

Study of quantum scattering T-matrix

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Abstract: We present an off-shell calculation of T-matrix elements for different kinds of potentials. In this report we review the basic concepts about this quantity, as well as its relation with the general quantum scattering problem, remarking its relevance when dealing with anisotropic and/or long ranged interactions. We emphasize the calculation of the generalized scattering lengths for the combination of a dipolar and a hard core potential (DHC), since it is of special interest in the field of ultra-cold quantum dipolar gases.

I. Introduction

Scattering theory is one of the most important fields in quantum mechanics, specially due to its associated practical applications concerning identification and characterization of unknown samples, biological applications, etc. However, in this report we approach quantum scattering in a more fundamental way, dealing exclusively with the problem of scattering of a particle by a potential. Although far from the practical paradigm previously mentioned, this problem is of interest in the field of ultra-cold quantum gases, remarkably in the calculation of pseudopotentials involved in mean field calculations in the framework of the Gross-Pitaevskii equation [1].

The ultimate goal of this project is the calculation of the s-wave scattering length for a dipole plus a hard core interaction, which presents anisotropy and long range behaviour. The reason behind this goal is a parallel work in progress in our research group where we analyze the experimental results presented in [2] using a *Path Integral Ground State (PIGS)* method, a numerical algorithm that is capable of reproducing the spatial structure of the ground state of a quantum many-body system with great accuracy. In that work, the authors show that close to a mean field instability, a system of Dy¹⁶⁴ atoms confined in a three dimensional harmonic trap forms *droplets*. This isotope of Dysprosium has a large dipole moment, which makes it ideal for experiments related to the study of the dipole interaction in ultracold gases. By tuning the scattering length of the short ranged part of the interaction between Dy¹⁶⁴ atoms using Feshbach resonances, authors show the transition from an homogeneous gas to a system of *droplets* as the scattering length of the short ranged part decreases.

Another simulation method that yields more accurate energies is the *Diffusion Monte Carlo (DMC)*, which we plan to use to determine more precisely the point where droplets start to form. In order to use the DMC method, we first need a *trial wave function*, which is typically taken as a product of two-body functions. One common choice for this factor is to take it as the low energy scattering solution of the two-body problem. As we shall see, the T-matrix elements yield the appropriate coefficients for

each partial wave in order to build a physically reasonable wave function.

This report is structured as follows: in Sec. II we review the main properties of the dipolar interaction. In Sec. III we present a brief overview of elastic quantum scattering. In Sec. IV we show the derivation of the system of integral equations to be numerically solved in order to get the T-matrix elements in the basis of the eigenstates of the free particle Hamiltonian with definite angular momentum. In Sec. IV A we provide an example of the numerical calculation of the T-matrix elements for a three dimensional soft core potential, together with the comparison between analytical and numerical results. In Sec. IV B we present an overview of the scattering properties of the main potential of interest in this work, the DHC potential. We also present the calculation of the aforementioned generalized scattering lengths. Finally, in Sec. VI we state the main conclusions of this work

II. The dipolar interaction

The dipolar interaction is of particular interest in the field of ultra-cold quantum gases because of its two key properties: it is *long ranged* and *anisotropic*. The properties of dilute gases (with densities ranging between 10^{14} and 10^{15} cm⁻³ [3]) with dipole interaction are quite different from the standard ones corresponding to usual short ranged interactions. Concerning the formal properties of the dipole interaction, the expression for this potential is:

$$V_{\text{dipolar}}(\vec{r}_i, \vec{r}_j) = \frac{d^2}{|\vec{r}_j - \vec{r}_i|^3} \times \left(\vec{p}_i \vec{p}_j - 3 \frac{[\vec{p}_i(\vec{r}_j - \vec{r}_i)][\vec{p}_j(\vec{r}_j - \vec{r}_i)]}{|\vec{r}_j - \vec{r}_i|^2} \right) \quad (1)$$

where d^2 is a constant, \vec{r}_i and \vec{p}_i are the position and unit polarization vectors of the i -th particle respectively and \vec{r}_j and \vec{p}_j are the position and unit polarization vectors of the j -th particle respectively. We consider the case where the polarization vectors are all parallel. Physically, this

corresponds to setting an external field which aligns the dipoles along one fixed direction. However, this field is not strong enough to produce any other significant effect. Thus, being \vec{p}_i and \vec{p}_j parallel, we can always use a reference frame in three dimensions where they are aligned along the \hat{z} axis. Denoting $\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$ and considering $\vec{p}_i = \vec{p}_j = \hat{z}$ Eq. (1) can be written as:

$$V_{\text{dipolar}}(\vec{r}_{ij}) = \frac{d^2 (1 - 3 \cos^2 \theta)}{r_{ij}^3} \quad (2)$$

where θ is the polar angle in spherical coordinates. This is the standard way the dipole interaction is presented in the literature. Notice that the dipole potential is invariant with respect to the azimuthal angle ϕ , so the anisotropic nature of the potential is present only through the $\cos^2 \theta$ dependence, and is the main responsible of the non-trivial structures present in dipole systems, ranging from the *stripe* phase emerging in a two dimensional homogeneous dipolar system ([4], [5]) to the droplets in a confined three dimensional system previously mentioned. The fact that the potential is negative for some values of θ leads to a collapse instability, although this instability is healed by the short ranged part of the interaction between atoms. The characteristic length of the dipole potential is:

$$D \equiv \frac{2Md^2}{\hbar^2} \quad (3)$$

with M the reduced mass. A more extensive presentation of the dipole interaction features can be found in [6]

III. Brief review of elastic scattering

In this section we review the main aspects of the standard three dimensional quantum elastic scattering theory. We consider the problem of scattering of a particle by a potential $V(\vec{r})$ as a two body problem in relative coordinates. The Schrödinger equation is:

$$-\frac{\hbar^2}{2M} \nabla^2 \psi + V\psi = E\psi \quad (4)$$

where \vec{r} is the relative position vector and M is the reduced mass. The solution of this equation can be written as:

$$\psi(\vec{r}) = e^{i\vec{k}\vec{r}} + \int dV G(\vec{r}, \vec{r}') \frac{2M}{\hbar^2} V(\vec{r}') \psi(\vec{r}') d\vec{r}' \quad (5)$$

with \vec{k} the wave vector corresponding to energy $E = \frac{\hbar^2 k^2}{2M}$, $k = |\vec{k}|$ and $G(\vec{r}, \vec{r}')$ the associated Green function. In scattering theory, we call the homogeneous part solution the **incident wave**, while the particular solution is called the **scattered wave**. This implies that the Green function has to take into account the boundary conditions associated to the scattered wave. For potentials

decaying faster than $1/r$ [7], the asymptotic behaviour of the solution at large distances is written as:

$$\lim_{r \rightarrow \infty} \psi(\vec{r}) = e^{i\vec{k}\vec{r}} + f(\theta, \phi, k) \frac{e^{ikr}}{r} \quad (6)$$

with $r = |\vec{r}|$ and (θ, ϕ) the polar and azimuthal angles of \vec{r} . The scattered wave is an outgoing spherical wave modified by the factor $f(\theta, \phi, k)$, which is the scattering amplitude. Notice that for the Coulomb potential a logarithmic phase shift appears inside the imaginary exponentials [7]. Identifying terms with Eq. (5):

$$f(\theta, \phi, k) \frac{e^{ikr}}{r} = \lim_{r \rightarrow \infty} \int dV G(\vec{r}, \vec{r}') \frac{2M}{\hbar^2} V(\vec{r}') \psi(\vec{r}') d\vec{r}' \quad (7)$$

Furthermore, Eq. (5) is an integral equation for $\psi(\vec{r})$. It can be shown that the Green function that incorporates the appropriate scattering boundary conditions in three dimensions is:

$$G(\vec{r}, \vec{r}') = -\frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \quad (8)$$

If the range of the potential is finite, at large distances we can write [8]:

$$|\vec{r}| \gg |\vec{r}'| \rightarrow |\vec{r} - \vec{r}'| \simeq r - \hat{r} \cdot \vec{r}'$$

where $\hat{r} \equiv \frac{\vec{r}}{r}$ is the unit position vector. This leads to a large distance approximation for the Green function:

$$G(\vec{r}, \vec{r}') \Big|_{|\vec{r}| \gg |\vec{r}'|} = -\frac{e^{ikr}}{4\pi r} e^{i\vec{k}' \cdot \vec{r}'} \quad (9)$$

and thus, using Eq. (7) one finds:

$$f(\theta, \phi, k) \frac{e^{ikr}}{r} = -\frac{M}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int dV e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}') \psi(\vec{r}') d\vec{r}' \quad (10)$$

where we have defined $\vec{k}' \equiv k\hat{r}$. The asymptotic form of the scattering wave function is then:

$$\lim_{r \rightarrow \infty} \psi(\vec{r}) = e^{i\vec{k}\vec{r}} - \frac{M}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int dV e^{i\vec{k}' \cdot \vec{r}'} V(\vec{r}') \psi(\vec{r}') d\vec{r}' \quad (11)$$

IV. Expression for the calculation of the T-matrix elements

The \hat{T} operator is defined by the relation:

$$\hat{V}|\psi\rangle \equiv \hat{T}|\phi\rangle \quad (12)$$

with $|\phi\rangle$ fulfilling $\langle \vec{r} | \phi \rangle = e^{i\vec{k}\vec{r}}$. Essentially, we are shifting the non-trivial part of the problem from the wave

function to the \hat{T} operator. It can be shown that the \hat{T} operator satisfies the **Lippman-Schwinger** equation [8], which is given by:

$$\hat{T}|\phi\rangle = \hat{V} \frac{1}{E - \hat{H}_0 \pm i\epsilon} \hat{T}|\phi\rangle + \hat{V}|\phi\rangle \quad (13)$$

where $\hat{H}_0 = \frac{\hat{p}^2}{2M}$ is the free particle Hamiltonian, $E = \frac{\hbar^2 k^2}{2M}$ is the energy of the incident and the scattered state and $\pm i\epsilon$ is an infinitesimal term introduced to avoid the singular behaviour of $\frac{1}{E - \hat{H}_0}$. The sign of this term is related to the boundary conditions of the scattered wave [8]: positive sign for an outgoing wave and negative sign for an incoming wave. Iterating Eq. (13) one reaches a series in terms of the potential \hat{V} , i.e. \hat{T} can be written as a perturbative expansion in terms of the potential. The first order term is $\hat{T}^{(1)} = \hat{V}$, which leads to the well-known Born approximation.

One can now project this equation on a given representation to solve for the matrix elements of \hat{T} . Considering $|\phi\rangle = (2\pi)^{d/2}|\vec{k}\rangle$, where d is the dimension of space, and projecting Eq. (13) on $\langle\vec{k}'|$ we have:

$$T(\vec{k}', \vec{k}) = \langle\vec{k}'|\hat{V} \frac{1}{E - \hat{H}_0 \pm i\epsilon} \hat{T}|\vec{k}\rangle + V(\vec{k}', \vec{k}) \quad (14)$$

where $T(\vec{k}', \vec{k}) \equiv \langle\vec{k}'|\hat{T}|\vec{k}\rangle$. Assuming the potential to be local (i.e. $\langle\vec{x}|\hat{V}|\vec{y}\rangle = V(\vec{x})\delta(\vec{x} - \vec{y})$), one has:

$$\begin{aligned} V(\vec{k}', \vec{k}) &= \int \int \langle\vec{k}'|\vec{x}\rangle \langle\vec{x}|\hat{V}|\vec{y}\rangle \langle\vec{y}|\vec{k}\rangle d\vec{x}d\vec{y} \\ &= \frac{1}{(2\pi)^d} \int e^{i(\vec{k} - \vec{k}')\cdot\vec{x}} V(\vec{x}) d\vec{x} = V(\vec{k} - \vec{k}') \end{aligned}$$

We can focus now in the other term of Eq. (14), which can be rewritten as:

$$\begin{aligned} &\langle\vec{k}'|\hat{V} \frac{1}{E - \hat{H}_0 \pm i\epsilon} \hat{T}|\vec{k}\rangle \\ &= \int V(\vec{q} - \vec{k}') \frac{1}{E - \frac{\hbar^2 q^2}{2M} \pm i\epsilon} T(\vec{q}, \vec{k}) d\vec{q} \end{aligned}$$

Using this and recalling that E is the eigenvalue of $|\vec{k}\rangle$ with energy $E = \frac{\hbar^2 k^2}{2M}$, we can rewrite Eq. (14) as:

$$T(\vec{k}', \vec{k}) = \int \frac{V(\vec{q} - \vec{k}')}{\left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M} \pm i\epsilon\right)} T(\vec{q}, \vec{k}) d\vec{q} + V(\vec{k} - \vec{k}') \quad (15)$$

which is the Lippmann Schwinger equation in momentum space. Although Eq. (15) can in principle be solved numerically, in order to perform efficient calculations in three dimensions it is convenient to first project Eq. (13) into the angular momentum representation (in particular, the eigenstates of the free particle Hamiltonian with

definite angular momentum $|E, l, m\rangle$). We first rewrite Eq. (13) as:

$$\hat{T} = \hat{V} \frac{1}{E - \hat{H}_0 \pm i\epsilon} \hat{T} + \hat{V} \quad (16)$$

Projecting on $\langle E_{k'}, l', m' |$ and $|E, l, m\rangle$:

$$\begin{aligned} T_{l', m'}^{l, m}(k', k) &= V_{l', m'}^{l, m}(k', k) \\ &+ \langle E_{k'}, l', m' | \hat{V} \frac{1}{E - \hat{H}_0 \pm i\epsilon} \hat{T} | E, l, m \rangle \end{aligned} \quad (17)$$

where $T_{l', m'}^{l, m}(k', k) \equiv \langle E_{k'}, l', m' | \hat{T} | E, l, m \rangle$, $E_{k'} \equiv \frac{\hbar^2 k'^2}{2M}$. Introducing an identity $\hat{I} = \sum_{l_2, m_2} \int dE_q |E_q, l_2, m_2\rangle \langle E_q, l_2, m_2|$ in Eq. (17) yields:

$$\begin{aligned} T_{l', m'}^{l, m}(k', k) &= V_{l', m'}^{l, m}(k', k) \\ &+ \frac{\hbar^2}{M} \sum_{l_2, m_2} \int \frac{V_{l', m'}^{l_2, m_2}(k', q) T_{l_2, m_2}^{l, m}(q, k)}{\left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M} + i\epsilon\right)} q dq \end{aligned} \quad (18)$$

with the matrix elements of the potential given by:

$$\begin{aligned} V_{l', m'}^{l, m}(k', k) &= i^l (-i)^{l'} \frac{2M}{\pi \hbar^2} \sqrt{kk'} \int_0^\infty r^2 j_l(kr) j_{l'}(k'r) \\ &\times \left[\int V(r, \theta, \phi) Y_l^m(\theta, \phi) Y_{l'}^{m'*}(\theta, \phi) d\Omega \right] dr \end{aligned} \quad (19)$$

We have used the identity [8]:

$$\langle \vec{r} | E, l, m \rangle = \frac{i^l}{\hbar} \sqrt{\frac{2Mk}{\pi}} j_l(kr) Y_l^m(\theta, \phi) \quad (20)$$

where $j_l(kr)$ denotes the spherical Bessel function of the first kind and $Y_l^m(\theta, \phi)$ the spherical harmonic with indexes l, m . If the potential is **central**, its matrix elements can be written as:

$$\begin{aligned} V_{l', m'}^{l, m}(k', k) &= \delta_{l, l'} \delta_{m, m'} i^l (-i)^{l'} \frac{2M}{\pi \hbar^2} \\ &\times \sqrt{kk'} \int_0^\infty r^2 j_l(kr) j_{l'}(k'r) dr \\ &\equiv \delta_{l, l'} \delta_{m, m'} \frac{2M}{\pi \hbar^2} \sqrt{kk'} v_l^l(k', k) \end{aligned} \quad (21)$$

In this case the potential elements are diagonal in the $|E, l, m\rangle$ base due to the orthonormality of the spherical harmonics.

Using Eqs. (10) and (12) we can relate the scattering amplitude with the T-matrix.

$$\begin{aligned} f(\theta, \phi, k) &= -\frac{M}{2\pi \hbar^2} \int e^{i\vec{k}'\cdot\vec{r}'} V(\vec{r}') \psi(\vec{r}') d\vec{r}' \\ &= -\frac{\sqrt{2\pi} M}{\hbar^2} \langle \vec{k}' | \hat{V} | \psi \rangle \\ &= -\frac{(2\pi)^2 M}{\hbar^2} \langle \vec{k}' | \hat{T} | \vec{k} \rangle \end{aligned} \quad (22)$$

It is a well known result from scattering theory that, for a **central, short ranged** potential, the scattering amplitude at low momentum converges to a constant known as the **s-wave scattering length** [9], which is the only parameter that determines the scattering properties. Using the last relation we reached, we can relate this important parameter with the T-matrix, obtaining:

$$\begin{aligned} f(\theta, \phi, k \rightarrow 0) &\rightarrow -a_{sc} = \lim_{k=k' \rightarrow 0} -\frac{(2\pi)^2 M}{\hbar^2} T(\vec{k}, \vec{k}') \\ &\rightarrow a_{sc} = \lim_{k \rightarrow 0} \frac{(2\pi)^2 M}{\hbar^2} T(\vec{k}) \end{aligned} \quad (23)$$

In this case, the dominant contribution to $T(\vec{k})$ arises from $T_{0,0}^{0,0}(k)$, so by applying a partial wave expansion to Eq. (23), one can reach an expression for the s-wave scattering length in terms of the partial 0-th wave T-matrix element $T_{0,0}^{0,0}(k)$ which reads:

$$a_{sc} = \lim_{k \rightarrow 0} \frac{\pi T_{0,0}^{0,0}(k)}{k} \quad (24)$$

A. Testing the three-dimensional formula: scattering by a soft core potential

The soft core potential is given by:

$$V(r) = \begin{cases} V_0 & r < R_0 \\ 0 & r > R_0 \end{cases} \quad (25)$$

It is convenient to rewrite Eq. (18) in order to solve it numerically. We need to use the Plemelj identity, which states that:

$$\frac{1}{x \pm i\epsilon} = \mathcal{P} \left\{ \frac{1}{x} \right\} \mp i\pi \delta(x) \quad \epsilon \rightarrow 0 \quad (26)$$

where $\mathcal{P} \{f(x)\}$ denotes the principal value of a function $f(x)$. Considering the potential is **central** and applying this identity to Eq. (18) leads to:

$$\begin{aligned} T_{l',m'}^{l,m}(k', k) &= \delta_{l,l'} \delta_{m,m'} \frac{2M}{\pi \hbar^2} \sqrt{kk'} v_{l'}^l(k', k) \\ &+ \frac{2}{\pi} \sqrt{k'} \mathcal{P} \left\{ \int \frac{v_{l'}^l(k', q) T_{l',m'}^{l,m}(q, k)}{\left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M}\right)} q^{3/2} dq \right\} \\ &- 2i \sqrt{k'} \int v_{l'}^l(k', q) T_{l',m'}^{l,m}(q, k) \delta \left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M} \right) q^{3/2} dq \end{aligned} \quad (27)$$

The integral with a delta function can be solved easily, and yields:

$$\begin{aligned} &\int v_{l'}^l(k', q) T_{l',m'}^{l,m}(q, k) \delta \left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M} \right) q^{3/2} dq \\ &= \frac{M}{\hbar^2} \sqrt{k} v_{l'}^l(k', k) T_{l',m'}^{l,m}(k, k) \end{aligned} \quad (28)$$

Splitting the T-matrix elements into real and an imaginary parts we can separate Eq. (28) into two equations: one for the real contributions and another for the imaginary ones. The T-matrix elements are written as:

$$T_{l',m'}^{l,m}(k', k) = \Sigma_{l',m'}^{l,m}(k', k) + i\Gamma_{l',m'}^{l,m}(k', k) \quad (29)$$

We also consider $V_{l',m'}^{l,m}(k, k')$ to be real. The aforementioned system of two equations then reads:

$$\begin{aligned} \Sigma_{l',m'}^{l,m}(k', k) &= \frac{2M}{\pi \hbar^2} \sqrt{kk'} v_{l'}^l(k', k) \delta_{l,l'} \delta_{m,m'} \\ &+ \frac{2}{\pi} \sqrt{k'} \mathcal{P} \left\{ \int_0^\infty \frac{v_{l'}^l(k', q) \Sigma_{l',m'}^{l,m}(q, k)}{\left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M}\right)} q^{3/2} dq \right\} \\ &+ \frac{2M}{\hbar^2} \sqrt{kk'} v_{l'}^l(k', k) \Gamma_{l',m'}^{l,m}(k, k) \end{aligned} \quad (30)$$

$$\begin{aligned} \Gamma_{l',m'}^{l,m}(k', k) &= \\ &\frac{2}{\pi} \sqrt{k'} \mathcal{P} \left\{ \int_0^\infty \frac{v_{l'}^l(k', q) \Gamma_{l',m'}^{l,m}(q, k)}{\left(\frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M}\right)} q^{3/2} dq \right\} \\ &- \frac{2M}{\hbar^2} \sqrt{kk'} v_{l'}^l(k', k) \Sigma_{l',m'}^{l,m}(k, k) \end{aligned} \quad (31)$$

with $v_{l'}^l(k', k)$ defined in Eq. (21). Notice how the isotropy of the potential makes $T_{l',m'}^{l,m}(k', k)$ be coupled only to itself. In order to solve numerically the system of integral equations, we fix k and discretize k' in a given interval in momentum space. We define the vectors:

$$\vec{v}_l^l(k) = [\sqrt{k'_0} v_l^l(k'_0, k) \quad \sqrt{k'_1} v_l^l(k'_1, k) \quad \dots \quad \sqrt{k'_N} v_l^l(k'_N, k)] \quad (32)$$

$$\vec{\Sigma}_{l',m'}^{l,m}(k) = [\Sigma_{l',m'}^{l,m}(k'_0, k) \quad \Sigma_{l',m'}^{l,m}(k'_1, k) \quad \dots \quad \Sigma_{l',m'}^{l,m}(k'_N, k)] \quad (33)$$

$$\vec{\Gamma}_{l',m'}^{l,m}(k) = [\Gamma_{l',m'}^{l,m}(k'_0, k) \quad \Gamma_{l',m'}^{l,m}(k'_1, k) \quad \dots \quad \Gamma_{l',m'}^{l,m}(k'_N, k)] \quad (34)$$

$$\vec{T}_{l',m'}^{l,m}(k) = [\vec{\Sigma}_{l',m'}^{l,m}(k) \quad \vec{\Gamma}_{l',m'}^{l,m}(k)] \quad (35)$$

We can now write the system of Eqs. (30) and (31) in matrix form:

$$A \vec{T}_{l',m'}^{l,m}(k) = -\frac{2M}{\pi \hbar^2} \sqrt{k} \vec{v}_l^l(k) \quad (36)$$

with $A \in M_{2N \times 2N}(\mathbb{R})$, and solve for $\vec{T}_{l',m'}^{l,m}(k)$.

It can be shown that, for a three dimensional short ranged central potential, the T-matrix elements can also be calculated as:

$$T_{l',m'}^{l,m}(k', k) = \frac{2M}{\hbar^2 \pi} \sqrt{\frac{k'}{k}} e^{i\delta_l} \vec{v}_l^l(k', k) \delta_{l,l'} \delta_{m,m'} \quad (37)$$

where:

$$\vec{v}_l^l(k', k) \equiv \int r^2 V(r) j_{l'}(k', r) h_{l,E_k}(r) dr \quad (38)$$

Here $h_{l,E_k}(r)$ is a $C^1(\mathbb{R})$ class function built from a linear combination of two independent solutions of the l -th partial wave radial Schrödinger equation fulfilling $h_{l,E_k}(0) = 0$, while δ_l is the l -th wave phase shift [10]. Notice that the \hat{T} operator is diagonal in the $|E, l, m\rangle$ base, which is also a consequence of the isotropic behaviour of the potential.

Using Eq. (37) we can calculate the T-matrix elements of the soft core potential. As a test, we show in Fig. (1) a comparison between the analytical and numerical calculations of $\Sigma_{0,0}^{0,0}(k', k)$ and $\Gamma_{0,0}^{0,0}(k', k)$. We take $\frac{\hbar^2 V_0}{2M} > k^2$ fixed. The analytical calculation yields:

$$\begin{aligned} \Sigma_{0,0}^{0,0}(k', k) &= \frac{2MV_0 \cos(\delta_0) \sin(kR_0 + \delta_0)}{\sqrt{k'k} \hbar^2 \pi (\lambda^2 + k'^2) \sinh(\lambda R_0)} \\ &\quad \times (\lambda \sin(k'R_0) \cosh(\lambda R_0) \\ &\quad - k' \cos(k'R_0) \sinh(\lambda R_0)) \end{aligned} \quad (39)$$

$$\Gamma_{0,0}^{0,0}(k', k) = \tan(\delta_0) \Sigma_{0,0}^{0,0}(k', k) \quad (40)$$

with $\lambda \equiv \sqrt{\frac{2MV_0}{\hbar^2} - k^2}$, $\tan(\delta_0) = \frac{-\tan(kR_0) + \frac{k}{\lambda} \tanh(\lambda R_0)}{\frac{k}{\lambda} \tanh(\lambda R_0) \tan(kR_0) + 1}$

B. DHC calculation: generalized scattering lengths

Since the previous way to obtain the T-matrix elements numerically involves the calculation of the matrix elements of the potential, we can not implement the exact hard core ($V_0 \rightarrow \infty$) part of the DHC interaction, because it leads to a divergence. Instead, we replace it by a high barrier soft core potential (HBSC) (defined in Eq. (25)), with finite $V_0 \gg 0$. However, as we shall see, we recover the values for the s-wave scattering length obtained by authors in [11], where a different numerical method that enables the full implementation of the hard core condition is used. This implies that, numerically, both the hard core and the HBSC potentials are equivalent. Under these considerations, the DHC potential is given by:

$$V(r, \theta) = \begin{cases} V_0 + V_{dd}(r, \theta) & r < R_0 \\ V_{dd}(r, \theta) & r > R_0 \end{cases} \quad (41)$$

with $V_{dd}(r, \theta) = \frac{d^2}{r^3}(1 - 3\cos^2\theta)$ and $V_0 \gg 0$. In order to obtain the set of integral equations to be solved, the matrix elements of the potential in the $|E, l, m\rangle$ basis must be calculated. Using Eq. (19) and substituting the potential:

$$\begin{aligned} V_{l',m'}^{l,m}(k', k) &= i^l (-i)^{l'} \frac{2M}{\pi \hbar^2} \sqrt{k'k'} [\delta_{l,l'} \delta_{m,m'} w_{l'}^l(k', k) \\ &\quad + u_{l'}^l(k', k) \left(\int (1 - 3\cos^2\theta) Y_l^m(\theta, \phi) Y_{l'}^{m'*}(\theta, \phi) d\Omega \right) \end{aligned} \quad (42)$$

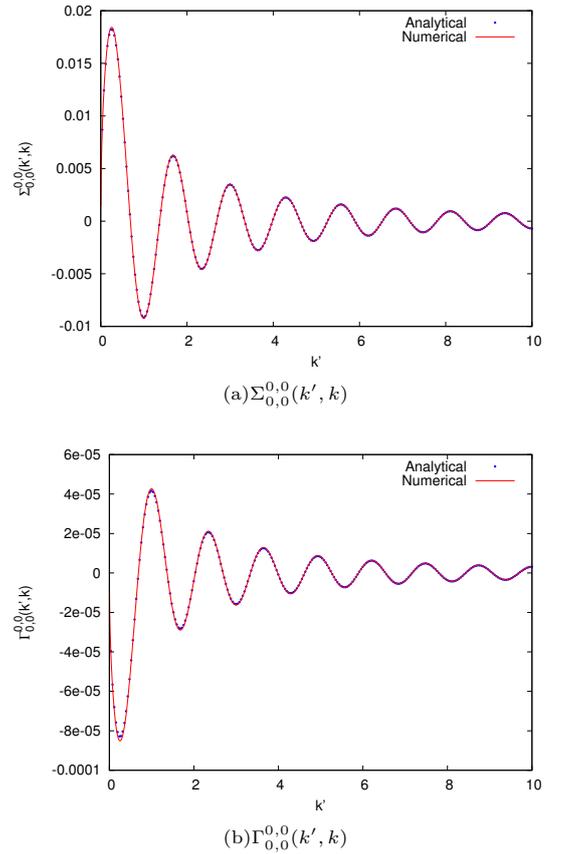


FIG. 1: Numerical and analytical calculations of $\Sigma_{0,0}^{0,0}(k', k)$ and $\Gamma_{0,0}^{0,0}(k', k)$ for the soft core potential. Results presented for $\frac{\hbar^2}{2M} = 1$. The simulation parameters are $k = 10^{-3}$, $V_0 = 5$, $R_0 = 5$. We have used a linear grid in momentum space with $N = 1200$ points, with a step of $\Delta k = 0.041$.

with:

$$w_{l'}^l(k', k) \equiv V_0 \int_0^R r^2 j_l(kr) j_{l'}(k'r) dr \quad (43)$$

$$u_{l'}^l(k', k) \equiv \int_0^\infty \frac{d^2}{r} j_l(kr) j_{l'}(k'r) dr \quad (44)$$

In order to compute the angular integral, we use the relation [12]:

$$\begin{aligned} \cos^2\theta Y_l^m(\theta, \phi) &= N_{l+2}^l \xi_{+2}(l, m) Y_{l+2}^m(\theta, \phi) \\ &\quad + \xi_0(l, m) Y_l^m(\theta, \phi) + N_{l-2}^l \xi_{-2}(l, m) Y_{l-2}^m(\theta, \phi) \end{aligned} \quad (45)$$

where:

$$N_{l'}^l \equiv \sqrt{\frac{2l+1}{2l'+1}} \quad (46)$$

$$\xi_{-2}(l, m) \equiv \frac{(l+m)(l-1+m)}{(2l+1)(2(l-1)+1)} \quad (47)$$

$$\xi_{+2}(l, m) \equiv \frac{(l-m+1)(l+2-m)}{(2l+1)(2(l+1)+1)} \quad (48)$$

$$\xi_0(l, m) \equiv \frac{(l-m+1)(l+1+m)}{(2l+1)(2(l+1)+1)} + \frac{(l+m)(l-m)}{(2l+1)(2(l-1)+1)} + 3\xi_{-2}(l'+2, m')N_{l'}^{l'+2}u_{l'}^{l'+2}(k', k)\delta_{l', l-2} \quad (49)$$

Substituting Eq. (45) into Eq. (42) and integrating, one finds:

$$V_{l', m'}^{l, m}(k', k) = \delta_{m, m'} \frac{2M}{\pi\hbar^2} \sqrt{kk'} \times \left[\left(w_{l'}^{l'}(k', k) + u_{l'}^{l'}(k', k) (1 - 3\xi_0(l', m')) \right) \delta_{l, l'} + 3\xi_{+2}(l' - 2, m)N_{l'}^{l'-2}u_{l'}^{l'-2}(k', k)\delta_{l, l+2} \right]$$

Notice that the invariance of $V_{l', m'}^{l, m}(k', k)$ with respect to ϕ makes its matrix elements diagonal in m, m' while its dependence on θ makes them non diagonal in l, l' . The invariance with respect to ϕ has another consequence: no physical quantities can depend on this variable. This implies that the only relevant T-matrix components are those with index $m = 0$.

With the explicit form of $V_{l', m'}^{l, m}(k', k)$ and splitting the T-matrix elements into real and imaginary parts, Eq. (18) can be rewritten as:

$$\Sigma_{l'}^l(k', k) = \frac{2}{\pi} \sqrt{k'} \int_0^\infty \left\{ \frac{q^{3/2} dq}{(F^2(k, q) - \epsilon^2)} \left[\left(w_{l'}^{l'}(k', q) + u_{l'}^{l'}(k', q) (1 - 3\xi_0(l')) \right) (F(k, q)\Sigma_{l'}^l(k', k) + \epsilon\Gamma_{l'}^l(k', k)) + 3\xi_{+2}(l' - 2)N_{l'}^{l'-2}u_{l'}^{l'-2}(k', q) (F(k, q)\Sigma_{l'-2}^l(k', k) + \epsilon\Gamma_{l'-2}^l(k', k)) + 3\xi_{-2}(l' + 2)N_{l'}^{l'+2}u_{l'}^{l'+2}(k', q) (F(k, q)\Sigma_{l'+2}^l(k', k) + \epsilon\Gamma_{l'+2}^l(k', k)) \right] \right\} + \frac{2M}{\pi\hbar^2} \sqrt{kk'} \left[\left(w_{l'}^{l'}(k', k) + u_{l'}^{l'}(k', k) (1 - 3\xi_0(l')) \right) \delta_{l, l'} + 3\xi_{+2}(l' - 2)N_{l'}^{l'-2}u_{l'}^{l'-2}(k', k)\delta_{l, l'-2} + 3\xi_{-2}(l' + 2)N_{l'}^{l'+2}u_{l'}^{l'+2}(k', k)\delta_{l, l'+2} \right] \quad (51)$$

$$\Gamma_{l'}^l(k', k) = \frac{2}{\pi} \sqrt{k'} \int_0^\infty \left\{ \frac{q^{3/2} dq}{(F^2(k, q) - \epsilon^2)} \left[\left(w_{l'}^{l'}(k', q) + u_{l'}^{l'}(k', q) (1 - 3\xi_0(l')) \right) (F(k, q)\Gamma_{l'}^l(k', k) - \epsilon\Sigma_{l'}^l(k', k)) + 3\xi_{+2}(l' - 2)N_{l'}^{l'-2}u_{l'}^{l'-2}(k', q) (F(k, q)\Gamma_{l'-2}^l(k', k) - \epsilon\Sigma_{l'-2}^l(k', k)) + 3\xi_{-2}(l' + 2)N_{l'}^{l'+2}u_{l'}^{l'+2}(k', q) (F(k, q)\Gamma_{l'+2}^l(k', k) - \epsilon\Sigma_{l'+2}^l(k', k)) \right] \right\} \quad (52)$$

with $F(k, q) \equiv \frac{\hbar^2 k^2}{2M} - \frac{\hbar^2 q^2}{2M}$. We have already discarded all $m \neq 0$ components, denoting $T_{l'}^l(k', k) = T_{l', 0}^{l, 0}(k', k)$. To solve the system numerically, we define the vectors:

$$\vec{\Sigma}_{l'}^l(k) = [\Sigma_{l'}^l(k'_0, k) \quad \Sigma_{l'}^l(k'_1, k) \quad \dots \quad \Sigma_{l'}^l(k'_N, k)] \quad (53)$$

$$\vec{\Sigma}^l(k) = [\vec{\Sigma}_0^l(k) \quad \vec{\Sigma}_2^l(k) \quad \dots \quad \vec{\Sigma}_{l'}^l(k) \quad \dots \quad \vec{\Sigma}_{l_f}^l(k)] \quad (54)$$

$$\vec{\Gamma}_{l'}^l(k) = [\Gamma_{l'}^l(k'_0, k) \quad \Gamma_{l'}^l(k'_1, k) \quad \dots \quad \Gamma_{l'}^l(k'_N, k)] \quad (55)$$

$$\vec{\Gamma}^l(k) = [\vec{\Gamma}_0^l(k) \quad \vec{\Gamma}_2^l(k) \quad \dots \quad \vec{\Gamma}_{l'}^l(k) \quad \dots \quad \vec{\Gamma}_{l_f}^l(k)] \quad (56)$$

$$\vec{T}^l(k) = [\vec{\Sigma}^l(k) \quad \vec{\Gamma}^l(k)] \quad (57)$$

with l_f the index of the last mode we include in the calculation and N the number of points. Ideally $l_f = \infty$ but in practice precise results are obtained with $l_f = 8$. The system of integral equations can thus be written in matrix form as:

$$A\vec{T}^l(k) = -\vec{v}^l(k) \quad (58)$$

with:

$$\vec{v}^l(k) = [0 \quad \dots \quad 0 \quad \vec{v}_{l'-2}^{l'}(k) \quad \vec{v}_{l'}^{l'}(k) \quad \vec{v}_{l'+2}^{l'}(k) \quad 0 \quad \dots \quad 0] \quad (59)$$

being $\vec{v}_{l'-2}^{l'}(k)$, $\vec{v}_{l'}^{l'}(k)$ and $\vec{v}_{l'+2}^{l'}(k)$ the discretized vector of the non-homogeneous contributions of the system. Due to the couplings between modes, the dimensions of A are now greater than in Sec. IV A, $A \in M_{2Nn_m \times 2Nn_m}(\mathbb{R})$ with n_m the number of modes. This increase in dimension implies a high memory cost, specially in low momentum calculations with $l = 0$. Because of that we use a special hybrid grid in momentum space, which concentrates a high quantity of points near the origin, such that the low momentum behaviour of the T-matrix elements can be well reproduced. The discretization used is:

$$k_i = \begin{cases} \exp\left(\log(k_0) + \frac{(\log(1) - d \log(k_0))}{(N_1 - 1)}(i - 1)\right) & k_i \leq 1 \\ 1 + \frac{(k_f - 1)}{(N_2 - 1)}(i - 1) & k_i > 1 \end{cases} \quad (60)$$

where $N = N_1 + N_2$, $i = 1, 2, \dots, N$, k_0 the first point of the grid and k_f the last one. In order to work with this grid, it is convenient to solve directly Eqs. (51) and (52), without applying the Plemelj identity. For $l \neq 0$ a standard linear grid provides the appropriate low k behaviour, and the application of the Plemelj identity to

Eqs. (51) and (52) is recommended. We present in Fig. (2) the solutions of the system of Eqs. (51) and (52) for $l = 0 = l'$ and $l = 0, l' = 2$.

Notice how the **anisotropy** of the potential originates couplings between different $T_{l'}^l(k', k)$ components, which makes the T-matrix elements be non diagonal in the $|E, l, m\rangle$ base. Since the potential of interest is also **long ranged**, the scattering amplitude no longer converges to the s-wave scattering length at low momentum, but several partial waves have a significant contribution [6]. We can define a set of **generalized scattering lengths** in analogy with Eq. (24), which was originally derived for a central, short ranged potential. Generalized scattering length are defined as:

$$a_{l'}^l \equiv \lim_{k \rightarrow 0} \frac{\pi T_{l'}^l(k, k)}{k} \quad (61)$$

These quantities are real, since for $k \rightarrow 0$, $\text{Re}\{T_{l'}^l(k, k)\} \gg \text{Im}\{T_{l'}^l(k, k)\}$. Numerical calculations indicate that already at $k = 10^{-2.5}$, $\text{Im}\{T_{l'}^l(k, k)\} / \text{Re}\{T_{l'}^l(k, k)\} \sim \mathcal{O}(10^{-2})$, as can be seen

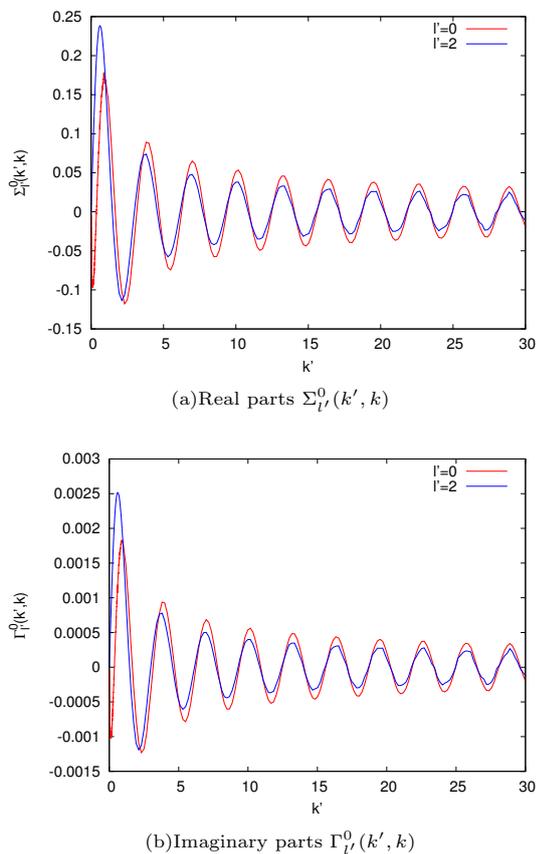


FIG. 2: Solutions of the system of equations (51) and (52) for $l = 0$. Results presented for $\frac{\hbar^2}{2M} = 1$. k is set to $k = 10^{-2.5}$, $V_0 = 10^{14}$, $d^2 = 16$, $R_0 = 2$, $n_m = 4$ and $\epsilon = 10^{-8}$. The number of points devoted to the exponential part of the grid is $N_1 = 900$ while that devoted to the linear part of the grid is $N_2 = 2400$ with $k_f = 450$.

in Fig.(2). Performing a partial wave expansion in Eq. (22) (which is still valid when the long ranged dipole part is present [11]) we can determine the dependence of the scattering amplitude on generalized scattering lengths at low momentum. The partial wave expansion yields:

$$\begin{aligned} f(\theta, k) &= -\frac{(2\pi)^2 M}{\hbar^2} T(\vec{k}', \vec{k}) \\ &= -\frac{(2\pi)^2 M}{\hbar^2} \langle \vec{k}' | \hat{T} | \vec{k} \rangle \\ &= -\frac{(2\pi)^2 M}{\hbar^2} \sum_{\substack{l, m \\ l', m'}} \int \int \left\{ \langle \vec{k}' | E_{q'}, l', m' \rangle \right. \\ &\quad \left. T_{l', m'}^{l, m}(q', q) \langle E_q, l, m | \vec{k} \rangle dE_q dE_{q'} \right\} \\ &= -\frac{(2\pi)^2}{k} \sum_{l, l'} T_{l'}^l(k) Y_{l'}^0(\theta_{k'}) Y_l^{0*}(\theta_k) \end{aligned} \quad (62)$$

where θ_k and $\theta_{k'}$ are the polar angle of the incident and scattered particles, respectively. Since $\vec{k}' = k \frac{\vec{r}}{r}$, we can write $\theta_{k'} = \theta$. We have used the identity [8]:

$$\langle E, l, m | \vec{k} \rangle = \frac{\hbar}{\sqrt{Mk}} Y_l^{m*}(\theta_k, \phi_k) \delta\left(E - \frac{\hbar^2 k^2}{2M}\right) \quad (63)$$

Since we can always use a reference system where the incident direction corresponds to the \hat{z} axis, we can set $\theta_k = 0$ without loss of generality. With this consideration, and taking the low momentum limit, one reaches:

$$f(\theta, k) \xrightarrow{k \rightarrow 0} -4\pi \sum_{l, l'} \sqrt{\frac{2l+1}{4\pi}} a_{l'}^l Y_{l'}^0(\theta) \quad (64)$$

The validity of Eq. (6) for the dipole interaction [13] implies that the partial wave superposition to build the scattering solution is analogous to the one presented for short ranged potentials. This implies that partial wave weights are [10]:

$$C_l^m = \frac{e^{i(\Delta_l + \frac{\pi l}{2})}}{k} \sqrt{4\pi(2l+1)} \quad (65)$$

with Δ_l the l -th phase shift, a quantity analogous to the one mentioned in Sec. IV A. Thus, the scattering amplitude can be written as [10]:

$$f(\theta, \phi) = \frac{1}{k} \sum_{l=0} \sqrt{4\pi(2l+1)} e^{i\Delta_l} \sin(\Delta_l) Y_l^0(\theta) \quad (66)$$

Combining Eq. (66) with Eq. (64) yields:

$$\sqrt{2l'+1} e^{i\Delta_{l'}} \sin(\Delta_{l'}) = -\pi \sum_l \sqrt{2l+1} T_{l'}^l(k) \quad (67)$$

Using the T-matrix elements we can find Δ_l , which enables us to build the appropriate superposition coefficients in Eq. (65) required to build the Monte Carlo trial wave function mentioned in the introduction of this work.

The generalized scattering lengths are also used in the construction of pseudopotentials, which are essential in the performance of mean field calculations through the Gross-Pitaevskii equation. In [1] the authors build a model pseudopotential for the interaction studied in this section from the $T_{l'}^l(k', k)$ elements. Another application of scattering lengths is the determination of the parameters of the potential which lead to the formation of bound states in the two body system [11], which arise in the case of the DHC potential from the attractive part of the dipole interaction. When a bound state is created, the generalized scattering lengths show a divergence for particular values of d^2 and R_0 . In order to show this, we present in Fig. (3) universal curves for a_0^0 and a_2^0 showing this effect. The curve presented for the s-wave scattering length reproduces the one from [11].

Interestingly, the low momentum values of $T_{l'}^l(k', k)$ obtained numerically agree almost exactly with the Born approximation for $(l, l') \neq (0, 0)$ away from resonances, which are given by:

$$\begin{aligned} a_{l'}^l \Big|_{\text{Born}} &= \lim_{k \rightarrow 0} \frac{\pi V_{l'}^l(k, k)}{k} & (68) \\ &= \lim_{k \rightarrow 0} \left\{ \delta_{m, m'} \frac{2M}{\hbar^2} \right. \\ &\times \left[\left(w_{l'}^{l'}(k, k) + u_{l'}^{l'}(k, k) (1 - 3\xi_0(l', m')) \right) \delta_{l, l'} \right. \\ &+ 3\xi_{+2}(l' - 2, m) N_{l'}^{l'-2} u_{l'}^{l'-2}(k, k) \delta_{l, l+2} \\ &\left. \left. + 3\xi_{-2}(l' + 2, m') N_{l'}^{l'+2} u_{l'}^{l'+2}(k, k) \delta_{l, l-2} \right] \right\} & (69) \end{aligned}$$

In order to evaluate this limit we must compute $w_{l'}^l(k, k)$ and $u_{l'}^l(k, k)$ with $k \rightarrow 0$, which are defined in Eqs. (43) and (44) respectively. To perform the calculations, it is convenient to introduce the variable:

$$z \equiv kr \rightarrow dz = kdr \quad (70)$$

The calculation for $w_{l'}^l(k, k)$ yields:

$$\begin{aligned} \lim_{k \rightarrow 0} w_{l'}^l(k, k) &= \lim_{k \rightarrow 0} V_0 \int_0^R r^2 j_l(kr) j_{l'}(kr) dr \\ &= \lim_{k \rightarrow 0} \frac{1}{k^3} V_0 \int_0^{kR} z^2 j_l(z) j_{l'}(z) dz \\ &= \lim_{k \rightarrow 0} \frac{V_0 k^2 R^3 j_l(kR) j_{l'}(kR)}{3k^2} \\ &= \frac{V_0 R^3}{3} \delta_{l, 0} \delta_{l', 0} & (71) \end{aligned}$$

where $\delta_{l, 0}$ is the Kronecker delta. We have used l'Hopital's rule and the low argument behaviour for $j_l(x)$ [12]. Using the variable z we can rewrite $u_{l'}^l(k, k)$ as:

$$u_{l'}^l(k, k) = \int_0^\infty \frac{d^2}{z} j_l(z) j_{l'}(z) dz = u_{l'}^l \quad (72)$$

which shows that $u_{l'}^l(k, k) = u_{l'}^l$, does not depend on k . The computation of the integral in Eq. (72) yields [14]:

$$u_{l'}^l = \frac{d^2 \pi \Gamma\left(\frac{l+l'}{2}\right)}{8 \Gamma\left(\frac{l-l'+3}{2}\right) \Gamma\left(\frac{l+l'+4}{2}\right) \Gamma\left(\frac{l'-l+3}{2}\right)} \quad (73)$$

where $\Gamma(l)$ is the gamma function. Eq. (73) only holds if $(l, l') \neq (0, 0)$, as $u_0^0 = \infty$. Particularizing for the l, l' couplings of interest leads to:

$$u_l^l = \frac{d^2}{2l(l+1)} \quad (74)$$

$$u_l^{l-2} = \frac{d^2}{6l(l-1)} \quad (75)$$

$$u_l^{l+2} = \frac{d^2}{6(l+2)(l+1)} \quad (76)$$

With these results, we can reach an expression for the generalized scattering lengths in the Born approximation,

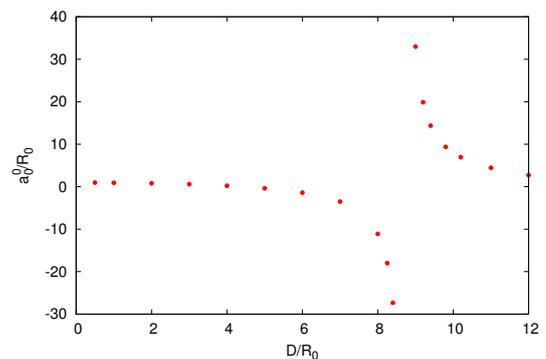
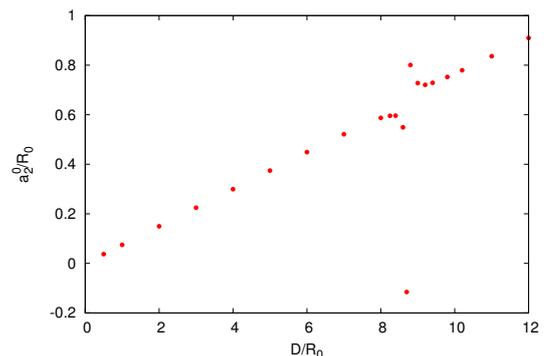

 (a) a_0^0

 (b) a_2^0

FIG. 3: Universal curves for the s-wave scattering length a_0^0 and for a_2^0 . The resonance, located at $\frac{D}{R_0} \simeq 8.7$, indicates the formation of a bound state in the two-body system. $D = \frac{2Md^2}{\hbar^2}$ is the dipole length.

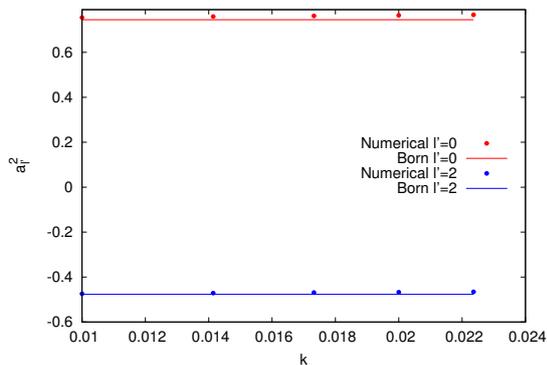


FIG. 4: Comparison between analytical values for a_0^2 and a_2^2 in the Born approximation and numerical results obtained by solving Eqs. (51) and (52) for $d^2 = 10$. Results are presented for $\frac{\hbar^2}{2M} = 1$.

which reads:

$$a_l^l \Big|_{\text{Born}} = -\frac{D}{(2l+3)(2l-1)} \quad (77)$$

$$a_l^{l-2} \Big|_{\text{Born}} = \frac{D}{2(2l-1)\sqrt{(2l-3)(2l+1)}} \quad (78)$$

for $(l, l') \neq (0, 0)$, which are consistent with the values presented in [15]. $D = \frac{2Md^2}{\hbar^2}$ is the characteristic dipole length defined in Eq. (3). We present, in Fig. (4) a comparison between the analytical Born approximation values for a_0^2 and a_2^2 , and the numerical results.

Although we have chosen a high barrier soft core (HBSC) potential to model the short ranged part of the full interaction, other similar options are also viable, such as a short ranged part modeled by $V_\sigma(r) = \left(\frac{\sigma}{r}\right)^{12}$. However, the s-wave scattering lengths of the full interaction obtained using a HBSC or a fast falling short ranged potential are very similar when both short ranged parts have the same scattering length and the system is not close to a resonance. This is shown in Tab. I. It is important to mention that we have introduced an infinitesimal cut-off parameter δ into $V_\sigma(r)$ in order to avoid divergences in the resolution of Eqs. (51) and (52). The effective potential to be used is $\tilde{V}_\sigma(r) = \frac{\sigma^{12}}{r^{12} + \delta}$. Under these conditions, appropriate results for the T-matrix can be obtained.

Finally, we present the s-wave scattering length of the full interaction used to model the droplet formation process of the system of trapped Dy¹⁶⁴ atoms mentioned in the introduction. From the PIGS simulations, where the $V_\sigma(r)$ short ranged model was used, we have observed that the formation of droplets involves a very narrow range of values of σ , mainly $\sigma \in [0.24, 0.28]$ (expressed in dipole units), with the first droplet state appearing at $\sigma = 0.28$. We present in Tab. II the values of the s-wave scattering lengths expressed in Bohr radius for the aforementioned values of σ .

V. Conclusions

In this report we have introduced the concept of the T-matrix while providing a numerical method to calculate it. We have presented how the anisotropy and the long range behaviour of an interaction affect its scattering properties: while anisotropy introduces couplings between different partial wave components of the T-matrix $T_{l',m'}^{l,m}(k',k)$ and makes them non diagonal in the partial wave basis of the free particle Hamiltonian, the long range behaviour makes several partial waves contribute to low energy scattering rather than just the s-wave, which is the dominant contribution for short ranged, isotropic potentials. This introduces the definition of a set of generalized scattering lengths $a_{l',m'}^{l,m}$. These facts have been illustrated with the calculation of the T-matrix elements for a dipole plus a hard core potential, which represents a model for the interaction between dipolar atoms such as Dy¹⁶⁴. For this potential, we have provided the appropriate partial wave superposition to build the asymptotic scattering solution as a function of the T-matrix elements, which can be used in the construction of a Diffusion Monte Carlo trial wave function. We have presented a universal curve for the generalized s-wave scattering length a_0^0 , which is crucial when building pseudopotentials [1], recovering the results in [11]. We have also shown the agreement between the analytical Born approximation and the numerical low momentum calculations away from a resonance for the generalized scattering lengths $a_{l'}^l$, with $(l, l') \neq (0, 0)$, as in [11].

By comparing scattering length calculations when setting the short ranged model interaction to be a high barrier soft core or a potential of the type $V_\sigma(r) = \left(\frac{\sigma}{r}\right)^{12}$ we conclude that the details of the short ranged part are not important in terms of the s-wave scattering length of the full interaction as long as it is not close to a resonance.

	HBSC	$\tilde{V}_\sigma(r)$
$d^2 = 2.83$	0.148	0.154
$d^2 = 3.54$	-0.270	-0.284
$d^2 = 4.24$	-0.992	-1.059
$d^2 = 4.95$	-2.489	-2.788
$d^2 = 5.66$	-7.873	-11.147

TABLE I: Comparison between the full interaction (dipole plus short ranged) s-wave scattering length when using a high barrier soft core (HBSC) or the $\tilde{V}_\sigma(r) = \frac{\sigma^{12}}{r^{12} + \delta}$ potential as a model for the short ranged part. Results presented for $\frac{\hbar^2}{2M} = 1$. Scattering length of both short ranged models is $a_{sc} = 0.70873$. The $d^2 = 5.66$ case corresponds to $\frac{D}{R_0} = 8$, which is rather close to the resonance located at $\frac{D}{R_0} \simeq 8.7$ (Fig. (3)). The parameters for the HBSC simulations are $k = 10^{-2.5}$, $V_0 = 10^{14}$ (soft core step), $R_0 = 0.70873$, $n_m = 4$, $N_1 = 900$, $N_2 = 2400$, $k_f = 450$, $\epsilon = 10^{-8}$, while for the decaying potential simulation $k = 10^{-2.5}$, $N_1 = 1700$, $N_2 = 900$, $k_f = 150$, $\epsilon = 10^{-8}$ and $\delta = 10^{-8}$.

σ	a_0^0
0.24	-560.736 a_B
0.25	-343.332 a_B
0.26	-244.728 a_B
0.27	-186.912 a_B
0.28	-148.141 a_B

TABLE II: S-wave scattering length of the full interaction $V(\vec{r}) = \tilde{V}_\sigma(r) + V_{dd}(r, \theta)$ as a function of σ for the range of droplet formation in the Dy^{164} system mentioned in the introduction. a_B is the Bohr radius. The simulation parameters are $k = 10^{-2.5}$, $N_1 = 1700$, $N_2 = 1000$, $k_f = 300$, $\epsilon = 10^{-8}$ and $\delta = 10^{-21}$.

Finally, we have presented the s-wave scattering length of the $V(\vec{r}) = \left(\frac{\sigma}{r}\right)^{12} + V_{dd}(r, \theta)$ potential, for $\sigma \in [0.24, 0.28]$ corresponding to the droplet formation regime seen in PIGS simulations of the system of trapped Dy^{164} atoms

[2] mentioned in the introduction.

VI. Acknowledgements

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