Off-shell *T* **matrices in one, two, and three dimensions**

S. A. Morgan, M. D. Lee, and K. Burnett

Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

(Received 25 May 2001; published 15 January 2002)

We discuss the calculation of the off-shell *T* matrix in one, two, and three dimensions using both the Beliaev-Galitskii relation and the inhomogeneous Schrödinger equation. The off-shell *T* matrix depends, in general, on three quantities: the incoming and outgoing momenta and the energy of the collision, all of which can be chosen independently. We give a simple proof of the fact that for low-momentum scattering the *T* matrix depends only on the energy of the collision. Using the inhomogeneous Schrödinger equation we derive analytical results for the fully off-shell *T* matrix in one, two, and three dimensions for hard-sphere central potentials. The usual form of the Beliaev-Galitskii relation is not quite correct for such potentials. We derive the appropriate correction term and show that it corresponds exactly to the contribution to the *T* matrix from the inhomogeneous term in the inhomogeneous Schrödinger equation.

DOI: 10.1103/PhysRevA.65.022706 PACS number(s): 03.65.Nk, 03.75.Fi

I. INTRODUCTION

The two-body *T* matrix provides a complete description of two-particle collisions and is, therefore, of fundamental importance in the theoretical description of dilute gases. In general, the *T* matrix depends on three quantities: the incoming and outgoing relative momenta of the atoms and the energy of the collision. For collisions in vacuum, only the on-shell *T* matrix is physically relevant. This corresponds to the case wherein the energy of the collision is the same as the asymptotic kinetic energy of the atoms before and after. In this paper, however, we are interested in the off-shell *T* matrix where the energy of the collision and the initial and final momenta can all be chosen independently. An example of a situation where off-shell *T* matrices are needed occurs in light-assisted collisions where the interaction with a laser beam changes the energy that is available to the colliding atoms $[1]$. The off-shell *T* matrix is also of crucial importance in the study of three-body collisions, where it is the fundamental input to the Fadeev equations $[2]$. Another example, of particular interest to the authors, occurs in the study of degenerate Bose gases, where particle collisions are described by a many-body *T* matrix that takes into account the effect of the medium (mean field) in which the collisions occur $[3-6]$. At low temperatures the many-body *T* matrix can be approximated by the off-shell two-body *T* matrix. This is of particular importance for the study of twodimensional systems, where the on-shell *T* matrix vanishes at zero momentum $[7]$. In this case the mean-field shift in the energy of the collisions is responsible for the finite interaction strength between particles in the lowest momentum states.

In this paper we present analytic results for the off-shell *T* matrix for hard-sphere central potentials in one, two, and three dimensions $(1D, 2D, 3D)$. We start in Sec. II with a brief review of the relevant scattering theory, leading to the inhomogeneous Schrödinger equation (ISE). The solutions of this equation, which satisfy appropriate asymptotic boundary conditions, can be used to obtain the off-shell *T* matrix. In Sec. III we describe the Beliaev-Galitskii (BG) relation, which provides an alternative means of calculating the offshell *T* matrix, using the half-on-shell *T* matrix as the input. The usual form of this relation does not treat hard-core potentials correctly, so we derive a modified form of the result that includes the appropriate correction term. In Sec. IV we give a simple proof of the fact that, in the limit of lowmomentum scattering, the *T* matrix depends only on the energy of the collision. This result is of some importance for the study of cold atoms as it means that particle interactions can be described by a contact potential. Sections V–VII are devoted to solving the ISE and obtaining analytical results for the off-shell *T* matrix in 1D, 2D, and 3D.

Although we have derived the correction that must be introduced into the BG relation to deal with hard-core potentials, an alternative approach is to use the usual form of the relation for a finite potential and then to take the infinite potential limit at the end. These calculations have been performed in 2D and 3D by Sheth, Chang, and Friedberg $[8]$, and in Sec. VII we present a similar calculation in 1D. The results obtained are consistent with the correction we have derived to the BG relation and also with the results from the ISE, which deals easily with hard-core potentials.

II. REVIEW OF SCATTERING THEORY

In this paper we are principally concerned with calculating the two-body *T* matrix. This is defined as a function of the complex variable *z* by the Lippmann-Schwinger equation $[9]$

$$
T(z) = V + VG_0(z)T(z) = V + VG(z)V,
$$
 (1)

where $G_0(z)$ and $G(z)$ are, respectively, the free and full Green's functions, defined by

$$
G_0(z) = \frac{1}{z - H_0}, \quad G(z) = \frac{1}{z - H}.
$$
 (2)

Here H_0 is the single particle Hamiltonian $(H_0 =$ $-\hbar^2\nabla^2/2\mu$, *H* is the full Hamiltonian for a pair of interacting atoms in the center-of-mass frame $(H = H_0 + V)$ and μ is the reduced mass. For the cases we are interested in, involving collisions of identical atoms of mass *m*, we have $\mu = m/2$.

We will denote the eigenstates of H_0 by $|\mathbf{k}\rangle$, so that H_0 **k** $>E_k$ **k** \rangle with $E_k = \hbar^2 k^2/2\mu$. The stationary scattering states will be denoted by $|\mathbf{k}+\rangle$. These are unbound eigenstates of *H* with energy E_k $[H|\mathbf{k}+\rangle=E_k|\mathbf{k}+\rangle]$, which at infinity have the form of an incoming plane wave of wave vector **k** and an outgoing scattered wave. Here and in the rest of this paper, wave functions are normalized according to $\langle \mathbf{k}' | \mathbf{k} \rangle = (2\pi)^D \delta(\mathbf{k}-\mathbf{k}')$ in *D* dimensions. This means that, although the *T* matrix has the dimensions of energy, its matrix elements have dimensions of $[E][L]^D$.

The two-body *T* matrix is important in scattering problems because its matrix elements $\langle \mathbf{k}' | T(z) | \mathbf{k} \rangle$ give the amplitude for scattering from state \bf{k} to \bf{k}' . For the case of two atoms colliding in a vacuum, only the on-shell matrix elements are physically relevant. These correspond to $k = k'$ and $z = E_k + i\delta$, where $k = |\mathbf{k}|$ and δ is a positive infinitesimal. In this paper, however, we are interested in the general off-shell *T* matrix for which **k**, k' , and *E* can all be chosen independently. This can be obtained by solving an inhomogeneous Schrödinger equation that can be derived directly from the Lippmann-Schwinger definition of the *T* matrix. Specializing to the case that $z = E + i \delta$, we can write Eq. (1) in the form

$$
\langle \mathbf{k'} | T(E) | \mathbf{k} \rangle = \langle \mathbf{k'} | V \left[1 + \frac{1}{E + i \delta - H} V \right] | \mathbf{k} \rangle = \langle \mathbf{k'} | V | \mathbf{k} + E \rangle,
$$
\n(3)

where the off-shell, outgoing, scattered wave $|\mathbf{k}+,\mathbf{E}\rangle$ is defined by

$$
|\mathbf{k} + E| = \left[1 + \frac{1}{E + i\,\delta - H}V\right] |\mathbf{k}\rangle.
$$
 (4)

In the position representation, Eq. (3) is

$$
\langle \mathbf{k'} | T(E) | \mathbf{k} \rangle = \int d^3 \mathbf{r} \, e^{-i\mathbf{k'} \cdot \mathbf{r}} V(r) \psi_+(\mathbf{r}, \mathbf{k}, E), \qquad (5)
$$

where $\psi_+(\mathbf{r}, \mathbf{k}, E) = \langle \mathbf{r} | \mathbf{k} + E \rangle$ and we have assumed that *V* is a local potential. The operator in square brackets in Eq. (4) is the Møller operator that acts on the initial wave to give the full scattered wave. The states $|\mathbf{k}+E\rangle$ are the off-shell generalization of the scattering states $|\mathbf{k}+\rangle$ introduced above, the relation between them being $|\mathbf{k}+\rangle=|\mathbf{k}+E=E_k\rangle$.

In the position representation, Eq. (4) becomes

$$
\psi_{+}(\mathbf{r}, \mathbf{k}, E) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^{3}\mathbf{r}' G_{0}^{+}(\mathbf{r}, \mathbf{r}', E) V(r') \psi_{+}(\mathbf{r}', \mathbf{k}, E). \tag{6}
$$

In 3D, the Green's function is given by the well-known expression $[10]$

$$
G_0^+(\mathbf{r}, \mathbf{r}', E) = \langle \mathbf{r} | \frac{1}{E - H_0 + i\delta} | \mathbf{r}' \rangle = -\frac{2\mu}{4\pi\hbar^2} \frac{e^{ik_E|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|},\tag{7}
$$

where $k_E = \sqrt{2\mu E/\hbar^2}$. In the asymptotic limit $r \rightarrow \infty$ we, therefore, have

$$
\psi_{+}(\mathbf{r}, \mathbf{k}, E) \xrightarrow{r \to \infty} e^{ikz} - \frac{2\mu}{4\pi\hbar^2} \frac{e^{+ik_{E}r}}{r} \langle k_{E}\hat{\mathbf{r}}|T(E)|\mathbf{k}\rangle,
$$
\n(8)

where we have used Eq. (5) and took the *z* axis in the direction of **k**.

Equation (8) shows that the half-on-shell *T* matrix $(k=k_E \neq k'$ or $k'=k_E \neq k$) describes the amplitude and angular distribution of the scattered wave, and is therefore proportional to the scattering amplitude (in 3D this is simply the coefficient of the outgoing spherical wave). For later convenience, we introduce an abbreviated notation for this quantity

$$
f(\mathbf{k}', \mathbf{k}) \equiv \langle \mathbf{k}' | T(E_k) | \mathbf{k} \rangle = \langle \mathbf{k}' | V | \mathbf{k} + \rangle, \tag{9}
$$

where \mathbf{k}' is any vector. The fully on-shell *T* matrix corresponds to the special case of this where $k' = k$. Equation (9) is proportional to the scattering amplitude in Eq. (8) because the *T* matrix is symmetric with respect to its momentum arguments $[11,12]$

$$
\langle \mathbf{k}' | T(E) | \mathbf{k} \rangle = \langle \mathbf{k} | T(E) | \mathbf{k}' \rangle. \tag{10}
$$

Equation (4) can also be used to obtain an inhomogeneous Schrödinger equation for $|\mathbf{k}+ \rangle$. Acting on both sides with $E + i\delta - H$ gives

$$
(E - H)|\mathbf{k} + E\rangle = (E - E_k)|\mathbf{k}\rangle, \tag{11}
$$

where we have used the fact that $H_0|\mathbf{k}\rangle = E_k|\mathbf{k}\rangle$. In the position representation this becomes

$$
[k_E^2 + \nabla^2 - U(\mathbf{r})] \psi_+(\mathbf{r}, \mathbf{k}, E) = (k_E^2 - k^2) e^{i\mathbf{k} \cdot \mathbf{r}}, \qquad (12)
$$

where $U(\mathbf{r})=2\mu V(\mathbf{r})/\hbar^2$. This equation must be solved subject to the boundary condition of Eq. (8) , and the off-shell T matrix can then be determined from Eq. (5) . Equation (12) has been used by Van Leeuwen and Reiner to study the *T* matrix in 3D for potentials consisting of chains of rectangular wells $[13]$. It can also be used as the basis of an efficient numerical algorithm for the calculation of the off-shell *T* matrix for more general potentials, as has been shown by Brumer and Shapiro $[14,15]$.

In Sec. V–VII, we will solve Eq. (12) and obtain the off-shell *T* matrix for hard-sphere central potentials in 1D, 2D, and 3D.

III. THE BELIAEV-GALITSKII RELATION

An important relation between off-shell and half-on-shell *T* matrix elements was derived by Beliaev and Galitskii $[16,17]$, and is often used as the basis of calculations of the off-shell *T* matrix. In this section we present a derivation of the Beliaev-Galitskii result. Our method follows that of Van Leeuwen and Reiner $[13]$ and includes an explicit formula for the correction to the usual form of the BG result, which must be included for infinite potentials. For hard-sphere potentials we show that this correction corresponds exactly to the contribution to the *T* matrix from the inhomogeneous term of the ISE.

We begin with the Lippmann-Schwinger definition of the *T* matrix for general complex *z* as given in Eq. (1) . This can be manipulated into the form

$$
G_0(z)T(z)G_0(z) = G(z) - G_0(z). \tag{13}
$$

Acting on the left with $\langle \mathbf{p}' |$ and on the right with $| \mathbf{p} \rangle$ gives

$$
\langle \mathbf{p'}|T(z)|\mathbf{p}\rangle = (z - E_{p'}) (z - E_p) \langle \mathbf{p'}|G(z) - G_0(z)|\mathbf{p}\rangle.
$$
\n(14)

We now write G in terms of the eigenstates of H as (see discussion at the end of this section)

$$
G(z) = \sum_{n} \frac{|n\rangle\langle n|}{z - E_n},
$$
\n(15)

where $H|n\rangle = E_n|n\rangle$. Substituting this into Eq. (14) and writing $z - E_p = (z - E_n) + (E_n - E_{p'})$ we obtain

$$
\langle \mathbf{p'} | T(z) | \mathbf{p} \rangle = \sum_{n} \left[\frac{(E_n - E_{p'}) (z - E_p) \langle \mathbf{p'} | n \rangle \langle n | \mathbf{p} \rangle}{z - E_n} \right]
$$

$$
+ (z - E_p) \sum_{n} \left[\langle \mathbf{p'} | n \rangle \langle n | \mathbf{p} \rangle - \langle \mathbf{p'} | \mathbf{p} \rangle \right]. \tag{16}
$$

For a finite potential, the second line of this expression would be zero due to the completeness of the states $\{|n\rangle\}.$ For a hard sphere potential, however, we have a modified completeness relation $\lceil 13 \rceil$

$$
\sum_{n} \langle \mathbf{r}' | n \rangle \langle n | \mathbf{r} \rangle = \delta(\mathbf{r} - \mathbf{r}'), \quad (|\mathbf{r}| \text{ and } |\mathbf{r}'| > a),
$$

= 0, (|\mathbf{r}| or |\mathbf{r}'| \le a). (17)

Using this in Eq. (16) gives the correction to the BG result for the hard-sphere potential

$$
\langle \mathbf{p'} | T_{\text{corr}}(z) | \mathbf{p} \rangle = - (z - E_p) \int_V d^D \mathbf{r} \, e^{i(\mathbf{p} - \mathbf{p'}) \cdot \mathbf{r}}, \qquad (18)
$$

where the integral is over the region of the potential *V*. In 3D, an equivalent result has been obtained previously by Van Leeuwen and Reiner $[13]$.

The first line of Eq. (16) can be manipulated into the standard form of the BG result by writing $z - E_p = (z - E_n)$ $+(E_n-E_p)$ and using $\langle \mathbf{p}'|(E_n-E_{p'})|n\rangle = \langle \mathbf{p}'|(H-H_0)|n\rangle$ $=\langle \mathbf{p}'|V|n\rangle$. If we also assume that *H* has only a continuous spectrum, then we can put $\Sigma_n \rightarrow \int d^D \mathbf{k}/(2\pi)^D$, $|n\rangle = |\mathbf{k}+\rangle$ and $E_n = E_k$ to obtain

$$
\langle \mathbf{p'} | T(z) | \mathbf{p} \rangle = \int \frac{d^D \mathbf{k}}{(2 \pi)^D} \Biggl[\langle \mathbf{p'} | V | \mathbf{k} + \rangle \langle \mathbf{k} + | \mathbf{p} \rangle + \frac{f(\mathbf{p'}, \mathbf{k}) f^*(\mathbf{p}, \mathbf{k})}{z - E_k} \Biggr]
$$

$$
- (z - E_p) \int_V d^D \mathbf{r} \, e^{i(\mathbf{p} - \mathbf{p'}) \cdot \mathbf{r}}, \qquad (19)
$$

where we also have used Eq. (9) [18]. Writing this out for $z_1 = E + i \delta$ and $z_2 = E_p + i \delta$ and subtracting gives

$$
\langle \mathbf{p'} | T(E) | \mathbf{p} \rangle = f(\mathbf{p'}, \mathbf{p}) - (E - E_p) \int_V d^D \mathbf{r} \ e^{i(\mathbf{p} - \mathbf{p'}) \cdot \mathbf{r}} + \int \frac{d^D \mathbf{k}}{(2 \pi)^D} f(\mathbf{p'}, \mathbf{k}) f^*(\mathbf{p}, \mathbf{k}) \left[\frac{1}{E - E_k + i \delta} - \frac{1}{E_p - E_k + i \delta} \right].
$$
\n(20)

The first and third terms form the usual Beliaev-Galitskii result. The second term is the correction that must be introduced to deal with the infinite potential. A comparison with Eqs. (5) and (12) shows that this contribution equals that from the inhomogeneous term of the ISE for a hard-sphere potential of radius *a*. However, this correspondence is somewhat surprising, as the inhomogeneous term in the ISE depends only on the width of the potential, not its height. Writing the correction out for the case $p' = p = 0$, gives the particularly simple result

$$
\langle \mathbf{0} | T_{\text{corr}}(E) | \mathbf{0} \rangle = -E \times (\text{Excluded volume}),
$$

= $-\frac{E4 \pi a^3}{3}$ (3D),
= $-E \pi a^2$ (2D),
= $-2E a$ (1D), (21)

where in each case $V(|\mathbf{r}|)$ is infinite for $|\mathbf{r}| \le a$ (see Secs. $V-VII$).

A simpler derivation of the BG relation that neglects the correction term can be obtained by substituting Eq. (15) for *G* directly into Eq. (1). The proof given here includes the correction because *G* appears as $G - G_0$ rather than on its own. For any finite potential, the contribution to *G* from states with energies greater than *V* will be canceled in large part by G_0 . Thus the sum over states converges better in G $-G₀$ than it does in *G* alone, allowing the infinite potential limit to be taken inside the summation and producing the correction term of Eq. (18) . However, we have not proved this rigorously, so the derivation given here is somewhat heuristic. Further justification for the validity of Eq. (18) comes from the fact that it agrees with the predictions of the ISE and also with results obtained by using the ordinary BG relation for a finite potential and taking the infinite potential limit at the end of the calculation. Although this greatly complicates evaluation of the *T* matrix, the calculations have been performed for $p' = p = 0$ in 2D and 3D by Sheth, Chang, and Friedberg $[8]$, and we discuss the 1D case in Sec. VII.

The BG result is useful because it relates the off-shell *T* matrix to the half-on-shell *T* matrix, which in turn can be calculated from the ordinary Schrödinger equation. However, in order to do the calculation, one must first calculate $f(\mathbf{p}', \mathbf{p})$ over the whole relevant range of the integral and then perform the integration. Either or both of these calculations may be nontrivial in practice. For the hard-sphere potentials we will consider in this paper, it is considerably simpler to use the ISE. This deals easily with infinite potentials and has the additional advantage that the *T* matrix can be obtained for all **k**' with very little extra effort over and above that required to obtain it for a single value.

IV. CONTACT INTERACTIONS FOR LOW-MOMENTUM SCATTERING

In this section we consider the general off-shell *T* matrix and show that its leading order contribution in the lowmomentum limit depends only on the energy *E* of the collision and not on the incoming or outgoing momenta. This result is important because it means that for low-momentum collisions the spatial representation of the *T* matrix can be taken to be a contact potential, $T(\mathbf{r}, \mathbf{r}', E) = g(E) \delta(\mathbf{r}) \delta(\mathbf{r})$ $-\mathbf{r}'$). This form of the *T* matrix greatly simplifies calculations of the properties of cold, dilute gases and is widely used in the theory of Bose-Einstein condensation.

The proof of this result is trivial if we use the Lippmann-Schwinger definition of the T matrix Eq. (1) in the momentum basis with the full Green's function for the interacting pair

$$
\langle \mathbf{k'} | T(E) | \mathbf{k} \rangle = \langle \mathbf{k'} | V | \mathbf{k} \rangle + \langle \mathbf{k'} | V \frac{1}{E - H + i\delta} V | \mathbf{k} \rangle,
$$

\n
$$
= \int d^D \mathbf{r} e^{-i\mathbf{k'} \cdot \mathbf{r}} V(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}
$$

\n
$$
+ \int \int d^D \mathbf{r} d^D \mathbf{r'} e^{-i\mathbf{k'} \cdot \mathbf{r}} V(\mathbf{r}) G^+(\mathbf{r}, \mathbf{r'}, E) V(\mathbf{r'}) e^{i\mathbf{k} \cdot \mathbf{r'}}.
$$
\n(22)

If we now suppose that the potential has a finite range r_0 so that *V*(**r**) is negligible for $r > r_0$, then in the limit kr_0 , $k' r_0$ ≤ 1 we can expand the exponentials as $e^{i\mathbf{k}\cdot\mathbf{r}} \approx 1 + O(kr_0)$. We can, therefore, write the low-momentum limit of the *T* matrix as

$$
\lim_{k',k \to 0} \langle \mathbf{k}' | T(E) | \mathbf{k} \rangle = g(E) + g_1(E) (k' r_0 + k r_0)
$$

+ $O[(k' r_0)^2, (k r_0)^2, k' k r_0^2]$, (23)

where $g(E)$ and $g_1(E)$ will in general depend on r_0 and we have used Eq. (10). Hence the leading-order contribution to the *T* matrix at low momentum is a function of the energy of the collision only and not the momentum. In many cases of practical interest, the condition $kr_0 \ll 1$ is well satisfied so the correction term is negligible and the *T* matrix is effectively independent of momentum. In this case its spatial representation can be taken to be a contact potential

$$
\langle \mathbf{r'} | T(E) | \mathbf{r} \rangle \sim \langle \mathbf{k'} = \mathbf{0} | T(E) | \mathbf{k} = \mathbf{0} \rangle \delta(\mathbf{r}) \delta(\mathbf{r'})
$$

= $g(E) \delta(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r'}),$ (24)

because this generates the same *T* matrix in momentum space at low momentum $[19]$. We note that a more stringent definition of momentum independence for the *T* matrix would require the derivatives with respect to k and k' to vanish at zero momentum [i.e., $g_1(E)=0$]. This is in fact true for central potentials (although not more generally), as is easily proved from Eq. (22) using symmetry arguments. In this case, the corrections to the contact potential form are of order $(kr_0)^2$, as we confirm for hard-sphere potentials in Secs. V–VII.

We note that the form of Eq. (24) is independent of dimensionality, which only enters in the explicit expression that must be used for $g(E)$. In 3D, $g(E)$ is independent of energy at low energy and for a hard-sphere potential of radius a it is given by (see Sec. V)

$$
g(E) = \frac{4\pi\hbar^2 a}{m} + O(k_E a)
$$
 (3D), (25)

where (as before) $k_E = \sqrt{2\mu E/\hbar^2}$ and $m = 2\mu$ is the mass of one of the colliding atoms. In $2D$ we have $(Sec. VI)$

$$
g(E) = \frac{4\,\pi\hbar^2/m}{\pi i - 2\,\gamma - \ln[(k_E a)^2/4]} + O\left(\frac{(k_E a)^2}{\ln(k_E a)}\right) \quad (2D),
$$
\n(26)

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant, while in $1D$ (Sec. VII)

$$
g(E) = -\frac{2\hbar^2}{ma} [ik_E a + (k_E a)^2].
$$
 (27)

These results show that while the *T* matrix is insensitive to momentum at low momentum, its energy dependence may be nontrivial.

V. THREE DIMENSIONS

In this section we solve the ISE in 3D and obtain analytical results for the off-shell *T* matrix. We consider the case of a hard-sphere interaction potential of radius a , $V(r) = 0$ for $r > a$, $V(r) = \infty$ for $r \le a$. This potential simply acts as a boundary condition, forcing the wave function to vanish for $r \leq a$. We take the direction of the initial wave to define the *z* axis, $\mathbf{k} = k\hat{\mathbf{z}}$. We make the usual transformation to partial waves and decompose the initial plane wave and the full scattered wave as $\lceil 20 \rceil$

$$
e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikz} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi (2l+1)} j_l(kr) Y_l^0(\theta), \qquad (28)
$$

OFF-SHELL *T* MATRICES IN ONE, TWO, AND THREE . . . PHYSICAL REVIEW A **65** 022706

$$
\psi_{+}(\mathbf{r}, \mathbf{k}, E) = \sum_{l=0}^{\infty} i^{l} \sqrt{4 \pi (2l+1)} \phi_{l}(r, k, E) Y_{l}^{0}(\theta), \quad (29)
$$

where $j_l(kr)$ and $Y_l^0(\theta)$ are the usual spherical Bessel functions and spherical harmonics, respectively. Substitution into Eq. (12) gives the equation for $\phi_l(r,k,E)$

$$
\left[k_E^2 + \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) - \frac{l(l+1)}{r^2} - U(r)\right] \phi_l(r,k,E)
$$

= $(k_E^2 - k^2) j_l(kr).$ (30)

Substituting Eqs. (28) and (29) into Eq. (5) gives the partial wave decomposition of the *T* matrix

$$
\langle \mathbf{k'} | T(E) | \mathbf{k} \rangle = \sum_{l=0}^{\infty} i^l \sqrt{4 \pi (2l+1)} t_l(k',k,E) Y_l^0(\theta_{\mathbf{k'}}),
$$
\n(31)

where

$$
t_l(k',k,E) = (-i)^l 4 \pi \int_0^\infty dr \, r^2 j_l(k'r) V(r) \phi_l(r,k,E),\tag{32}
$$

and $\theta_{\mathbf{k}'}$ is the angle of \mathbf{k}' relative to **k**.

Equation (30) can be solved using the fact that the spherical Bessel function $j_l(kr)$ is the regular solution of the equation

$$
\left[k^2 + \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l(l+1)}{r^2}\right]j_l(kr) = 0.
$$
 (33)

We will also be interested in the spherical Neumann function $n_l(kr)$ that is the irregular solution, and the Hankel function of the first kind $h_l^{(1)}(kr) = j_l(kr) + i n_l(kr)$, which corresponds to an outgoing wave in the asymptotic limit $kr \rightarrow \infty$.

A comparison of Eqs. (30) and (33) shows that the general solution for $\phi_l(r,k,E)$ for $r > a$ has the form

$$
\phi_l(r,k,E) = j_l(kr) + (A_l - 1)j_l(k_E r) + B_l n_l(k_E r), \quad (34)
$$

where we have included the -1 in the coefficient of $j_l(k_Er)$ so that A_l has its usual value in the on-shell limit $k_E = k$. The boundary condition at infinity gives $B_l = i(A_l - 1)$, which is clearly required so that the scattered wave is proportional to $h_l^{(1)}(k_E r)$ and hence to an outgoing wave (this result is proved more formally in the Appendix). The condition that the wave function vanishes at $r=a$ then gives

$$
A_l - 1 = \frac{-j_l(ka)}{h_l^{(1)}(k_E a)}.
$$
 (35)

The solution for $\phi_i(r, k, E)$, which matches the boundary conditions is, therefore,

$$
\phi_l(r,k,E) = j_l(kr) - \frac{j_l(ka)}{h_l^{(1)}(k_E a)} h_l^{(1)}(k_E r) \quad (r > a),
$$

$$
\phi_l(r,k,E) = 0 \quad (r \le a). \tag{36}
$$

The boundary condition at infinity can also be used to give an expression for the half-on-shell T matrix with k' $=k_E \neq k$, as shown in the Appendix. However, we want the completely general case so we need to substitute the result for $\phi_i(r, k, E)$ into Eq. (32) and evaluate the integral. On first inspection this appears difficult because we have an infinite potential multiplied by a zero wave function. However, this difficulty can be avoided, if we follow the method of Schick [7], which involves manipulating Eqs. (30) and (33) to obtain an alternative expression for the integral. Specifically, we multiply Eq. (30) by $j_l(k'r)$ and Eq. (33) (with $k \rightarrow k'$) by $\phi_l(r, k, E)$, subtract and integrate. Choosing the limits of integration to be from θ to α , this gives

$$
\int_{0}^{a} dr \, r^{2} j_{l}(k'r) U(r) \phi_{l}(r,k,E)
$$
\n
$$
= \left[j_{l}(k'r) r^{2} \frac{d\phi_{l}}{dr} \right]_{0}^{a} - \left[\phi_{l} r^{2} \frac{d j_{l}(k'r)}{dr} \right]_{0}^{a}
$$
\n
$$
+ (k_{E}^{2} - k'^{2}) \int_{0}^{a} dr \, r^{2} j_{l}(k'r) \phi_{l}
$$
\n
$$
- (k_{E}^{2} - k^{2}) \int_{0}^{a} dr \, r^{2} j_{l}(k'r) j_{l}(kr), \qquad (37)
$$

where integration by parts has been used on the kineticenergy term.

For a hard-sphere potential, $\phi_l(r,k,E)$ vanishes for $r \le a$ so the second and third terms on the right-hand side (RHS) of Eq. (37) are zero, while $U(r)$ vanishes for $r > a$ so the left-hand side is proportional to $t_l(k',k,E)$ [cf. Eq. (32)]. The last term on the RHS can be evaluated using Bessel function identities, while the first term can be calculated using Eq. (36) and the fact that the Bessel functions satisfy

$$
\frac{dj_l(x)}{dx} = \frac{ij_l(x)}{x} - j_{l+1}(x). \tag{38}
$$

We, therefore, obtain the general result (obtained previously by Van Leeuwen and Reiner \vert 13 \vert)

$$
t_{l}(k',k,E) = -(-i)^{l}U_{0}\left\{\frac{(x_{E}^{2}-x'^{2})}{(x^{2}-x'^{2})}xj_{l}(x')j_{l+1}(x) -\frac{(x_{E}^{2}-x^{2})}{(x^{2}-x'^{2})}x'j_{l}(x)j_{l+1}(x') -x_{E}j_{l}(x)j_{l}(x')\frac{h_{l+1}^{(1)}(x_{E})}{h_{l}^{(1)}(x_{E})}\right\},
$$
(39)

where $U_0 = 4\pi\hbar^2 a/m$, $x = ka$, $x' = k'a$, and $x_E = k_E a$. Substitution into Eq. (31) then gives the final expression for the off-shell *T* matrix.

Various limits of this result are of interest. If we take the half-on-shell case $k = k_E \neq k'$ and use Bessel function identities, we obtain

$$
t_l(k',k,E_k) = (-i)^{l+1} U_0 \frac{j_l(x')}{x h_l^{(1)}(x)},
$$
\n(40)

which has an elegent simplicity. Inserting this result into Eq. (31) gives

$$
\langle \mathbf{k'} | T(E_k) | \mathbf{k} \rangle = -i U_0 \sum_{l=0}^{\infty} \sqrt{4 \pi (2l+1)}
$$

$$
\times \frac{j_l(k'a)}{(ka)h_l^{(1)}(ka)} Y_l^0(\theta_{\mathbf{k'}}).
$$
(41)

This result can also be derived by consideration of the asymptotic boundary condition (i.e., without using the method of Schick) as is shown in the Appendix. The other half-on-shell *T* matrix $(k' = k_E \neq k)$ can be found by exchanging k and k' , which follows from Eq. (10).

For small x the spherical Bessel functions have the form $j_l(x) \sim x^l$, so we see from Eq. (39) that in the limit $ka, k'a$ ≤ 1 the *T* matrix is independent of *k* and *k'* with errors of order $(ka)^2$ as predicted in Sec. IV. Setting $k=k'=0$ we get

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = U_0 \left[1 - ik_E a - \frac{1}{3} (k_E a)^2 \right].
$$
 (42)

This result was derived for $E > 0$. Analytically continuing to $E<0$ and using units $\hbar=2\mu=1$, we get

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = U_0 \left[1 - i \sqrt{E} a - \frac{1}{3} E a^2 \right] \quad (E > 0), \tag{43}
$$

$$
=U_0 \left[1 + \sqrt{|E|}a - \frac{1}{3}Ea^2\right] \quad (E<0),
$$
 (44)

where the positive square root should be taken in each case. This is the same result as that obtained by Chang and coworkers $[8]$ and includes their correction (the last term) to the result predicted by the naive use of the BG relation for the infinite potential (discussed below).

A. The Beliaev-Galitskii prediction

It is interesting to compare the above results with the BG prediction. For the case $k=k'=0$ the usual form of this relation is

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = f(\mathbf{0}, \mathbf{0}) + \frac{E}{(2\pi)^3} \int d^3 \mathbf{k} \frac{|f(\mathbf{0}, \mathbf{k})|^2}{(E_k - i\delta)(E - E_k + i\delta)}.
$$
\n(45)

Taking $f(\mathbf{0}, \mathbf{k})$ from Eq. (41) gives

$$
\langle \mathbf{0} | T(E_k) | \mathbf{k} \rangle = f(\mathbf{0}, \mathbf{k}) = U_0 e^{-ika}.
$$
 (46)

The BG relation, therefore, becomes

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = U_0 + \left(\frac{2 U_0 a}{\pi} \right) \left(\frac{2mE}{\hbar^2} \right) \int_0^\infty dk \frac{1}{k_E^2 - k^2 + i \delta},
$$

= U_0 (1 - ik_E a). (47)

A comparison with the exact result of Eq. (42) shows that the contribution of order $(k_Ea)^2$ is missing. This is as expected, because we have used the BG relation after taking the limit of an infinite potential and so the correction term of Eq. (18) must be included. The comparison of Eqs. (21) and (42) shows that this gives the correct result. The alternative procedure is to use the BG relation for finite $V(r)$ and take the infinite potential limit at the end. This calculation has been performed by Sheth, Chang, and Friedberg [8], and the correction they obtain is precisely the last term of Eq. (42) .

VI. TWO DIMENSIONS

The analysis in 2D is very similar to that in 3D, the main difference being the replacement of spherical Bessel, Neumann, and Hankel functions with their two-dimensional counterparts. In this section we give a brief outline of the calculation and a discussion of the results obtained. We consider again a hard-disk potential for which $V(r)=0$ for *r* $>a, V(r) = \infty$ for $r \le a$.

We take the direction of the incident wave to define the *x* axis. The usual partial wave decomposition gives $[21]$

$$
e^{ikx} = \sum_{m=0}^{\infty} \epsilon_m i^m \infty \cos(m\theta) J_m(kr), \qquad (48)
$$

$$
\psi_{+}(\mathbf{r}, \mathbf{k}, E) = \sum_{m=0}^{\infty} \epsilon_m i^m \cos(m\theta) \phi_m(r, k, E), \qquad (49)
$$

where $\epsilon_0 = 1$, $\epsilon_i = 2$ ($i \neq 0$). $J_m(kr)$ is the usual Bessel function that satisfies the equation

$$
\left[k^2 + \frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right) - \frac{m^2}{r^2}\right]J_m(kr) = 0,\tag{50}
$$

while $\phi_m(r, k, E)$ satisfies

$$
\[k_{E}^{2} + \frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right) - \frac{m^{2}}{r^{2}} - U(r)\] \phi_{m}(r, k, E)
$$

= $(k_{E}^{2} - k^{2})J_{m}(kr).$ (51)

The partial wave decomposition of the *T* matrix is

$$
\langle \mathbf{k}' | T(E) | \mathbf{k} \rangle = \sum_{m=0}^{\infty} \epsilon_m i^m \cos(m \theta_{\mathbf{k}'}) t_m(k', k, E), \quad (52)
$$

where $\theta_{\mathbf{k}}$ is the angle of **k**' relative to **k** and

OFF-SHELL *T* MATRICES IN ONE, TWO, AND THREE . . . PHYSICAL REVIEW A **65** 022706

$$
t_m(k',k,E) = (-i)^m 2\pi \int_0^\infty dr \, r J_m(k'r) V(r) \phi_m(r,k,E).
$$
\n(53)

Comparing Eqs. (50) and (51) it is clear that the general solution for $\phi_m(r, k, E)$ in the region $r > a$ has the form

$$
\phi_m(r,k,E) = J_m(kr) + (A_m - 1)J_m(k_Er) + B_m N_m(k_Er),
$$
\n(54)

where the Neumann function $N_m(kr)$ is the irregular solution of Eq. (50) . The boundary condition at infinity gives B_m $=i(A_m-1)$ as before, so the condition at $r=a$ gives

$$
A_m - 1 = \frac{-J_m(ka)}{H_m^{(1)}(k_E a)},
$$
\n(55)

where $H_m^{(1)}(x) = J_m(x) + iN_m(x)$ is the Hankel function of the first kind and corresponds asymptotically to an outgoing circular wave. The solution for $\phi_m(r, k, E)$, which matches the boundary conditions is, therefore,

$$
\phi_m(r,k,E) = J_m(kr) - \frac{J_m(ka)}{H_m^{(1)}(k_E a)} H_m^{(1)}(k_E r) \quad (r > a),
$$

$$
\phi_m(r,k,E) = 0 \quad (r \le a), \tag{56}
$$

in direct correspondance with the $3D$ result of Eq. (36) .

To evaluate the *T* matrix, this result should be substituted into Eq. (53) . As in the 3D case, however, the singular nature of the potential makes direct evaluation of the integral difficult and so we use the method of Schick $[7]$ to reexpress it in terms of well-defined quantities. We do this by multiplying Eq. (51) by $J_m(k'r)$ and Eq. (50) (with $k \rightarrow k'$) by $\phi_m(r, k, E)$, subtracting and integrating. Choosing the limits of integration to be from 0 to *a* gives

$$
\int_{0}^{a} dr \, r J_{m}(k'r) U(r) \phi_{m}(r,k,E)
$$
\n
$$
= \left[J_{m}(k'r) r \frac{d \phi_{m}}{dr} - \phi_{m} r \frac{d J_{m}(k'r)}{dr} \right]_{0}^{a}
$$
\n
$$
+ (k_{E}^{2} - k'^{2}) \int_{0}^{a} dr \, r J_{m}(k'r) \phi_{m}
$$
\n
$$
- (k_{E}^{2} - k^{2}) \int_{0}^{a} dr \, r J_{m}(k'r) J_{m}(kr), \qquad (57)
$$

where integration by parts has been used on the kineticenergy term. Following similar steps as in the 3D case, and using Eq. (56) and Bessel function identities, this becomes

$$
t_m(k',k,E) = -(-i)^m \frac{2\pi\hbar^2}{2\mu} \left\{ \frac{(x_E^2 - x'^2)}{(x^2 - x'^2)} x J_m(x') J_{m+1}(x) - \frac{(x_E^2 - x^2)}{(x^2 - x'^2)} x' J_m(x) J_{m+1}(x') - x_E J_m(x) J_m(x') \frac{H_{m+1}^{(1)}(x_E)}{H_m^{(1)}(x_E)} \right\},
$$
(58)

where $x = ka$, $x' = k'a$ and $x_E = k_Ea$ as before. Substitution into Eq. (52) then gives the final result for the fully off-shell *T* matrix in 2D.

Various limits of this result are of interest. We consider again the half-on-shell case $k = k_E \neq k'$ where Bessel function identities simplify the expressions considerably. Using Eq. (52) we obtain

$$
\langle \mathbf{k'} | T(E_k) | \mathbf{k} \rangle = \frac{\hbar^2}{2\mu} \sum_{m=0}^{\infty} 4 \epsilon_m \frac{J_m(k'a)}{i H_m^{(1)}(ka)} \cos(m \theta_{\mathbf{k'}}).
$$
\n(59)

For small *x* the Bessel functions have the form $J_m(x) \sim x^m$, so in the limit ka , $k'a \le 1$, Eq. (58) shows that the *T* matrix is independent of *k* and k' with errors of order $(ka)^2$ as predicted in Sec. IV. Setting $k=k'=0$ we obtain

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = 2 \pi \left(\frac{\hbar^2}{2\mu} \right) \left[\frac{k_E a H_1^{(1)}(k_E a)}{H_0^{(1)}(k_E a)} - \frac{(k_E a)^2}{2} \right],
$$
\n(60)

where the last term is the contribution from the inhomogeneous part of the ISE. In the limit $x_F \le 1$ and using $\hbar = 2\mu$ $=1$ this becomes

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = \frac{4 \pi}{\pi i - 2 \gamma - \ln(Ea^2/4)} + O\left[\frac{Ea^2}{\ln(Ea^2)}\right],\tag{61}
$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant. Although this result has been derived for $E > 0$, it can also be used for $E<0$ by straightforward analytic continuation. Equation (61) is a well-known result for the low-energy limit of the offshell *T* matrix in 2D [3]. Adhikari has shown that its functional form follows from a consideration of the analytic properties of the T matrix at low energy $[22]$. Equation (61) also shows that the *T* matrix vanishes at zero energy, which is why the medium in which collisions occur must be taken into consideration in the study of cold 2D gases.

Figure 1 shows the comparison between the exact result of Eq. (60) and the approximation of Eq. (61) . It is clear that the approximation works better for the real part at positive energies than it does at negative energies or for the imaginary part.

A. The Beliaev-Galitskii prediction

For $k=k'=0$ the usual BG relation for the off-shell *T* matrix is

FIG. 1. Real and imaginary parts of the zero-momentum, offshell *T* matrix $\langle 0|T(E)|0 \rangle$ in 2D. The solid lines are the exact result of Eq. (60) and the dotted lines are the low-energy approximation of Eq. (61). Units of $\hbar = 2\mu = 1$ have been used.

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = f(\mathbf{0}, \mathbf{0}) + \frac{E}{(2\pi)^2} \int d^2 \mathbf{k} \frac{|f(\mathbf{0}, \mathbf{k})|^2}{(E_k - i\delta)(E - E_k + i\delta)}.
$$
\n(62)

Taking $f(\mathbf{0}, \mathbf{k})$ from Eq. (59) gives

$$
\langle \mathbf{0} | T(E_k) | \mathbf{k} \rangle = f(\mathbf{0}, \mathbf{k}) = \left(\frac{\hbar^2}{2\mu} \right) \frac{4}{i H_0^{(1)}(ka)}.
$$
 (63)

 $f(\mathbf{0},\mathbf{0})$ is, therefore, zero and the BG relation becomes

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = \frac{16E}{(2\pi)^2} \int d^2 \mathbf{k}
$$

$$
\times \frac{1}{|H_0^{(1)}(ka)|^2} \frac{1}{(k^2 - i\delta)(k_E^2 - k^2 + i\delta)}.
$$
(64)

To our knowledge this integral has not been calculated exactly, although it can be done approximately in the limit $k_{E}a \ll 1$ [7]. Furthermore, it does not give exactly the right result as the limit of an infinite potential has already been taken. It is possible, however, to calculate the correction that must be introduced to deal with this, and this has been done by Chang and Friedberg $[8]$. They obtain the result $[23]$

$$
\langle \mathbf{0} | T(E) | \mathbf{0} \rangle = [
$$
Result of Eq. (64)] – $\pi E a^2$. (65)

As in the 3D case, the correction term is precisely the contribution derived in Eq. (21) . However, the advantages of using the ISE over the BG relation (even in its modified form) are particularly clear in this case. An analytical result for the fully off-shell *T* matrix can be obtained where the infinite potential is dealt with correctly and the difficult integral of Eq. (64) does not have to be evaluated.

VII. ONE DIMENSION

In 1D, the ISE is

$$
\left[k_E^2 + \frac{d^2}{dx^2} - U(x)\right]\psi_+(x,k,E) = (k_E^2 - k^2)e^{ikx}.
$$
 (66)

The analog of a central potential is a symmetric potential, so we consider the case that $U(x) = U(-x)$. In particular, we will consider an infinite barrier potential for which

$$
U(x) = \infty \quad (|x| \le a),
$$

$$
U(x) = 0 \quad (|x| > a). \tag{67}
$$

The analog of a partial wave expansion in 1D is, therefore, a parity expansion as described in $[24]$, but we will not introduce this here as the calculation is sufficiently simple that it is not necessary.

As before, the *T* matrix is related to the solution of the ISE by

$$
\langle k' | T(E) | k \rangle = \int dx \, e^{-ik'x} V(x) \psi_+(x, k, E). \tag{68}
$$

In this equation, k' can be positive or negative corresponding to waves traveling in the $+x$ or $-x$ directions, respectively. In all subsequent equations, however, we will take wave vectors to be positive and denote the direction of motion by writing the sign explicitly.

The solution to Eq. (66) , which matches the boundary conditions, is

$$
\psi_{+}(x,k,E) = e^{ikx} + \int dx' G_0^{+}(x,x',E)V(x')\psi_{+}(x',k,E),
$$
\n(69)

where the free particle Green's function is given by $[10]$

$$
G_0^+(x, x', E) = -\left(\frac{2\mu}{\hbar^2}\right) \frac{i}{2k_E} e^{ik_E|x - x'|}.
$$
 (70)

The asymptotic limit of the solution, therefore, has the form

$$
\psi_{+}(x,k,E) \xrightarrow{|x| \to \infty} e^{ikx} + f(\epsilon) e^{ikE|x|}, \tag{71}
$$

where $\epsilon \equiv x/|x| = +1$ (-1) for $x > 0$ ($x < 0$). Substituting Eq. (70) into Eq. (69) and comparing with Eq. (68) gives

$$
f(\pm 1) = -\left(\frac{2\mu}{\hbar^2}\right) \frac{i}{2k_E} \langle \pm k_E | T(E) | k \rangle. \tag{72}
$$

The solution to Eq. (66) for $|x| > a$ is

$$
\psi_{+}(x,k,E) = e^{ikx} + (A_{+} - 1)e^{ik_{E}x} + B_{+}e^{-ik_{E}x} \quad (x > a),
$$
\n(73)

$$
\psi_{+}(x,k,E) = e^{ikx} + (A_{-} - 1)e^{ikEx} + B_{-}e^{-ikEx} \quad (x < -a).
$$
\n(74)

Comparison with Eq. (71) gives

$$
B_{+} = (A_{-} - 1) = 0,\t(75)
$$

so the boundary condition at $x = \pm a$ then gives

$$
(A_{+}-1) = -e^{i(k-k_{E})a},
$$

$$
B_{-} = -e^{i(k+k_{E})a}.
$$
 (76)

The solution to the ISE, which matches all the boundary conditions is, therefore,

$$
\psi_{+}(x,k,E) = e^{ikx} - e^{i(k-k_E)a} e^{ik_E x} \quad (x > a),
$$

$$
\psi_{+}(x,k,E) = e^{ikx} - e^{i(k+k_E)a} e^{-ik_E x} \quad (x < -a),
$$

$$
\psi_{+}(x,k,E) = 0 \quad (|x| \le a). \tag{77}
$$

Comparison with Eq. (72) gives the result for the half-onshell *T* matrix

$$
\langle \pm k_E | T(E) | k \rangle = \left(\frac{\hbar^2}{2\mu} \right) \frac{2k_E}{i} e^{-i(k_E \mp k)a}.
$$
 (78)

To obtain an expression for the fully off-shell *T* matrix, we once again use the method of Schick $[7]$. The plane wave satisfies

$$
\left[k'^2 + \frac{d^2}{dx^2}\right] e^{\pm ik'x} = 0.
$$
 (79)

Multiplying this by $\psi_+(x,k,E)$ and Eq. (66) by $e^{-ik'x}$, subtracting and integrating from $-a$ to *a* gives

$$
\int_{-a}^{+a} dx \, e^{-ik'x} U(x) \psi_{+} = \left[e^{-ik'x} \frac{d\psi_{+}}{dx} - \psi_{+} \frac{d(e^{-ik'x})}{dx} \right]_{-a}^{a}
$$

$$
+ (k_{E}^{2} - k'^{2}) \int_{-a}^{+a} dx \, e^{-ik'x} \psi_{+}
$$

$$
+ 2 \frac{(k^{2} - k_{E}^{2})}{k - k'} \sin(k - k') a. \tag{80}
$$

Using Eqs. (68) and (77) , this gives the final result for the fully off-shell *T* matrix in 1D

$$
\langle k' | T(E) | k \rangle = \frac{\hbar^2}{2\mu} \left\{ \frac{2(k'k - k_E^2)}{k - k'} \sin(k - k')a - 2ik_E \cos(k - k')a \right\}.
$$
 (81)

This reduces to Eq. (78) for $k' = \pm k_E$ as it should. It is apparent from this expression that in the limit $ka, k'a \leq 1$, the T matrix is independent of k and k' with corrections of quadratic order, as expected from the analysis of Sec. IV.

If we take the limit $k=k_E=\pm k'$ we get the fully on-shell *T* matrix, which is

$$
\langle k|T(E_k)|k\rangle = \left(\frac{\hbar^2}{2\mu}\right)\frac{2k}{i},\tag{82}
$$

$$
\langle -k|T(E_k)|k\rangle = \left(\frac{\hbar^2}{2\mu}\right)\frac{2k}{i}e^{-2ika}.\tag{83}
$$

In this limit, Eq. (77) shows that $\psi_+(x, k, E)$ is zero for *x* $>a$, while the reflection coefficient has modulus 1 as we would expect. Of course, this requires a nonzero forward scattering amplitude so that the incident wave can be canceled in the region $x > a$ and so that the optical theorem is satisfied.

Using units, $\hbar = 2\mu = 1$, the zero-momentum limit of the fully off-shell *T* matrix is

$$
\langle 0|T(E)|0\rangle = -\frac{2}{a}(i\sqrt{E}a + Ea^2). \tag{84}
$$

For $Ea^2 \ll 1$ and positive energies, the leading-order contribution to the *T* matrix in 1D is therefore imaginary. This result can also be used for $E < 0$ by straightforward analytic continuation where the *T* matrix is always real

$$
\langle 0|T(E)|0\rangle = \frac{2}{a}(\sqrt{|E|}a - Ea^2) \quad (E<0). \tag{85}
$$

Although we have focused on hard-sphere potentials in this paper, it is also of interest to calculate the *T* matrix in 1D for a δ function potential, $V(r) = V_0 \delta(r)$. This is a meaningful potential in 1D in the sense that it leads to a well-defined *T* matrix without the need for any ultraviolet renormalization, in contrast with higher dimensions. This potential is also of interest because it appears in the exactly soluble many-body boson models considered by Girardeau $[25]$ and by Lieb and Liniger $[26]$. In this case the *T* matrix is also a contact potential so the Lippmann-Schwinger equation, Eq. (1) , reduces to an algebraic equation whose solution is

$$
\langle k|T(E)|k\rangle = g(E) = \frac{V_0}{1 + V_0 \left(\frac{2m}{\hbar^2}\right) \left(\frac{i}{2k_E}\right)}.
$$
 (86)

In the limit of an impenetrable δ function ($V_0 \rightarrow \infty$) this agrees with the $a \rightarrow 0$ limit of Eq. (81) as it should.

A. The Beliaev-Galitskii prediction

It is interesting to compare the above results with the prediction of the BG relation. For the case $k=k'=0$ this is

$$
\langle 0|T(E)|0\rangle = f(0,0) + \frac{E}{2\pi} \int_{-\infty}^{\infty} dk \frac{|f(0,k)|^2}{(E_k - i\delta)(E - E_k + i\delta)}.
$$
\n(87)

We will calculate this initially for the case that $f(0,k)$ corresponds to the hard-sphere potential; i.e., the limit $U \rightarrow \infty$ has already been taken. In this case Eq. (81) gives

$$
f(0,k) = \left(\frac{\hbar^2}{2\mu}\right) \frac{2k}{i} e^{-ika},\tag{88}
$$

so the BG relation becomes

$$
\langle 0|T(E)|0\rangle = \left(\frac{\hbar^2}{2\mu}\right)\frac{2k_E^2}{\pi}\int_{-\infty}^{\infty} dk \frac{1}{k_E^2 - k^2 + i\delta} = \left(\frac{\hbar^2}{2\mu}\right)\frac{2k_E}{i}.\tag{89}
$$

Comparison with the exact result of Eq. (84) shows that we are missing the contribution of relative order $Ea²$. This is because we have used the BG relation after taking the limit of an infinite potential, whereas we should have used it for finite *U* and taken the limit at the end of the calculation. To do this we must first calculate $f(0,k)$ for finite *U*. Since this is an on-shell matrix element, it can be obtained from the ordinary Schrödinger equation. The wave function for $|x|$ $\leq a$ has the form

$$
\psi_{+}(x,k,E) = Ae^{iKx} + Be^{-iKx}, \tag{90}
$$

where $K^2 = k^2 - k_u^2$ and $k_u^2 = U$. The solution for $|x| > a$ is given by Eqs. (73) – (75) with $k_E = k$ as before, but Eq. (76) no longer applies because the wave function does not vanish at $|x|=a$ for a finite potential. Instead we must ensure continuity of the wave function and its derivative at $x = \pm a$. This allows the coefficents *A* and *B* to be determined and the *T* matrix can then be evaluated directly from its definition of Eq. (68) . The result of the calculation is

$$
f(0,k) = 2U\frac{\hbar^2}{2\mu}\left(\frac{\sin Ka}{K}\right)\frac{ike^{-ika}}{K\sin Ka+ik\cos Ka}.
$$
 (91)

This reduces to Eq. (88) for $k_u \ge k$ but is very different for k_u $\lt k$.

The BG integral now becomes

$$
\langle 0|T(E)|0\rangle = \left(\frac{\hbar^2}{2\mu}\right) \frac{2k_E^2 U^2}{\pi} \int_{-\infty}^{\infty} dk
$$

$$
\times \frac{\sin^2 Ka}{K^2} \frac{1}{(K^2 + k_u^2 \cos^2 Ka)(k_E^2 - k^2 + i\delta)},\tag{92}
$$

which can be evaluated by contour integration. We see that as well as the pole at $k = k_E$ (which is all we had previously when we took the limit $k_u \rightarrow \infty$ inside the integral), there is also a whole series of poles that occur when $k > k_u$. Since we are ultimately interested in the limit $k_u \rightarrow \infty$ we can evaluate the position and residues of these poles on the assumption that k_u is very large. The new poles occur when $Ka = (2n)$ $(1+i)^{\pi}$ (1 $\pm i/k_u a$)/2 for integer *n*. Only the poles with a positive imaginary part contribute to the integral and the corresponding residues in the large k_u limit are $\mathcal{R}(n)$ $=4iEa/[\pi^3(2n+1)^2]$. Summing over these residues using $\sum_{-\infty}^{\infty} [1/(2n+1)^2] = \pi^2/4$ (and including a factor of $2\pi i$ from the residue theorem) gives a contribution to the T matrix that is $-(\hbar^2/2\mu)2k_E^2a = -2Ea$. This is just the term in Eq. (84) that was missing in the earlier calculation of Eq. (89) and is consistent with the prediction of Eq. (21)

VIII. CONCLUSIONS

In this paper we have used the inhomogeneous Schrodinger equation to derive analytic results for the general offshell *T* matrix for the case of hard-sphere central potentials in one, two, and three dimensions. For the potentials considered, this approach is considerably simpler than using the Beliaev-Galitskii relation. The ISE has the additional advantage that it deals easily with infinite potentials. In contrast, the usual form of the BG relation can only be applied directly to finite potentials. We have derived the correction term that must be introduced to deal with hard-core potentials and found that it corresponds exactly to the contribution to the *T* matrix from the inhomogeneous term of the ISE.

We have also shown that for all potentials with a finite range r_0 (not just the hard-spheres considered elsewhere in the paper), the low-momentum limit of the off-shell T matrix $(kr_0 \ll 1)$ depends only on energy and not on the incoming or outgoing relative momenta of the particles involved. This result is independent of dimensionality, which only affects the form of the remaining energy dependence of the *T* matrix. The result is important because it means that lowmomentum collisions can be represented by a contact potential. This greatly simplifies theoretical calculations of the properties of cold, dilute gases, such as Bose-Einstein condensates.

ACKNOWLEDGEMENTS

This research was supported by the Engineering and Physical Science Research Council of the United Kingdom, and by the European Union via the ''Cold Quantum Gases'' network. In addition, M.D.L. was supported by Queen's College, Oxford, and S.A.M. would like to thank Trinity College, Oxford, for financial support.

APPENDIX: THE ASYMPTOTIC BOUNDARY CONDITION

In this Appendix we use the boundary condition at infinity to derive a result used in the main text. This boundary condition also leads to an expression for the half-on-shell *T* matrix with $k' = k_F$, without the need to use the method of Schick.

In 3D, the asymptotic boundary condition that the solution of Eq. (12) must satisfy is given in Eq. (8) , which we reproduce here for convenience

$$
\psi_{+}(\mathbf{r}, \mathbf{k}, E) \xrightarrow{r \to \infty} e^{ikz} - \frac{2\mu}{4\pi\hbar^2} \frac{e^{+ik_{E}r}}{r} \langle k_{E} \hat{\mathbf{r}} | T(E) | \mathbf{k} \rangle.
$$
\n(A1)

The asymptotic limit of the spherical Bessel and Neumann functions is $[10]$

$$
j_l(x) \xrightarrow{x \to \infty} \frac{\sin(x - l\pi/2)}{x},
$$

$$
n_l(x) \xrightarrow{x \to \infty} -\frac{\cos(x - l\pi/2)}{x}.
$$
 (A2)

Using these expressions and the results of Eqs. (29) and (34) in Eq. (A1) and equating coefficients of $e^{\pm i k_E r}$ gives

$$
-\frac{2\mu}{4\pi\hbar^2}\langle k_E \hat{\mathbf{r}}|T(E)|\mathbf{k}\rangle = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} Y_l^0(\theta)
$$

$$
\times \left[\frac{(A_l - 1)e^{-il\pi/2}}{2ik_E} - \frac{B_l e^{-il\pi/2}}{2k_E} \right],
$$
(A3)

$$
0 = \sum_{l=0}^{\infty} i^l \sqrt{4 \pi (2l+1)} Y_l^0(\theta) \left[\frac{-(A_l - 1)e^{il\pi/2}}{2i} - \frac{B_l e^{il\pi/2}}{2} \right],
$$
\n(A4)

where θ is the angle between $\hat{\bf{r}}$ and the *z* axis.

- $[1]$ K. Burnett, Phys. Rep. **118**, 339 (1985) .
- [2] L.D. Fadeev, Zh. Eksp. Teor. Fiz. 39, 1459 (1960) [Sov. Phys. JETP 12, 1014 (1961)].
- [3] H.T.C. Stoof and M. Bijlsma, Phys. Rev. E 47, 939 (1993).
- [4] M. Bijlsma and H.T.C. Stoof, Phys. Rev. A **55**, 498 (1997).
- @5# N.P. Proukakis, K. Burnett, and H.T.C. Stoof, Phys. Rev. A **57**, 1230 (1998).
- $[6]$ S.A. Morgan, J. Phys. B 33, 3847 (2000) .
- $[7]$ M. Schick, Phys. Rev. A 3, 1067 (1971) .
- [8] C. Chang and R. Friedberg, Phys. Rev. A 49, 913 (1994); S. Sheth and R. Friedberg (unpublished).
- [9] J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972).
- [10] G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists*, 4th ed. (Academic Press, San Diego, 1995).
- $[11]$ A.S. Reiner, Nuovo Cimento A **51**, 1 (1967) .
- [12] K.L. Kowalski, Phys. Rev. 144, 1239 (1966).
- [13] J.M.J. Van Leeuwen and A.S. Reiner, Physica (Amsterdam) **27**, 99 (1961).
- $[14]$ P. Brumer and M. Shapiro, J. Chem. Phys. 63 , 427 (1975) .
- $[15]$ M. Shapiro and P. Brumer, Phys. Rev. C 12 , 1371 (1975) .
- [16] S.T. Beliaev, Zh. Eksp. Teor. Fiz. 34, 433 (1958) [Sov. Phys. JETP 7, 299 (1958)].
- [17] V.M. Galitskii, Zh. Eksp. Teor. Fiz. 34, 151 (1958) [Sov. Phys. JETP 7, 104 (1958)].

Equating coefficients of $Y_l^0(\theta)$ we obtain

$$
B_l = i(A_l - 1),\tag{A5}
$$

which is a result used in the text. Substituting this into Eq. $(A3)$ and using Eq. (35) for $(A₁-1)$ (which comes from the boundary condition at $r=a$), we get an expression for the half-on-shell *T* matrix

$$
\langle k_E \hat{\mathbf{r}} | T(E) | \mathbf{k} \rangle = -i U_0 \sum_{l=0}^{\infty} \sqrt{4 \pi (2l+1)}
$$

$$
\times \frac{j_l(ka)}{(k_E a) h_l^{(1)}(k_E a)} Y_l^0(\theta). \tag{A6}
$$

The symmetry of the *T* matrix with respect to its arguments [cf. Eq. (10)] shows that this result agrees with that of Eq. (41) obtained using the method of Schick. A similar analysis can be carried out in 2D.

- [18] We note that the quantity $\langle \mathbf{p}'|V|\mathbf{k}+\rangle$ in Eq. (19) appears ill defined for an infinite potential since it involves infinity times zero ($|\mathbf{k}+\rangle$ vanishes in the region of the potential). However, this quantity cancels when we obtain Eq. (20) and is in fact finite (it is just the on-shell T matrix) as the subsequent calculations of Secs. V–VII demonstrate.
- [19] R. H. Landau, *Quantum Mechanics II: A Second Course in* Quantum Theory (Wiley, New York, 1990).
- [20] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechan* ics (Wiley, New York, 1977), Vol. II.
- [21] I. Richard Lapidus, Am. J. Phys. **50**, 45 (1982).
- [22] Sadhan K. Adhikari, Am. J. Phys. 54, 362 (1986).
- [23] R. Friedberg (private communication). We are grateful to Professor Friedberg for pointing out to us that the 2D results of $[8]$ are missing factors of $2/\pi$. In particular, the equation directly below Eq. (22) should contain a factor of $2/\pi$, and all subsequent 2D equations should contain a factor of $2/\pi$ for each power of the scattering amplitude f . This means that Eqs. (64) and (66) of [8] should contain a factor of $(2/\pi)^2$ that makes them consistent with our result of Eq. (60) .
- [24] J.H. Eberly, Am. J. Phys. 33, 771 (1965); see also J. Formanek, *ibid.* **44**, 778 (1976).
- [25] M. Girardeau, J. Math. Phys. 1, 516 (1960).
- [26] E.H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963); E.H. Lieb, *ibid.* **130**, 1616 (1963).