to

$$\tau^{\Lambda'}(k,k,E)=-\frac{(A(E),B(E))}{(A(E),A(E))}, \quad (28)$$

where we denote the optimal choice of the cutoff parameter by Λ'.

Summarizing, the algorithm runs as follows.

(1) Choose a $\Lambda > k$ and calculate $\tau^{\Lambda}(p,p',E)$.

(2) Determine the matrices $A(p,p',E)$ and $B(p,p',E)$, which are independent of Λ.

(3) Find the optimal on-shell matrix element $\tau^{\Lambda'}(k,k,E)$ determined by Eq. (28).

(4) Use the matrices A and B to obtain $\tau^{\Lambda'}(p,p',E)$ and Eq. (25) to find the optimal separable approximation.

As an example of this procedure we consider nucleon-nucleon scattering using the Malfliet-Tjon III potential.[15] We use the convenient measure $\mu(p)=\ln(p)$ to stress small momenta where the T matrix is large. In Fig. 3 we present the V matrix, the exact T matrix at an energy of 1 MeV, our optimized separable approximation T^{SA} and

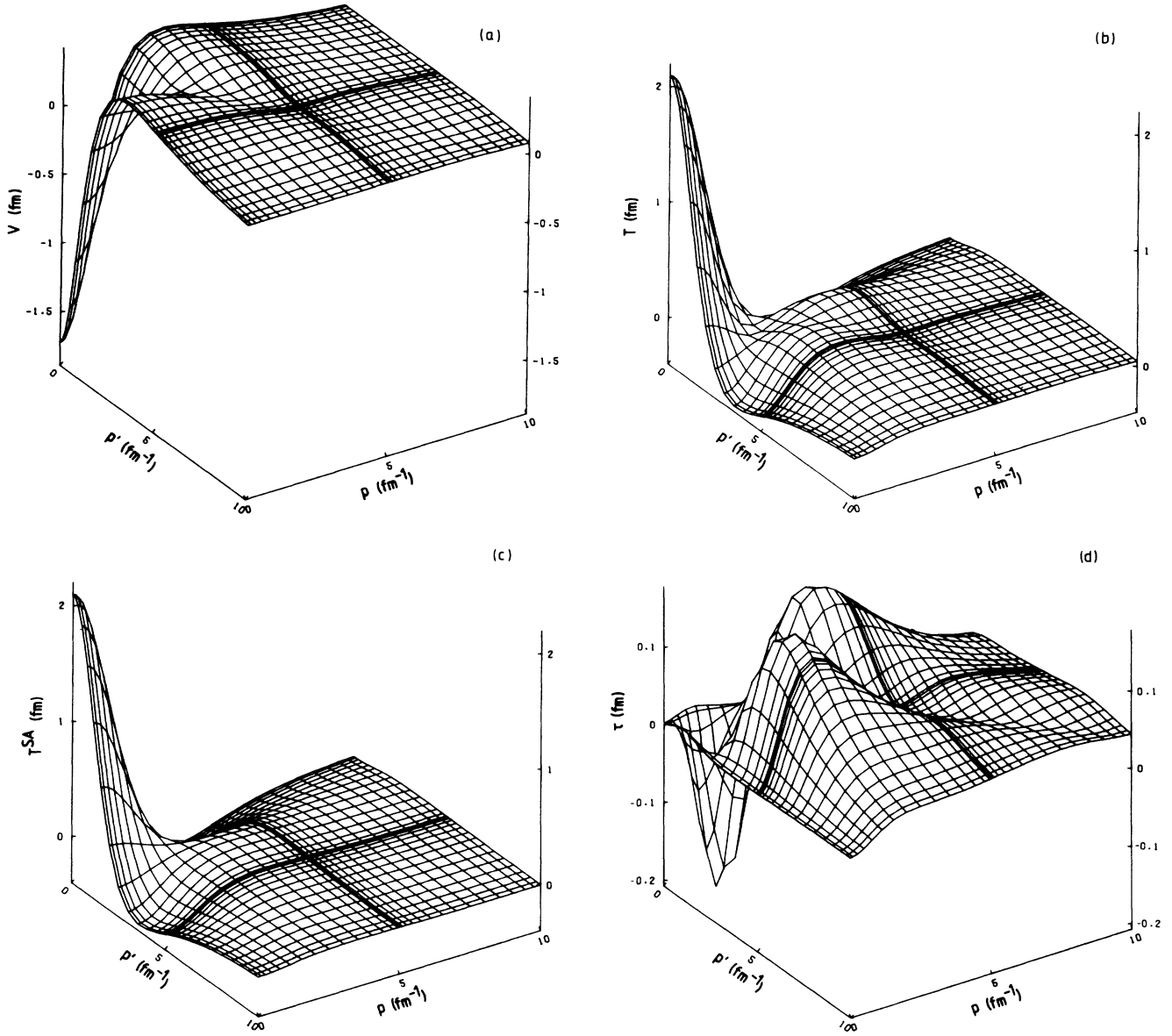

FIG. 3. Illustration of the accuracy of the separable approximation T^{SA} in the case of a Malfliet-Tjon III potential and a total angular momentum $l=0$. (a) Potential surface $V(p,p')$. (b) Exact T matrix at an energy of 1 MeV. (c) Separable approximation T^{SA} obtained by using the measure $\mu(p)=\ln(p)$ in the optimalization procedure and (d) the $\tau^{\Lambda'}$ matrix representing the difference between T and T^{SA}.

$\tau^{\Lambda'}$, i.e., the difference between T and T^{SA}. Apparently, the latter is relatively small in the part of the (p,p') plane where the T matrix is large. Furthermore, we note that in this way the unphysical poles in the τ^{Λ} matrix, which are introduced because Λ is finite, are always avoided because the norm $\|\tau^{\Lambda}(E)\|$ would else be infinite.

Finally, we would like to point to the huge amount of freedom available to improve in particular on the last comparison by extending the τ method in a similar way as proposed by Adhikari;[16] the function $\Theta(\Lambda-p')$ in Eq. (4) defining τ^{Λ} can in principle be replaced by any function with the value 1 for $p'=k$ without invalidating the method. Note, however, that the approaches still differ. Our proposal leads to an explicit energy dependence of all scattering observables, without resorting to Jost functions which have to be evaluated numerically. It would be interesting to find out to what extent further improvements of the separable approximation may be achieved in this way.

VI. CONCLUSIONS

Summarizing, we recall that the nonsingular equation for the τ matrix is numerically easy to handle and has a solution that is well behaved close to the energy $E=0$. Due to this feature the τ matrix can be used to formulate an effective-range theory in arbitrary dimension and to find the (small-E) energy dependence of all kinds of important scattering quantities, such as the wave function and the phase shift.

In the context of three-body calculations, the method introduced may be useful for analyzing the singularities involved in the kernel of the Faddeev equation for three asymptotically free particles and to find a satisfactory separable approximation to the T matrix that avoids unphysical poles and is applicable to negative energies.

ACKNOWLEDGMENTS

We thank W. Glöckle and W. Plessas for useful and stimulating discussions. This research is supported by the Nederlandse Organisatie voor Zuiver-Wetenschappelijk Ondezoek (ZWO) (Werkgroep Gebruik Supercomputers).

APPENDIX

In this appendix we study the behavior of the τ^{Λ} matrix as a function of the momentum and energy variables in the special situation of $n=2$ and $l=0$, which is the most important case with respect to applications in the context of low-energy scattering. Moreover, we will prove that $\tau^{\Lambda}(p,p',E)$ and also its on- and half-shell counterparts are well-behaved functions of energy, with an asymptotic expansion for $E\downarrow 0$.

Studying the E dependence by means of Eq. (4) is not very convenient, because it is not an integral equation of the Fredholm type. To avoid this problem we introduce a new matrix $\rho^{\Lambda}(p,p',E)$, which is defined by

$$\rho^{\Lambda}(p,p',E)=V(p,p')+\int_0^{\infty}dp''\frac{p''}{E-(p'')^2}\left[V(p,p'')-\Theta(\Lambda-p'')\frac{V(p,k)V(k,p'')}{V(k,k)}\right]\rho^{\Lambda}(p'',p',E) \tag{A1}$$

and in terms of which $\tau^{\Lambda}(p,p',E)$ can be expressed as

$$\tau^{\Lambda}(p,p',E)=\rho^{\Lambda}(p,p',E)-\frac{\rho^{\Lambda}(p,k,E)\int_0^{\Lambda}dp''\frac{p''}{E-(p'')^2}[V(k,k)\rho^{\Lambda}(k,p',E)-V(k,p'')\rho^{\Lambda}(p'',p',E)]}{V(k,k)+\int_0^{\Lambda}dp''\frac{p''}{E-(p'')^2}[V(k,k)\rho^{\Lambda}(k,k,E)-V(k,p'')\rho^{\Lambda}(p''k,E)]} . \tag{A2}$$

Due to the last relation, which involves only proper integrals with regular integrand, τ^{Λ} is found to be a well-behaved function of energy with an asymptotic expansion for $E\downarrow 0$, if the same is true for the dependence of the ρ^{Λ} matrix on all its arguments. We start by considering the explicit energy dependence and return to the problem associated with the momentum variables later on.

We consider Eq. (A1) as a problem in the Hilbert space $L_2(\mathbb{R}^+)$ of the p variable and rewrite it in an abstract notation,

$$|\rho^{\Lambda}(p',E)\rangle=|V(p')\rangle+K_{\Lambda}(E)|\rho^{\Lambda}(p',E)\rangle , \tag{A3}$$

where we explicitly show the special role of p' as a dummy variable, which plays no role in the integral equation itself. Note that the phase-space factor p'' in Eq. (A1) is included in $K_{\Lambda}(E)$.

Our proof is now based on the following theorem. If (i) $K_{\Lambda}(E)$ is bounded for $0\le E<\epsilon$; (ii) $[1-K_{\Lambda}(E)]^{-1}$ exists for $0\le E<\epsilon$, which means that 1 should not be in the spectrum of $K_{\Lambda}(E)$; and (iii) $K_{\Lambda}(E)$ has an asymptotic expansion,

$$K_{\Lambda}(E)=\sum_{i=0}^{m}K_i^{\Lambda}E^i+R_{\Lambda}(E) ,$$
$$\lim_{E\downarrow 0}\|R_{\Lambda}(E)\|/E^m=0 , \tag{A4}$$

with bounded operators K_i^{Λ}, then Eq. (A3) has a solution in $L_2(\mathbb{R}^+)$ equal to $[1-K_{\Lambda}(E)]^{-1}|V(p')\rangle$ having an asymptotic expansion given by

$$|\rho^{\Lambda}(p',E)\rangle=\sum_{i=0}^{m}E^i|\rho_i^{\Lambda}(p')\rangle+|\sigma^{\Lambda}(p',E)\rangle ,$$
$$\lim_{E\downarrow 0}\|\,|\sigma^{\Lambda}(p',E)\rangle\|/E^m=0 . \tag{A5}$$

Here $\|O\|$ is the usual notation for the norm of the opera-

tor O. The theorem is easily proved by using the resolvent identity

$$[1-K_\Lambda(E)]^{-1}=(1-K_0^\Lambda)^{-1} +(1-K_0^\Lambda)^{-1}\left[\sum_{i=1}^{m} K_i^\Lambda E^i+R_\Lambda(E)\right] \times[1-K_\Lambda(E)]^{-1} \tag{A6}$$

and substituting it into

$$|\rho^\Lambda(p',E)\rangle=[1-K_\Lambda(E)]^{-1}\,|V(p')\rangle$$

to find the equation

$$|\rho^\Lambda(p',E)\rangle=(1-K_0^\Lambda)^{-1}\,|V(p')\rangle +(1-K_0^\Lambda)^{-1}\left[\sum_{i=0}^{m} K_i^\Lambda E^i+R_\Lambda(E)\right] \times|\rho^\Lambda(p',E)\rangle\ .$$

Iterating m times leads to an asymptotic expansion of the form given by Eq. (A5), because all vectors and operators involved are bounded due to the assumptions of the theorem.

Furthermore, if $K_\Lambda(E)$ is bounded, if $|V(p')\rangle$ has an asymptotic expansion that is schematically denoted by

$$|V(p')\rangle \underset{p'\downarrow 0}{\sim} \sum_{i=1}^{m}(p')^{2i}\,|V_{2i}\rangle+o((p')^{2m})\ ,$$

and if all the vectors $|V_{2i}\rangle$ are elements of $L_2(\mathbb{R}^+)$, then we find by substituting this expansion into the formal solution of Eq. (A3) that $|\rho^\Lambda(p',E)\rangle$ has a similar asymptotic expansion in p'^2 for $p'\downarrow 0$.

To complete the discussion about the energy and momentum dependence of $\rho^\Lambda(p,p',E)$, we will now show that for a realistic potential $V(r)$ the requirements of the above theorems are fulfilled. The transformation to momentum space of the potential ($n=2$ and $l=0$) is given by

$$\tilde{V}(Q)=\int_0^\infty dr\, rV(r)J_0(Qr)\ ,$$
$$V(p,p')=\frac{1}{2\pi}\int_0^{2\pi}d\phi\,\tilde{V}[(p^2+p'^2-2pp'\cos\phi)^{1/2}]\ . \tag{A7}$$

The lemma of Riemann-Lebesgue[17] states that $\tilde{V}(Q)\sim o(1/\sqrt{Q})$ as $Q\to\infty$, if $V(r)$ is continuous and the integral

$$\int_0^\infty dr\sqrt{r}\,V(r)$$

is absolutely convergent. In particular, the potential of the $2\frac{1}{2}$-dimensional model (Fig. 1) behaving as $-\ln(r)$ for small r and r^{-6} for large r, obeys these conditions. Because $\tilde{V}(Q)$ exists for every $Q\geq 0$ we can formulate the following upper bound with a proper positive value for μ:

$$|\tilde{V}(Q)|\leq\frac{C}{(1+Q)^{1/2+\mu}}\ , \tag{A8}$$

and therefore also

$$|V(p,p')|\leq\frac{C}{(1+|p-p'|)^{1/2+\mu}}\ , \tag{A9}$$

which is sufficient to show that $|V(p')\rangle$ is indeed for all p' an element of the Hilbert space $L_2(\mathbb{R}^+)$. To show that the kernel is bounded we look at the Hilbert-Schmidt norm $\|K_\Lambda(E)\|_{\rm HS}$. As in the treatment of Osborn[13] we write the norm squared as the sum of terms $L_\Lambda(E)$ and $M_\Lambda(E)$,

$$L_\Lambda(E)=\int_0^\infty dp\int_{k+1}^\infty dp'\,|K_\Lambda(p,p',E)|^2\ ,$$
$$M_\Lambda(E)=\int_0^\infty dp\int_0^{k+1}dp'\,|K_\Lambda(p,p',E)|^2\ .$$

Furthermore, because of our interest in low-energy scattering we assume for simplicity $0\leq E<\epsilon<1$.

Using Eq. (A9) we find that $L_\Lambda(E)<\infty$, but to analyze $M_\Lambda(E)$ we need the smoothness condition

$$|V(p+\Delta p,p')-V(p,p')|\leq\frac{C'|\Delta p|}{(1+|p-p'|)^{3/2+\mu}}\ , \tag{A10}$$

because of the pole involved in the integration over p'. This condition is easily derived by applying the mean value theorem and using

$$\left|\frac{\partial V(p,p')}{\partial p}\right|\leq\frac{C'}{(1+|p-p'|)^{3/2+\mu}}\ , \tag{A11}$$

for $V(r)$ obeying the requirements of the Riemann-Lebesgue theorem. On the basis of Eq. (A10) we can now show that $M_\Lambda(E)$ is finite and therefore that the operator $K_\Lambda(E)$ is bounded.

Finally, we need to consider the operators

$$K_i^\Lambda\equiv\frac{1}{i!}\frac{d^iK_\Lambda(E)}{dE^i}\bigg|_{E=0}$$

and the vectors

$$|V_i\rangle\equiv\frac{1}{i!}\frac{d^i|V(p')\rangle}{dp'^i}\bigg|_{p'=0}\ .$$

The problem for $K_0^\Lambda=K_\Lambda(0)$ and $|V_0\rangle=|V(0)\rangle$ has already been solved, but in the case of $i>0$ the partial derivatives $\partial^iV(p,p')/\partial p'^i|_{p'=0}$ come into play. They have the upper bound

$$\left|\frac{\partial^iV(p,p')}{\partial p'^i}\bigg|_{p'=0}\right|\leq\frac{C_i}{(1+p)^{i+1/2+\mu}}\ , \tag{A12}$$

with $C_i=0$ for odd i. This leads to the conclusion that $K_i^\Lambda(p,p')$ decreases for large p and p' at least as fast as $K_0^\Lambda(p,p')$. Because of this and the fact that $K_i^\Lambda(p,p')$ contains no poles its Hilbert-Schmidt norm exists, so that the operator K_i^Λ is bounded. In addition, Eq. (A12) is sufficient to prove that also the norm of $|V_i\rangle$ is finite.

Summarizing, we have shown that $\rho^{\Lambda}(p,p',E)$ and therefore $\tau^{\Lambda}(p,p',E)$ is a well-behaved function of energy and momentum, with an asymptotic expansion for $E \downarrow 0$. This has also been shown to be true for the on- and half-shell τ-matrix elements. Our conclusion, formulated in Sec. II, that the singular energy dependence of the T matrix is concentrated in the function $I_{\Lambda}(E)$ is therefore justified.

[1]I. F. Silvera and J. T. M. Walraven, Phys. Rev. Lett. **44**, 164 (1980).

[2]R. Sprik, J. T. M. Walraven, G. H. van Yperen, and I. F. Silvera, Phys. Rev. B **34**, 6172 (1986); D. A. Bell, H. F. Hess, G. P. Kochanski, S. Buchman, L. Pollack, Y. M. Xiao, D. Kleppner, and T. J. Greytak, *ibid.* **34**, 7670 (1986); T. Tommila, S. Jaakkola, M. Krusius, I. Krylov, and E. Tjukanov, Phys. Rev. Lett. **56**, 941 (1986).

[3]L. P. H. de Goey, T. H. M. v. d. Berg, N. Mulders, H. T. C. Stoof, B. J. Verhaar, and W. Glöckle, Phys. Rev. B **34**, 6183 (1986).

[4]B. J. Verhaar, L. P. H. de Goey, J. P. H. W. van den Eijnde, and E. J. D. Vredenbregt, Phys. Rev. A **32**, 1424 (1985).

[5]W. Glöckle, *The Quantum Mechanical Few-Body Problem* (Springer-Verlag, Berlin, 1983), and references therein.

[6]D. Bollé and F. Gesztesy, Phys. Rev. Lett. **52**, 1469 (1984); Phys. Rev. A **30**, 1279 (1984).

[7]R. M. C. Ahn, J. P. H. W. van den Eijnde, C. J. Reuver, B. J. Verhaar, and I. F. Silvera, Phys. Rev. B **26**, 452 (1982).

[8]I. B. Mantz and D. O. Edwards, Phys. Rev. B **20**, 4518 (1979).

[9]B. J. Verhaar, J. P. H. W. van den Eijnde, M. A. J. Voermans, and M. M. J. Schaffrath, J. Phys. A **17**, 595 (1984).

[10]S. K. Adhikari, W. G. Gibson, and T. K. Lim, J. Chem. Phys. **85**, 5580 (1986).

[11]L. P. H. de Goey, H. T. C. Stoof, B. J. Verhaar, and W. Glöckle, Phys. Rev. B (to be published).

[12]K. L. Kowalski, Phys. Rev. Lett. **15**, 798 (1965); H. P. Noyes, *ibid.* **15**, 538 (1965).

[13]T. A. Osborn, Nucl. Phys. **A138**, 305 (1969).

[14]E. A. Bartnik, H. Haberzetl, and W. Sandhas, Phys. Rev. C **34**, 1520 (1986).

[15]R. A. Malfliet and J. A. Tjon, Nucl. Phys. **A127**, 161 (1969); G. L. Payne, W. H. Klink, W. N. Polyzou, J. L. Friar, and B. F. Gibson, Phys. Rev. C **30**, 1132 (1984).

[16]S. K. Adhikari, Phys. Rev. C **19**, 1729 (1979).

[17]G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1962), and references therein.