Dipolar confinement-induced molecular states in harmonic waveguides

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Abstract
The bound states of two identical dipoles in a harmonic waveguide are investigated. In the regime of weak dipole–dipole interactions, the local frame transformation method is applied to determine the spectrum of dipolar confinement-induced bound states analytically. The accuracy of the local frame transformation approach is discussed by comparing the analytical results with the numerical ones based on a solution of the close-coupling equations. It is found that close to the threshold energy in the waveguide, the local frame transformation method needs to include more partial wave states to obtain accurate bound state energies. As the binding energy increases, the local frame transformation method using a single partial wave state becomes more accurate. We also compare the bound states in waveguides and in free space. For the bosonic case, the s-wave dominated bound state looks like a free-space state when its energy is below a certain value. For the fermionic case, the p-wave dominated bound state energies in waveguides and in free-space coincide even close to zero energy.

Keywords: ultracold dipole gas, atomic waveguide, dipolar confinement-induced bound state, local frame transformation approach

(Some figures may appear in colour only in the online journal)

1. Introduction
Ultracold gases in tightly confining traps have attracted much attention particularly since one can realize effective one- [1, 2] and two- [3] dimensional systems by tuning their geometry. The tight confinement modifies significantly the interparticle collisional properties, and specifically leads to confinement-induced resonances (CIRs) which have been predicted theoretically [4–7] and observed experimentally [1, 8]. The capability to tune the two-body interaction via Feshbach resonances and/or CIRs enabled the investigation of strongly correlated many-body physics in low dimensions [9]. Tight traps also affect the two-body bound state properties, and confinement-induced molecular (CIM) states have been observed for isotropic interparticle interaction [1, 2].

Dipolar gases [10–15] possess anisotropic dipole–dipole interaction (DDI) [16] which makes it interesting to investigate the influence of a tight trap on such systems. It has been demonstrated that adding a trap in one direction can suppress the reactive scattering collisions in a polar molecular gas [17]. In addition, one can control the reactive collisions by tuning the orientation of the dipoles with respect to the confined direction [18]. The influence of a two-dimensional trap on the dipolar reactive collision has been studied in [19, 20]. In the non-reactive case, the modification of the DDI by traps has been analyzed theoretically in [21, 22] thereby demonstrating that dipolar confinement-induced resonances (DCIR) occur in harmonic waveguides [23]. For the case that the confining potential is anharmonic, inelastic DCIRs have been predicted [24]. The relative orientation between dipoles and the waveguide axis can also be used to tune the two-body interaction in a quasi-one dimensional geometry [25]. While the scattering properties of
two dipoles in traps have been theoretically investigated, the
dipolar CIM (DCIM) state properties of such system have been
addressed much less.

In this work, we consider two identical dipoles, which can be
either bosonic or fermionic, in a harmonic waveguide. The
dipoles are aligned along the longitudinal direction (z axis) of
the waveguide. The local frame transformation approach [23, 26–37]
is applied to calculate the DCIM states when the DDI is weak. A
dipolar bound state equation is derived which allows one to
determine the energies of the DCIM states analytically with the
free-space scattering information as input. Moreover, the dipolar
bound state equation within the Born approximation shows
explicitly the influence of the DDI in determining the bound state
energies. By comparing the local frame transformation results
with corresponding numerical calculations, it is found that,
below threshold, the local frame transformation approach with
the single partial wave approximation is accurate even in the
presence of DDI. Close to threshold, one needs to include higher
partial wave states in the local frame transformation approach to
get accurate bound state energies. The dependence of the DCIM
states on the DDI strength is explored. Based on numerical
calculations, both the weak and strong DDI regimes are inves-
tigated. We find that qualitatively the dependence of the DCIM
states on the DDI is similar in these two regimes. The DCIM
state becomes increasingly bound as the DDI increases. The
l > 0-wave dominant bound states are more sensitive to the
variation of the DDI compared to the s-wave dominant states.
DCIM states can emerge by increasing the DDI.

The paper is organized as follows. Section 2 introduces
our computational methods. The set of close-coupling
equations is provided in a partial wave basis, and the dipolar
bound state equations based on the local frame transformation
approach are presented. In section 3, the properties of the
DCIM states are discussed. Both the bosonic and fermionic
cases are analyzed. Section 4 contains our conclusions.

2. Computational method

In harmonic waveguides, the center of mass motion and
relative motion are separable. The Hamiltonian of the relative
motion, which contains a short-range isotropic interaction in
conjunction with DDI, is expressed as

\[ H = T + V_c(r) + V_d(r) + V_{dd}(r), \]

where T is the kinetic energy, \( V_c(r) \) is the transverse trapping
potential, and is assumed to be an isotropic two-dimensional
harmonic potential \( V_c(r) = \frac{1}{2} \mu \omega^2 r^2 \), where \( \mu \) is the reduced
mass, \( \omega \) is the trapping frequency, and \( r \) is the magnitude of
the transverse component of the interparticle vector \( r \). \( V_d(r) \) is the
short-range isotropic potential, and depends on the species
under consideration. \( V_{dd}(r) \) is modeled by a Lennard–Jones
potential \( V_{dd}(r) = C_6/r^6 - C_10/r^{10} \), which possesses a van
der Waals potential tail (note that \( r = |r| \)). \( V_d(r) \) is the DDI,
and has the usual form \( V_d(r) = \frac{d^2}{r^2} (1 - 3 \cos^2 \theta) \) where \( d \) is
the dipole moment, and \( \theta \) is the angle between the z axis and
the interparticle vector \( r \). We remark that the singularity of the
DDI at the origin is remedied by the corresponding behavior of
the short range potential at the origin. The threshold energy of
two dipoles without the confinement is chosen to be the
zero energy point. The energy of the scattering threshold in
waveguides is given by \( E_{th} = \frac{h^2}{2d^2} \).

The three potential terms in equation (1) determine three
length scales in the system. The length scale associated with the
transverse confinement is the harmonic oscillator length \( a_t = \frac{\sqrt{\hbar}}{\mu \omega} \), whereas the length scale of the short-range interaction
term is the van der Waals length given by the relation \( \beta_{vdw} = (2\mu C_6/h^3)^{1/4} \). Finally the DDI is characterized by the dipole
length \( l_d = \mu d^2/h^2 \). Below we will introduce two methods to
determine the bound state belonging to the Hamiltonian (1). One
approach is the close-coupling method which solves the problem
numerically. In the weak DDI regime, the dipole length and the
van der Waals length are far smaller than the harmonic oscillator
length. The local frame transformation method is in this case
applied to derive the DCIM states (semi)analytically.

2.1. Close-coupling method

We expand the two-body wavefunction \( \psi \) in the partial wave
basis

\[ \psi(r, \theta, \phi) = \sum_{m} \psi_m(\theta, \phi), \]

where \( \psi_m(\theta, \phi) \) are the partial wave functions, \( Y_{lm} \) are the spherical
harmonics, and \( l \) and \( m \) are the partial wave quantum number and
the magnetic quantum number, respectively. Since the system
under investigation is cylindrically symmetric, the magnetic
quantum number is conserved. In the following \( m \) is set to zero,
and is consequently omitted. The kinetic term T and the short-
range potential \( V_c(r) \) are diagonal in the partial wave basis. The
dipole potential \( V_d(r) \) and the transverse trapping potential \( V_{dd}(r) \)
couple different partial wave states. The matrix elements of \( V_d(r) \) and
\( V_{dd}(r) \) in the partial wave basis are given, respectively, by [38]

\[ V_{dd}(r) = \langle l|V_{dd}|l'\rangle = \frac{2d^2}{r^3} \sqrt{(2l + 1)(2l' + 1)} \begin{pmatrix} 1 & 2 \end{pmatrix}, \]

\[ V_{dd}(r) = \langle l|V_{dd}|l'\rangle = \frac{3}{4} \mu \omega^2 r^2 \delta_{ll'}, \]

where \( \delta \) is the Kronecker delta function, and the large curved
brackets are 3-j symbols. In the partial wave basis, the Schrö-
dinger equation is a set of close-coupling equations satisfied by
the radial wavefunction \( f_l(r) \)

\[ \left[ \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_c(r) + V_{dd}(r) \right] f_l(r) + \sum_{l'} \left( V_{dd}(r) + V_{dd}(r) \right) f_{l'}(r) = E_l(r), \]

where \( V_c(r) = \frac{l(l+1)}{2\mu r^2} \) is the centrifugal term, and \( E_l \) is the total
energy. With the boundary condition that the bound state
wavefunction vanishes at \( r \to 0 \) and \( r \to \infty \), the set of close-
coupling equations given in equation (5) is solved numerically based on the log-derivative algorithm [39]. To obtain the bound state energy $E_b$ and the wavefunction $\psi$ the approach of [40] is employed.

In the numerical calculation, the dimensionless version of equation (5) is used, in which the length and energy are scaled by $a_\perp$ and $\hbar\omega_\perp$, respectively. The coefficient $C_6$ in the Lennard–Jones potential is fixed, such that $\beta_b/a_\perp = 0.018$, which is an experimentally achievable value. For example, the van der Waals coefficient of two ground state $^{166}\text{Er}$ atoms is 1723 au [41], and the corresponding van der Waals length $\beta_b$ is 151 au. In [42], a transverse trapping potential with frequency $\omega_\perp \sim 600 \text{ Hz}$ is realized experimentally for Er atoms. The corresponding harmonic oscillator length $a_\perp$ is 8518 au, and the ratio $\beta_b/a_\perp$ amounts to 0.018. For other systems, the van der Waals lengths would be different. Nevertheless one can tune the transverse trapping frequency $\omega_\perp$ to achieve the desired value for $\beta_b/a_\perp$. The coefficient $C_{10}$ in the Lennard–Jones potential is varied such that the scattering length of the Lennard–Jones potential can be changed significantly, and moreover, the number of bound states supported by the Lennard–Jones potential can be tuned.

### 2.1.1. Partial wave probability density of the DCIM states.

The partial wave probability densities (PD) of the DCIM state $P^l_b = |f|^2$ are calculated via close-coupled method [39, 40]. By examining the partial wave PDs, regions dominated by different terms in the Hamiltonian (1) are identified.

The partial wave PDs for a bosonic DCIM state are shown in the upper panel of figure 1 (solid line). The energy of the DCIM state is $E_b/\hbar\omega_\perp = 0.5$. The scaled $C_{10}'/C_{10}/(\hbar\omega_\perp a_\perp^{10})$, which is dimensionless, is set to be $6.7 \times 10^{-19}$. The ratio $l_d/a_\perp$ is 0.026. In the range $r/a_\perp \ll 1$, the trapping potential is far smaller than the short-range potential and DDI, and can be neglected. As a demonstration, we performed the free space scattering calculation by dropping the term $V_d(r)$ in equation (1). The partial wave PD $P^l_b$ of the scattering state at energy $E_b$ is also shown in the upper panel of figure 1 (dotted line). The lower panel of figure 1 is a zoom-in plot of the upper panel in the short-range region $r/a_\perp \ll 1$, and clearly shows that $P^l_b$ has the same nodal structure in this region. This indicates that the trapping potential is negligible for $r/a_\perp \ll 1$, and the two dipoles interact essentially like in free space.

The partial wave PDs shown in figure 1 offer more information. The DCIM state (solid line in figure 1) involves many partial wave components, and for the depicted state, the dominant one is the s-wave component. The oscillatory behavior of $P^l_b$ in the short-range region $r/a_\perp \ll 1$, shown in the lower panel of figure 1, is due to the presence of the potential well of the interaction potential $V_{\text{int}}(r) = V_d(r) + V(r)$. It is noted that there are maxima for $P^l_b$ with $l > 0$ at large distances $r/a_\perp > 1$. By examining the potential curves in the partial wave basis, we encounter potential wells at distances $r/a_\perp > 1$ for $l > 0$ partial wave channels as shown in figure 2. Considering weak DDI, the potential well results from the competition between the decreasing centrifugal potential $V_{\text{cent}}$ and the increasing trapping potential $V(r)$ as the interparticle distance increases. The positions of the maxima for the high partial wave PDs coincide with the positions of the minima of the outer potential wells at $r/a_\perp > 1$.

In the region $r/a_\perp > 1$, the short-range potential $V_d(r)$ and the DDI potential $V_l(r)$ decay to zero, and the trapping potential $V(r)$ becomes dominant. In this region the system is mainly governed by $V_l(r)$, and is nearly independent of $V_d(r)$ and $V(r)$. In order to confirm this, we compare in figure 3 the partial wave PDs of two DCIM states calculated with different short-range potential $V_d(r)$ and DDI potential $V_l(r)$. The bound state PD $P^l_b$ shown in figure 1 is also shown in figure 3 (solid line). As stated before, in the calculation of $P^l_b$ the Lennard–Jones potential supports ten bound states, and the

![Figure 1](image1.png)

**Figure 1.** (Upper panel) Bound state partial wave probability density $P^l_b$ of two identical bosonic dipoles in a waveguide is shown (solid line). The free-space scattering state probability density $P^l_b$ is also provided (dashed line). $C_{10}' = 6.7 \times 10^{-19}$ and the Lennard–Jones potential supports ten bound states. The ratio $l_d/a_\perp$ is 0.026. The bound state energy and the scattering energy are the same $E_f/\hbar\omega_\perp = 0.5$. $P^l_b$ is renormalized at $r_0/a_\perp = 0.01$, so that $P^l_b(r_0/a_\perp) = P^l_b_0 - q(r_0/a_\perp)$. (Lower panel) A zoom-in picture at short distances.
diode moment \( l_d/a_0 \) is 0.026. Another bound state PD \( P^{|l|}_{in} \), the energy of which is also \( E_{in} \), is additionally shown (dotted line). The Lennard–Jones potential supports here one bound state and \( l_d/a_0 \) is zero in the calculation of \( P^{|l|}_{in} \). Due to the different \( V_d(r) \) and \( V_L(r) \) used in the calculations, the short-range parts of the two bound state PDs are significantly different. Nevertheless, in the region \( r/a_0 > 1 \), the two bound state PDs are nearly the same, and are, to a large extend, determined by the trapping potential.

Based on the above observation of length scale separation in the system, we introduce the local frame transformation approach below, which can connect the two-body properties in waveguides with the scattering properties in free space analytically.

### 2.2. Local frame transformation approach

The concept of the local frame transformation approach was introduced in [26, 27] to calculate the Stark effect of non-hydrogenic Rydberg spectra. Subsequently the method was generalized to study the photodetachment of negative ions in magnetic fields [28, 29] and the photoionization of atoms [30, 31]. The application of the local frame transformation approach to ultracold collisions in quasi-low dimensional geometry was pioneered in [32]. Until now, it has been applied to understand different aspects of ultracold collisions in harmonic waveguides, such as higher wave CIR [33], energy dependence of the CIRs [34], multi-open-channel collisions [35] and the dipolar CIRs [23]. Ultracold collisions in other confining geometries have been discussed in [36]. Recently the local frame transformation approach has been adopted to treat the two-body scattering analytically in the presence of spin–orbit coupling [43]. Here we provide a further application of the local frame transformation approach, and show that one can obtain a comprehensive analysis of the DCIM states. In the following, the key idea of the local frame transformation approach is briefly introduced (see [32–34] for more details) and then the bound state equation for two dipoles in waveguides is presented. Finally, within the Born approximation, the dipolar bound state equation is simplified to show the dependence on the DDI explicitly.

#### 2.2.1. Local frame transformation method for bound states: a brief review

As shown in figures 1 and 3, the length scales of the short-range potential \( V_d(r) \), DDI potential \( V_d(r) \) and of the trapping potential \( V_t(r) \) are separated in the weak DDI regime. In the region \( r/a_0 \ll 1 \), \( V_t(r) \) is small compared to \( V_d(r) \) and \( V_d(r) \), and the two dipoles effectively interact as if there is no confinement. The partial wave basis is then employed to construct the wavefunction matrix \( \Psi(r) \) in this region

\[
\Psi(r) = f(r) - G(r)K^{3D},
\]

(6)

where \( f = \text{diag} \{ f_1, f_2, \ldots \} \) and \( G = \text{diag} \{ G_1, G_2, \ldots \} \) are diagonal matrices, \( f_i = j_i(r)P_i(\cos \theta) \) and \( G_i = n_i(r)j_i(\cos \theta) \) are the spherical Bessel functions and spherical Neumann functions, respectively. \( P_i(\cos \theta) \) are the Legendre polynomials. The effect of the two-body interaction is encapsulated in the free space \( K \) matrix, denoted as \( K^{3D} \).

In the region \( r/a_0 \gg 1 \), the interchange interaction \( V_d(r) + V_d(r) \) vanishes, and the system can be treated as two non-interacting particles in a waveguide. The wavefunction in this region can be written as

\[
\Psi(r) = F(r) - G(r)K^{3D},
\]

(7)

where \( F = \text{diag} \{ F_1, F_2, \ldots \} \) and \( G = \text{diag} \{ G_1, G_2, \ldots \} \) are diagonal matrices. \( F_i \) and \( G_i \) are the regular and irregular solutions of the Hamiltonian (1) without the short-range potential \( V_d(r) \) and the DDI potential \( V_d(r) \). For identical bosons, \( F_i(\rho, z) = \Phi_i(\rho)\cos q_dz \) and \( G_i(\rho, z) = \Phi_i(\rho)\sin q_dz \). For identical fermions, \( F_i(\rho, z) = \Phi_i(\rho)\text{Sign}(z)\sin q_dz \) and
$G_n(z) = -\Phi_n(r)\text{Sign}(z)\sin q_n z$ (for details see [32, 33]), where $z$ is the $z$ component of the interparticle vector $r$, $\Phi_n(r)$ is the eigenfunction of the 2D harmonic oscillator, $\text{Sign}(z)$ is the sign function, $q_n$ the channel momentum along the waveguide axis determined by $\frac{q^2a^2}{2}\omega_z^2 = E - \hbar\omega_z^2(2n + 1)$, and $K^{1D}$ is the $K$ matrix at large distances.

In the intermediate region $\beta_n/a_l, \lambda_l/a_l < r < 1$, both $V_s(r) + V_0(r)$ and $V_t(r)$ are small compared to the kinetic energy. Then in this region, both the partial wave basis \{\Omega\}_l and the asymptotic basis \{F_n, G_n\}, can be used to describe the wavefunction. A local transformation matrix $U$ can be defined which connects the two basis sets [28]

$$F_n = \sum_l \delta_{ll} U_{ln}, \quad G_n = \sum_l \delta_{ll} (U^T)_{ln}^{-1}.$$  \hspace{1cm} (8)

The element of the transformation matrix $U$ reads [34, 37]

$$U_{ln} = \sqrt{\frac{\beta_n}{a_l}} \frac{(\beta_n a_l)^{l+1}}{a_l \beta_n k a_l} \bigg(\frac{2l+1}{k a_l^2} p_l(q_n/k)\bigg),$$  \hspace{1cm} (9)

where $n$ is the transverse harmonic oscillator quantum number, $d_0$ is $l/2$ for even $l$ and $(l + 1)/2$ for odd $l$. $k = (2\mu E/h^2)^{1/2}$ is the collisional momentum.

The local frame transformation $U$ can be used to express $K^{1D}$ in terms of $K^{3D}$ according to the relation [34]

$$K^{1D} = UK^{3D}U^T.$$  \hspace{1cm} (10)

From the $K^{1D}$ matrix, one can deduce both bound state and scattering information in waveguides [34]. We are interested in the bound state spectrum here. By imposing asymptotically an exponentially decaying boundary condition in the wavefunction (7), one obtains the following relation for $K^{1D}$ [33, 34]

$$\text{det}(I - iK^{1D}) = 0,$$  \hspace{1cm} (11)

where the roots of equation (11) provides us with the energies of the confinement-induced bound state $E_{b\nu}$.

### 2.2.2. Dipolar bound state equation

Next we examine the explicit expression for the $K^{3D}$ matrix in the presence of DDI, and derive the dipolar bound state equation in terms of the $K^{3D}$ matrix. For systems consisting of atoms governed by the van der Waals interaction, the single partial wave approximation works quite well in the ultracold regime [34]. In the presence of DDI, different partial wave states are coupled [44]. To be specific, the $l$ partial wave is coupled to the $l'$ partial wave with $l' = l, l \pm 2, |l - l'| = 0$ is an exceptional case which is not coupled by the DDI. In the determination of DCCR [23], the local frame transformation approach with three partial wave states can accurately reproduce the numerical results in the weak DDI regime. Therefore, we include up to three lowest partial wave states in the derivation of the bound state equation either for bosons or fermions. For identical particles, the free space $K^{3D}$ matrix including three partial wave states can be expressed as [23]

$$K^{3D} = \begin{pmatrix} K_{l_h l_l} & K_{l_h l_{l'}} & 0 \\ K_{l_{l'} l_l} & K_{l_{l'} l_{l'}} & K_{l_{l'} l_{l''}} \\ 0 & K_{l_{l''} l_l} & K_{l_{l''} l_{l'}} \end{pmatrix}.$$  \hspace{1cm} (12)

where $l_h, l_l$ and $l_l'$ label the quantum numbers of the lowest three partial wave states in ascending order. For identical bosons, the lowest three partial wave states are the $s, d$ and $g$ wave states. For identical fermions, these are the $p, f$ and $h$ wave states. In the expression of $K^{3D}$ (see equation (12)), direct couplings between different partial waves due to the DDI are included, such as $K_{l_h l_l}, K_{l_h l_{l'}}$ and $K_{l_{l'} l_l}, K_{l_{l'} l_{l''}}$. Since the weak DDI is considered here, the indirect couplings between partial wave states which are mediated by another state are set to zero, such as $K_{l_h l_{l''}}, K_{l_{l'} l_h}, K_{l_{l'} l_{l''}}$.

From the $K^{3D}$ matrix, the generalized scattering length $a_{1,1'}$ is introduced as [45]

$$a_{1,1'} = -\frac{K_{l_h l_l}}{k}.$$  \hspace{1cm} (13)

By substituting equations (10) and (12) into equation (11), the dipolar bound state equation including three partial wave states can be written as

$$a_{b, b'} = \frac{i}{k} \frac{\Delta_N}{\Delta_D},$$  \hspace{1cm} (14)

where

$$\Delta_N = -1 + 2im_{l_l l_h} K_{l_h l_l} + m_{l_l l_h} K_{l_h l_l}^2$$

$$+ i m_{l_l l_h} K_{l_h l_l} - m_{l_h l_{l'}} K_{l_{l'} l_h} + 2m_{l_l l_{l'}} K_{l_{l'} l_h} K_{l_h l_l}$$

$$+ m_{l_h l_{l'}} K_{l_{l'} l_h}^2 (1 - i m_{l_{l'} l_h} K_{l_h l_l})$$

$$+ m_{l_h l_{l'}} (-2m_{l_{l'} l_h} K_{l_h l_l} - m_{l_{l'} l_{l''}} K_{l_{l'} l_h} K_{l_{l''} l_h})$$

$$+ m_{l_h l_{l'}} K_{l_{l'} l_h}^2 (-1 + i m_{l_{l'} l_h} K_{l_h l_l} + m_{l_{l'} l_{l'}} K_{l_{l''} l_h}(i + m_{l_{l''} l_{l'}} K_{l_{l''} l_h}))$$

$$+ 2m_{l_{l'} l_{l''}} K_{l_{l''} l_h}(i + m_{l_{l''} l_{l'}} K_{l_{l''} l_h})$$

$$+ m_{l_{l'} l_{l''}} (K_{l_{l''} l_h} + i m_{l_{l''} l_{l'}} K_{l_{l''} l_h} K_{l_{l''} l_h}),$$

$$\Delta_D = -2m_{l_l l_h} m_{l_{l'} l_h} (i K_{l_h l_l} + m_{l_{l'} l_h} K_{l_h l_l}^2 - m_{l_h l_{l'}} K_{l_{l'} l_h} K_{l_{l'} l_h})$$

$$+ m_{l_l l_h} (m_{l_{l'} l_h} K_{l_h l_l}^2 - K_{l_h l_l} (i + m_{l_{l'} l_h} K_{l_h l_l}))$$

$$+ m_{l_l l_h} (-i K_{l_h l_l} + m_{l_{l'} l_h} K_{l_h l_l}^2 - K_{l_h l_l} K_{l_{l'} l_h})$$

$$+ m_{l_l l_h} (-1 + 2i m_{l_{l'} l_h} K_{l_h l_l} + i m_{l_{l'} l_{l'}} K_{l_{l''} l_h})$$

$$+ m_{l_{l'} l_{l''}} (K_{l_{l''} l_h}^2 - K_{l_{l''} l_h} K_{l_{l''} l_h})$$

$$+ m_{l_{l'} l_{l''}} (-m_{l_{l''} l_{l'}} K_{l_{l''} l_h}^2 + K_{l_{l''} l_h}(i + m_{l_{l''} l_{l'}} K_{l_{l''} l_h})),$$

(15)

and $M_{l, l'}$ is the trace $\sum_j U_{lj}^* U_{l'j}$ over all the closed transverse harmonic oscillator modes, and are known analytically [34]. The explicit expressions for $M_{l, l'}$ are given in the appendix for the cases of identical bosons and fermions considered in this work.

In the dipolar bound state equations (14), two sets of quantities are needed to determine the DCIM state. One set is the $M_{l, l'}$, which contain the geometrical information of the waveguide and are known analytically (see appendix). The other set is the elements of the free-space $K^{3D}$ matrix, or equivalently the generalized scattering length $a_{1,1'}$ which encapsulate the effect of the interparticle interaction.
Equation (14) provides us with the spectrum of the DCIM states once the free-space $\mathbf{K}^{3D}$ is known. This is one of the main results of this paper.

By setting $K_{l_1l_1} = K_{l_1l_1} = K_{l_1l_1} = 0$ in equations (15) and (16), one can obtain the bound state equation including two partial wave states. By setting all the other elements of the $\mathbf{K}^{3D}$ matrix to zero except $K_{l_1l_1}$, the bound state equation with a single partial wave state is obtained.

2.2.3. Dipolar bound state equation within Born approximation.

One can obtain the $a_{l_1l_1}$ by solving the free space scattering problem numerically [38]. Alternatively, the Born approximation can be adopted to compute analytically $a_{l_1l_1}$ away from resonances [38]

$$a_{l_1l_1} = -\frac{2l_1}{(2l_1-1)(2l_1+3)},$$

and

$$a_{l_1l_2} = -\frac{l_1}{(2l_1-1)(2l_1+1)(2l_1+3)},$$

We note that the Born approximation cannot be used to calculate the term $a_{ss}$ [38].

Applying the Born approximation to calculate the high partial wave elements of the $\mathbf{K}^{3D}$ matrix, the dipolar bound state equation (14) for the bosonic dipoles is simplified to

$$a_{ss} = \frac{i - 1 + \eta_1^F l_1 + \eta_2^F l_2 + \eta_3^F l_3}{\sigma_0^B + \sigma_1^B l_2 + \sigma_2^B l_3^2},$$

where

$$\eta_1^B = \frac{2ik}{1155}(55M_{dd} + 77\sqrt{5}M_{ds} + 11\sqrt{5}M_{gd} + 15M_{gg}),$$

$$\eta_2^B = \frac{k^2}{3465}(77M_{ds}^2 - 7M_{gd}^2 + 2M_{dd}(11M_{gd} + 6\sqrt{5}M_{gg})$$

$$12\sqrt{5}M_{gd}M_{gs} + M_{dd}(7M_{gg} - 22M_{gs} - 77M_{ss})),$$

$$\eta_3^B = \frac{-2ik^3}{3465}(M_{dd}^2M_{gg} - 2M_{dd}M_{gd}M_{gs} + M_{gd}^2M_{ss}$$

$$+ M_{dd}(M_{gs}^2 - M_{gg}M_{ss})),$$

and

$$\sigma_0^B = -M_{ss},$$

$$\sigma_1^B = \frac{-2ik}{1155}(55M_{dd}^2 + 11\sqrt{5}M_{ds}M_{gs} + 15M_{gg}^2$$

$$- (55M_{dd} + 11\sqrt{5}M_{gd} + 15M_{gg})M_{ss}$$

$$- (55M_{dd} + 11\sqrt{5}M_{gd} + 15M_{gg})M_{ss}),$$

$$\sigma_2^B = \frac{k^2}{495}(M_{dd}^2M_{gg} - 2M_{dd}M_{gd}M_{gs} + M_{gd}^2M_{ss}$$

$$+ M_{dd}(M_{gs}^2 - M_{gg}M_{ss})).$$

The dipolar bound state equation for the $p$-wave dominated fermionic DCIM state, which exists in the vicinity of free space resonance of $a_{pp}$, is simplified within the Born approximation to

$$a_{pp} = \frac{i - 1 + \eta_1^F l_1 + \eta_2^F l_2 + \eta_3^F l_3^2}{\sigma_0^F + \sigma_1^F l_2 + \sigma_2^F l_3^2},$$

where

$$\eta_1^F = \frac{2ik}{45045}(1001M_{df} + 429\sqrt{2}M_{pp}$$

$$+ 65\sqrt{77}M_{hf} + 385M_{hh}),$$

$$\eta_2^F = \frac{k^2}{675675}(1287M_{df}^2 - 405M_{hf}$$

$$+ 10M_{fp}(13\sqrt{33}M_{df} + 22\sqrt{2}M_{hf}$$

$$- 220\sqrt{2}M_{gd}M_{gs} + M_{dd}(405M_{hh}$$

$$- 130\sqrt{33}M_{pp} - 1287M_{pp})),$$

$$\eta_3^F = \frac{-2ik^3}{61425}(M_{df}^2M_{hh} - 2M_{df}M_{hf}M_{pp} + M_{hf}^2M_{pp}$$

$$+ M_{hf}(M_{pp} - M_{hh}M_{pp})),$$

and

$$\sigma_0^F = -M_{pp},$$

$$\sigma_1^F = \frac{-2ik}{45045}(1001M_{df} + 65\sqrt{77}M_{df}M_{pp} + 385M_{pp}$$

$$+ (1001M_{df} + 65\sqrt{77}M_{hf} + 385M_{hh})M_{pp}),$$

$$\sigma_2^F = \frac{-3k^2}{5005}(M_{df}^2M_{hh} - 2M_{df}M_{hf}M_{pp} + M_{hf}^2M_{pp}$$

$$+ M_{hf}(M_{pp}^2 - M_{hh}M_{pp})).$$

Compared to the dipolar bound state equations (14), (19) and (22) depend explicitly on $l_2$ revealing in this manner the influence of the DDI in determining the energies of DCIM states. The influence of the waveguide is contained in the two sets of parameters $\eta$ and $\sigma$ in equations (19) and (22) which are expressed in terms of $M_{ff}$. These equations allow us to investigate the dependence of DCIM states on $a_{ss}$ (bosonic dipoles) or $a_{pp}$ (fermionic dipoles) for fixed DDI analytically, which will be studied in the following section.

3. DCIM states

In the following the dipolar confinement-induced bound states are investigated. Both the identical bosonic and fermionic dipoles are considered. In each case, two sets of calculations have been performed. In a first set, the dipole moment $d$ is fixed, $C_{10}$ is varied and accordingly the generalized scattering lengths $a_{l_1}$ change. Such a situation can be realized experimentally by tuning the short-range interaction $V_{sr}(r)$ via Feshbach resonances [46] while keeping the DDI unchanged. We consider the bound state dominated by its lowest partial wave state, i.e. the $s$-wave dominated bound state for identical bosonic dipoles or $p$-wave dominated bound state for identical fermionic dipoles. The variation of the binding energy as a function of $a_{ss}$ or $a_{pp}$ is examined. For the second set we fix
C_{10} and allow the dipole moment d to vary. This case can be achieved experimentally, for example in the case of electric dipoles, by tuning external electric fields. The dependence of the bound state energy on the DDI, more specifically the dipole length, is studied.

3.1. Bosonic DCIM states

For bosonic DCIM states and for a fixed DDI strength \( l_d/a_0 = 0.026 \), the scaled binding energy \( E_{\text{bi}}^s = E_{\text{bi}}/\hbar a_0 \) is shown in the upper panel of figure 4 as a function of \( a_s/a_0 \). We note that the binding energy in waveguides is given by \( E_{\text{bi}} = E_{\text{bi}}^s - E_0 \). The numerical data obtained from the close-coupling method are shown as a black solid line. \( C_{10} \) is varied here in the region where the corresponding Lennard–Jones potential supports either one or no bound state in free space. We consider the DCIM states in the energy range \( 0 < E_0/\hbar a_0 < 1 \). Once a bound state is determined for a specific \( C_{10} \), then the free-space scattering calculation is performed to calculate \( a_{ss} \) at the bound state energy.

The bound state energy obtained by the local frame transformation approach including one (green dotted line), two (blue dotted–dashed line) and three (red dashed line) partial wave states are also shown in the upper panel of figure 4. In this set of local frame transformation calculations, \( a_{ss} \) can be treated as a parameter, and all the other generalized scattering lengths needed in the bound state equations can be calculated within the Born approximation. The local frame transformation approach including a single partial wave state reproduces the numerical results well when the binding energy \( E_{\text{bi}}^s \) is larger than 0.1. Approaching the scattering threshold in the waveguide \( E_{\text{bi}}^s \to 0 \), there will be a large portion of the bound state wavefunction spanning over large distances \( r/a_0 > 1 \) where the trapping potential dominates and different partial wave states are strongly coupled together.

In this energy region, the deviation between the bound state energy based on the local frame transformation approach with a single partial wave state and the numerical bound state energy becomes large. The upper panel of figure 4 shows that including one more partial wave state (blue dotted–dashed line) in the local frame transformation approach can give a more accurate bound state energy below the threshold for the considered regime. Including three partial wave states (red dashed line) improves further the accuracy of the local frame transformation approach in the energy region \( E_{\text{bi}}^s < 0.1 \).

In the local frame transformation calculation with \( s, d \) and \( s, d, g \) partial wave states (blue dotted–dashed line and red dashed line in figure 4), an avoided crossing appears in the binding energy curve in the energy region \( E_{\text{bi}}^s \to 0 \) to one, i.e. \( E_b \) close to zero, which is not observed in the numerical result and in the local frame transformation approach with s-wave state only. The lower panel of figure 4 shows magnification in the vicinity of the avoided crossing. The appearance of the avoided crossing is attributed to the inaccuracy of the local frame transformation for higher partial wave states in the energy region \( E_{\text{bi}}^s \to 0 \). To apply the local frame transformation, an intermediate regime is needed where the kinetic energy dominates the interparticle interaction potential \( V_{\text{g}}(r) + V_{\text{t}}(r) \) and the trapping potential \( V_{\text{t}}(r) \). As stated before we assume an intermediate region exists between \( \beta_s/a_s < r/a_s < 1 \). As shown in figure 2, the channel potentials for higher partial wave states are positive between \( \beta_s/a_s < r/a_s < 1 \) while the channel potential energy changes from negative to positive values for the s-wave state. If the energy \( E_b \) is close to 0, there is no well-defined intermediate region where the local frame transformation can be applied accurately for higher partial waves. This results in the unphysical avoided crossing in the local frame transformation approach including \( d \) and \( g \) wave states. It is worth noting that in the energy region where the avoided crossing appears for higher partial wave states, the bound state energy based on the local frame transformation approach with a single s-wave state agrees very well with the numerical results. In addition, these calculation shows that DCIM states also exist in the region \( a_{ss} < 0 \). It demonstrates the impact of

![Figure 4](image-url)
the confinement on the dipolar system since in free space case dipolar bound states arise only for \( a_\omega > 0 \).

In the following, we investigate the dependence of the bosonic DCIM states on the DDI strength, characterized by the scaled dipole length \( l_d/a_\perp \). The bound state spectrum in the waveguide is calculated numerically via the close-coupling method, and the scaled bound state energy \( E'_h = E_h/h_\omega \) is shown in figure 5 (black solid line). The bound state energies based on the local frame transformation approach are shown as red circles. The bound state energies in free space without the transverse trapping potential are also obtained numerically and are depicted as blue squares. In the numerical calculation, \( C_{10} \) is fixed to \( 2.18 \times 10^{-16} \). The Lennard–Jones potential supports one bound state which is close to \( E = 0 \), the scattering threshold in free space. Varying the coefficient \( C_{10} \), the general features of \( E'_h \) as a function of \( l_d/a_\perp \) remain the same as those shown in figure 5. In the local frame transformation calculation, the dipolar bound state equation (14) including three partial waves, which is quite accurate close to the threshold \( E_{th} \), is used to determine the bound state in the energy region \( E_h/h_\omega \in (1/2, 1) \). Away from the threshold, the bound state equation (14) can be less accurate as shown in figure 4. Hence, we use the bound state equation including one partial wave in the energy region \( E_h/h_\omega \in (0, 1/2) \). The generalized scattering lengths needed in the bound state equations are calculated numerically. As shown in the upper panel of figure 5, the bound state energy determined via the local frame transformation approach agrees very well with the numerical results.

As the DDI increases, the interparticle interaction potential becomes deeper [47]. As a result, new bound states emerge as shown in the upper panel of figure 5. The bound state around \( l_d/a_\perp = 0.13 \) is more sensitive to the variation of the DDI compared to the other bound states. An analysis of the wavefunction reveals that this is a \( g \)-wave dominant bound state, and all the other bound states are dominated by a \( s \)-wave component.

As shown in figure 5, the bound state energy decreases as the DDI strength increases. When the bound state energy is well below the threshold \( E_{th} \), the dipoles are localized at distances \( r/a_\perp \ll 1 \), and the dipolar bound state wavefunction exponentially vanishes prior to the region where \( V_l(r) \) becomes important. Therefore, in this case the bound state in waveguides is essentially like a bound state in free space. This situation is examined in figure 5 that, due to the presence of the confinement, the DCIM state exists in larger energy region and dipole moment region compared to the free-space dipolar bound state. As shown in the upper panel of figure 5, the bound state energies with and without trapping potential coincide with each other except for the energy region \( E'_h \) close to 0. A magnification in the vicinity of \( l_d/a_\perp = 0.055 \) is shown in the lower panel.

The bound state which is close to \( E = 0 \) in free space is shifted in the presence of the waveguides. As its energy lowers, this shift becomes smaller. When \( E'_h = -1 \), i.e. the bound state energy is \(-h_\omega^2\), the effect of the waveguide is already negligible, and the bound state energies in the waveguide and in free space are almost the same.

In the strong DDI regime, where the dipole length \( l_d \) is comparable to the harmonic oscillator length \( a_\perp \), the dependence of the scaled bound energy \( E'_h \) of the DCIM states on \( l_d/a_\perp \) is determined numerically and is depicted in figure 6 (black solid line). The local frame transformation approach cannot be applied to calculate the DCIM states in the strong DDI regime since the length scale separation does not apply. The numerical free-space dipolar bound state energies are also shown in figure 6 (blue squares). In the strong DDI regime, different partial wave channels are strongly mixed. As shown
in figure 6, there are more bound states which are dominated by higher partial wave components and are sensitive to the variation of the DDI strength. Moreover, unlike the situation in the weak DDI regime, where the DCIM states are dominated by a single partial wave component, the DCIM states in the strong DDI regime contain a significant number of different partial wave components of the same order of magnitude. For example, the first DCIM state from the left in figure 6 contains both $s$ and $d$ wave components significantly. The qualitative features of the dependence of the DCIM states on the DDI in the strong DDI regime are similar to those in the weak DDI regime. New DCIM states emerge as the DDI strength increases. In the following discussion on the fermionic DCIM states, we will focus on the weak DDI regime.

Above we examined the variation of the binding energies of the DCIM states as a function of general scattering length and DDI strength. In the following we investigate the variation of the binding energies of the DCIM states as one tunes the scattering length between the atoms can be tuned by the magnetic Feshbach resonances both for Dy and Er [49]. The $C_{10}$ is chosen such that the scattering length is negative.

The choice of the negative scattering length is to emphasize that the bound states discussed in figure 7 are induced by the confinement, since there is no bound state for negative scattering length in free space. For positive scattering length, there exist weakly bound states in free space, whereas the confining trap yields a shift to their corresponding binding energies. Different choices of the absolute values for the scattering length show the same shift for the bound state as one tunes the confining frequency. In the calculation corresponding to figure 7, the absolute value for the scattering length is set to be the background scattering length for $^{162}$Dy and $^{166}$Er, which is 120 au [48] and 72 au [50], respectively.

In figure 7, the scaled binding energy $E_{b}^\star$ is shown as a function of the harmonic oscillator length $a_\perp$. The local frame transformation approach using a single partial wave state (black solid line) and for $^{166}$Er (red dashed line). A weakly bound state is formed when a weak transverse trapping potential is added, i.e. when $a_\perp$ is large. The DCIM state becomes more bounded as the trapping becomes more tight.

3.2. Fermionic DCIM states

Let us now focus on the fermionic DCIM states. For fixed DDI strength $l_d/a_\perp = 0.026$, the variation of the scaled binding energy with $a_\perp/a_{pp}$ is shown in figure 8. The fermionic bound state energy curve has similar features as the bosonic case. As shown in the corresponding lower panel, the local frame transformation approach using a single partial wave state (green dotted line) deviates from the numerical results (black solid line) only close to the threshold. By including more partial wave states (red dashed line), the local frame transformation approach provides a more accurate bound state energy when $E_{b_1}^\star$ tends to zero, and also produces the spurious avoided crossing when $E_{b_1}^\star$ tends to 1, see the upper panel of figure 8. The dependence of the scaled fermionic bound state energy $E_{b_1}^\star$ on the DDI strength, namely $l_d/a_\perp$, is provided in figure 9. Here $C_{10}^\star = 1.11 \times 10^{-16}$ and the short range potential $V_\sigma$ supports a $p$-wave bound state.
very close to $E = 0$. Other choices of the value for $C_{10}$ lead to a similar behavior. The solid line in figure 9 depicts the numerical bound state energies. A series of new bound states emerges as the DDI strength increases. Among the bound states shown in the upper panel of figure 9, the one around $l_d/a_\perp = 0.095$ is a $l = 5$-wave dominant bound state, and the other states are $p$-wave dominated. All these bound states are more sensitive to the variation of the DDI strength compared to the $s$-wave dominant bound state shown in figure 5. This can be understood as follows. The potential matrix element $V^{(l)}(r)$ vanishes for the $s$-wave channel, and is nonzero for $l > 0$ channels. The $l > 0$ wave channel potentials are directly affected by the DDI. Hence the bound states dominated by higher partial wave components are more sensitive to the variation of the DDI. The bound state energies calculated via the local frame transformation approach are shown in red circles in figure 9. The calculation follows the same procedure as described for the bosonic case. It is shown that the local frame transformation approach is also capable to calculate the bound state energies accurately for the fermionic case.

The numerical free-space bound state energies are shown in blue squares in figure 9. Focusing on the bound state in the vicinity of $l_d/a_\perp = 0.0884$ shown in lower panel, one can observe that, for the fermionic case, the bound state energies in waveguides and in free space coincide with each other even in the energy region $E_b \rightarrow 0$. The reason for this is that there are centrifugal potential barriers for all the channels, including the lowest $p$-wave channel. The potential barrier tends to constrain the bound state wavefunction in the short-range region where the trapping potential is negligible. This is clearly shown in figure 10 where the partial wave PD of a bound state at $E_b = 0$ in the waveguide is depicted. The bound state barely feels the trapping potential, and is almost a bound state in free space.
4. Conclusions

We have investigated the dipolar confinement-induced molecular (DCIM) states in harmonic waveguides. Identical bosonic and fermionic dipoles are considered. In the weak DDI regime, in which the dipole length is smaller than the harmonic oscillator length, the local frame transformation approach is utilized to connect the bound state in waveguides with the scattering properties in free space analytically. By examining the numerical partial wave PD of the DCIM states, we show that length scale separation exists in the weak DDI regime which is crucial for the application of the local frame transformation approach.

The dipolar bound state equation based on a local frame transformation is derived, which enables us to address analytically the conditions under which the CIM states between two bosonic/fermionic dipoles emerge. This is one of the main result of this work. The bound state energies calculated via local frame transformation approach are compared with the numerical ones. Since both DDI and the trapping potential couple different partial wave states, one expects that multiple partial wave states are involved in the local frame transformation approach. Indeed, close to the scattering threshold in waveguides $E = \hbar \omega_{ij}$, the local frame transformation approach including the lowest partial wave state fails to provide accurate bound state energies, and higher partial wave states are needed. However, when $E$ tends to zero, the bound state energies based on the local frame transformation approach including higher partial wave states deviate from the numerical ones. The reason is that one cannot find an intermediate region for higher partial wave channels where the kinetic energy is significantly larger than the interparticle interaction potential and the trapping potential. The local frame transformation in such a case is less accurate, and this results in spurious avoided crossings. Nevertheless, one can still use the local frame transformation approach in this energy region since the single partial wave approximation is valid according to the comparison with the numerical calculations.

The dependence of the DCIM states on the DDI has been investigated, and both the weak and strong DDI regimes have been studied. As the DDI strength increases, a series of DCIM states emerges. The $s$-wave dominated DCIM states are less sensitive to the variation of the DDI strength as compared to the higher partial wave ($l > 0$) dominated DCIM states. This is due to the fact that the matrix elements of the DDI potential vanish for the $s$-wave channel and are nonzero for $l > 0$. The $l > 0$ channel potentials are affected directly by the DDI. We also compared the bound states in waveguides and in free space. It is found that for the bosonic case, the bound state in waveguides is almost like a free-space state when the bound state energy is smaller than $-\hbar \omega_{ij}$. For the fermionic case, the centrifugal potential barrier in the channel potentials localizes the bound state wavefunction in the short-range region where the trapping potential is weak. The fermionic bound states in waveguides start to behave as free space bound states just below the zero energy threshold.

A full investigation of the bound state properties of two identical dipoles in an external potential is important for an understanding of the corresponding many-body physics. In [51], it is shown that the wavefunction of the $p$-wave molecule in waveguides is stretched by the transverse confinement. This leads to less weight of the molecule in the short-range regime, and hence the atom loss could be suppressed. Similar to the $p$-wave molecular states discussed in [51], the DCIM states are also extended in the longitudinal direction of the waveguide. One may therefore expect that the DCIM states play an important role in stabilizing ultracold dipolar gases in waveguides. Besides, the detailed knowledge about the bound states close to the threshold is important to locate the scattering resonances [37] which can be used to tune the interaction in many-body systems.

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Appendix

For identical bosons, $s$, $d$ and $g$ wave states are involved, and the explicit expressions for $M_{l,f}$ read as follows

$$M_{ls} = -i\frac{\frac{1}{2} - \epsilon}{2\sqrt{1/2 + \epsilon}},$$ (25)

$$M_{ld} = -\sqrt{5}\left\{\frac{3i\epsilon}{4(\frac{1}{2} + \epsilon)^{3/2}} + i\frac{\frac{1}{2} - \epsilon}{4\sqrt{1/2 + \epsilon}}\right\},$$ (26)
\[ M_{dd} = 5 \left( -9\zeta \left[ \frac{3}{2}, -\epsilon \right] \right) \left( \frac{8(1 + \epsilon)^{3/2}}{(1 + \epsilon)^{5/2}} \right) - \frac{3i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{4(1 + \epsilon)^{3/2}} \],
\[ M_{dd} = 3 \left( -3i\zeta \left[ -\frac{3}{2}, -\epsilon \right] \right) \left( \frac{4(1 + \epsilon)^{3/2}}{(1 + \epsilon)^{5/2}} \right) - \frac{15i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{8(1 + \epsilon)^{3/2}} \],
\[ M_{df} = -\sqrt{5} \left( -3i\zeta \left[ -\frac{5}{2}, -\epsilon \right] \right) \left( \frac{125i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{32(1 + \epsilon)^{5/2}} \right) + \frac{3i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{2(1 + \epsilon)^{5/2}} + \frac{3i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{2(1 + \epsilon)^{5/2}} \],
\[ M_{gh} = 9 \left( -1225i\zeta \left[ -\frac{7}{2}, -\epsilon \right] \right) \left( \frac{525i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{128(1 + \epsilon)^{9/2}} \right) + \frac{555i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{64(1 + \epsilon)^{9/2}} + \frac{125i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{32(1 + \epsilon)^{9/2}} \],
\[ M_{gh} = 7 \left( 25i\zeta \left[ -\frac{5}{2}, -\epsilon \right] \right) \left( \frac{15i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{8(1 + \epsilon)^{5/2}} \right) + \frac{9i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{8(1 + \epsilon)^{3/2}} \],
\[ M_{gf} = \sqrt{33} \left( 63i\zeta \left[ -\frac{5}{2}, -\epsilon \right] \right) \left( \frac{35i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{8(1 + \epsilon)^{5/2}} \right) + \frac{15i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{16(1 + \epsilon)^{3/2}} \],
\[ M_{hh} = 11 \left( 3969i\zeta \left[ -\frac{9}{2}, -\epsilon \right] \right) \left( \frac{2205i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{128(1 + \epsilon)^{11/2}} \right) + \frac{3395i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{64(1 + \epsilon)^{11/2}} + \frac{525i\zeta \left[ -\frac{5}{2}, -\epsilon \right]}{32(1 + \epsilon)^{11/2}} \],
\[ M_{hh} = 1 \left( -\frac{3}{2}, -\epsilon \right) \right) \left( \frac{225i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{128(1 + \epsilon)^{3/2}} \right) + \frac{225i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{128(1 + \epsilon)^{3/2}} \].

where \( \epsilon = \frac{E - h^2 \omega^2}{2m} \), and \( E \) is the total energy. \( \zeta(a, s) \) is the Hurwitz zeta function.

For identical fermions, \( p, f \) and \( h \) waves are involved in the local frame transformation calculation. The explicit expressions for \( M_{IF} \) read then

\[ M_{gp} = \frac{3i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{2(1 + \epsilon)^{3/2}} \],
\[ M_{gp} = -\sqrt{21} \left( -5i\zeta \left[ -\frac{3}{2}, -\epsilon \right] \right) \left( \frac{3i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{4(1 + \epsilon)^{3/2}} \right) \],
\[ M_{gf} = 7 \left( 25i\zeta \left[ -\frac{5}{2}, -\epsilon \right] \right) \left( \frac{15i\zeta \left[ -\frac{3}{2}, -\epsilon \right]}{8(1 + \epsilon)^{5/2}} \right) + \frac{9i\zeta \left[ -\frac{1}{2}, -\epsilon \right]}{8(1 + \epsilon)^{3/2}} \].

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