Quantum few-body bound states of dipolar particles in a helical geometry

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Abstract
We study a quantum mechanical system consisting of up to three identical dipoles confined to move along a helical shaped trap. The long-range interactions between particles confined to move in this one dimension leads to an interesting effective two-particle potential with an oscillating behavior. For this system we calculate the spectrum and the wave functions of the bound states. The full quantum solutions show clear imprints of the tendency for the system to form chains of dipoles along the helix, i.e. a configuration in which the dipoles are sitting approximately one winding of the helix apart so that they can take maximal advantage of the strong head-to-tail attraction that is a generic feature of the dipole–dipole interaction.

Keywords: few-body physics, dipolar particles, quantum bound states

1. Introduction

Cold atomic gas physics has advanced to the stage at which simulation and exploration of quantum phenomena can now be done at unprecedented levels of accuracy and with great potential for engineering systems that are otherwise very hard to access in other fields of research [1–5]. An important recent advance is the ability to create homo- and heteronuclear molecules or trap atoms with large permanent magnetic moments at low temperatures which has many interesting applications [6–14]. The head-to-tail attraction between such molecules with dipole moments is a concern, as it limits the timescales at which an experiment can operate due to strong losses. One way to solve this is to confine the molecules in lower dimensional traps, where the head-to-tail attraction can be suppressed [15, 16].

Dipolar particles in low-dimensional traps are particularly interesting due to the long-range nature of the dipole–dipole interaction and its relation to the movement allowed by the dipolar particles in the trapping geometry. In particular, the long-range interaction may mediate an interaction across otherwise distant regions of the space in which the dipoles move. A case in point is the geometry of a one-dimensional helix. Dipolar particles moving on a helix will interact not only with particles in close proximity, but also with particles that are sitting at a distance of one or more revolutions of the helix due to the long-range dipolar force. The detailed interplay between the non-trivial long-range interaction of both charged ions and dipolar particles on a helical geometry has given rise to a number of theoretical studies into these setups [17–25]. A helical trapping potential can be realized with Laguerre–Gaussian beams with nonzero angular momentum [26–32] or by trapping the atoms in the evanescent field surrounding an optical fiber [33–36]. The current study envisions the combination of such helical traps with dipolar particles in future experiments. The central question that we ask here is the structure of states with a few particles on the helix in the quantum regime, i.e. we consider what kind of bound states are possible and what their structures are.

In this work we consider dipolar particles on a single helix which confines the movement of the dipoles. We will be assuming that the helical trap is strongly confined in the directions that are locally perpendicular to the helix such that we may ignore the motion of the particles in these transverse directions. In this setup we investigate the formation of quantum mechanical bound states of two and three particles on the helix, we study their structure and the criteria for formation. The paper is organized as follows. In section 2 we introduce the helix and the dipole–dipole interaction. In section 3 we look at two dipoles on a helix, we calculate the bound states and look at their energy and their size. In
section 4 we introduce another dipole and look at the bound states of three dipoles on a helix. We conclude in section 5.

2. The helix model

A helix is defined by two parameters, the radius $R$, and the pitch $h$. The radius defines the circumference while the pitch defines how far one moves along the symmetry axis of the helix during one revolution. The geometry of the helical setup is illustrated in figure 1. To describe the position along the helix it is convenient to use the arc length $s$ measured along the helix, but for numerical purposes we will instead use the angle around the central symmetry axis $\phi = s/\alpha$, where $\alpha = \sqrt{R^2 + \left(\frac{h}{2\pi}\right)^2}$. It is worth noting, that this angle $\phi$ is not limited to be smaller than $2\pi$, anything more than that just means more than one revolution on the helix. The relation between the coordinates on the helix, and the Cartesian coordinates in three-dimensional space is

\[
(x, y, z) = \left(R \sin \phi, R \cos \phi, h \phi \right) / 2\pi.
\] (1)

where $R$ is positive and $\phi$ runs through an interval between $\phi_{\text{min}}$ and $\phi_{\text{max}}$. On the helix we place between one and three dipoles, all of equal mass $m$, and dipole moment $d$, all the dipoles are aligned by an external field.

The long-range interaction of two particles on the helix are given by the usual dipole–dipole interaction between two dipoles in three-dimensional space. The two-body interaction potential, $V$, between two dipoles at position $r_i$ and $r_j$ is

\[
V(r_i, r_j) = \frac{1}{4\pi \varepsilon_0} \frac{1}{r_i} \left[ d \cdot d - 3(d \cdot \hat{r})(d \cdot \hat{r}) \right].
\] (2)

where $r = |r_i - r_j|$ is the distance between the dipoles, and $\hat{r} = (r_i - r_j)/r$ is the unit vector in the direction connecting the two dipoles. We use the unit $\frac{1}{4\pi \varepsilon_0}$, where $\varepsilon_0$ is the permittivity, corresponding to electric dipoles, but in principle the formalism is applicable for magnetic dipoles if we use the unit $\frac{\mu_0}{4\pi}$, where $\mu_0$ is the vacuum permeability. Here we will assume that an external field is used to align the dipole moments of all particles along the symmetry axis which we take to be the z-axis (see figure 1). As mentioned above, instead of describing the position of the dipoles by their Cartesian coordinates it turns out to be easier to use their position along the helix. This can be done through the coordinate transformation in equation (1). If the position of the two dipoles along the helix are $\phi_i$ and $\phi_j$ the two-dipole potential in equation (2) becomes

\[
V(\phi_i, \phi_j) = \frac{d^2}{4\pi \varepsilon_0} \left[ 1 - \cos(\phi_i - \phi_j) \right] - 2 h^2 \left( \frac{\phi_i - \phi_j}{2\pi} \right)^2 \left( \phi_i - \phi_j \right)^2 / 2\pi \varepsilon_0 \left( 1 - \cos(\phi_i - \phi_j) \right) + h^2 \left( \frac{\phi_i - \phi_j}{2\pi} \right)^2 / 2\pi \varepsilon_0 \left( 1 - \cos(\phi_i - \phi_j) \right)
\] (3)

We see that for dipoles trapped on the helix with dipole moments pointing in the the z-direction the two-dipole potential in equation (3) only depends on the distance between the two dipoles $\phi = \phi_i - \phi_j$ measured along the helix.

The two-dipole potential as a function of this dipole separation, is shown in figure 2. The long range part of the potential falls of as $\phi^2$ like the distance dependence from equation (2) in three-dimensions. But the potential also contains oscillations at smaller distances. They disappear when $\phi > 1 + (2\pi)^2 R h / 2\pi$. The corresponding minima in the potential arise whenever the dipoles are above each other. It is worth
noting that the minima are not exactly at multipla of 2π, which would correspond to the dipoles being directly above each other. Instead the minima are located at a distance from each other that is slightly smaller than 2π as it is a compromise between optimizing the angle, and minimizing the three-dimensional distance between the dipoles.

When two dipolar particles come very close to each other we expect that strong interactions will cause for instance chemical reactions and losses from our setup. This is not the regime we are interested in and we therefore look for a parameter regime in which the short-range behavior of the dipole–dipole potential is purely repulsive. In this regime, we may safely ignore any chemical reactions and strong losses. This requirement puts limitations on the geometry of the helix. If \( \frac{h}{R} > \sqrt{2\pi} \), then the two-dipole potential becomes attractive, and would allow distances where f.x. van der Waals forces would dominate. We thus restrict ourselves to cases where \( \frac{h}{R} < \sqrt{2\pi} \).

3. The two-body problem

We now place two dipoles on the helix. The kinetic energy operator, \( T = T_1 + T_2 \), is the sum of the two individual contributions expressed either in arc lengths, \( s_i \), or angles, \( \phi_i \), corresponding to each of the particles, \( i = 1, 2 \), that is [22, 37]

\[
T_i = \frac{-\hbar^2}{2m} \beta_i^2 + \frac{\hbar^2}{2m \alpha_i^2} \frac{\partial^2}{\partial \phi_i^2},
\]

where, \( m \) is the mass of one particle, \( \phi_i = \alpha s_i \). Here it is appropriate to emphasize that one must be careful with the quantization in geometries with non-trivial curvature. However, in the present paper we consider only the regular helix with constant curvature. The transformation we use from Cartesian to the curvilinear coordinates is then straightforward [22, 37].

We shall from now on use only the angular coordinates. It is convenient to change the coordinates from those of two individual dipoles, \( \phi_1 \) and \( \phi_2 \), to relative angular, \( \phi = \phi_1 - \phi_2 \), and center-of-mass, \( \Phi = (\phi_1 + \phi_2)/2 \), coordinates. The two-body kinetic energy operator is then as usual a sum of relative and center-of-mass contributions. The interaction between the pair of particles only depends on the relative angular distance between the dipoles as expressed in equation (3). The relative and center-of-mass motion are then decoupled, where the latter free particle motion can be trivially and independently calculated for given boundary conditions. In this paper we will ignore the center-of-mass motion which has no influence on the formation and structure of relative bound states.

The Hamiltonian, \( H \), governing the relative motion of the two dipoles takes the form

\[
H = \frac{-\hbar^2}{2m \alpha^2} \frac{\partial^2}{\partial \phi^2} + V(\phi),
\]

where \( \mu = m/2 \) is the reduced mass of the two dipoles. It is convenient to write this relative Hamiltonian in natural units, \( \hat{H} \), which has the form

\[
\hat{H} = \frac{\hbar^2}{2m \alpha^2} \frac{\partial^2}{\partial \phi^2} + \beta \hat{V}(\phi),
\]

where \( \beta \) is the potential strength given by

\[
\beta = \frac{\mu d^2}{2\pi \epsilon_0 R \hbar^2} \left( \frac{\alpha}{R} \right)^2
\]

and \( \hat{V} \) is the reduced potential where

\[
\hat{V}(\phi) = \frac{1 - \cos \phi - \left( \frac{\hbar \phi}{2\pi R} \right)^2}{2[1 - \cos \phi] + \left( \frac{\hbar \phi}{2\pi R} \right)^2}.
\]

We thus measure lengths in units of \( \alpha \) and energies in units of \( \hbar^2/\mu \alpha^2 \). Because \( V(\phi) \to \infty \) as \( \phi \to 0 \), the wavefunction \( \psi(\phi) \) has to be zero at \( \phi = 0 \). This means, that we only need to calculate the wavefunction for \( \phi > 0 \), and then construct the wavefunction to be either odd or even depending on whether dipoles are identical fermions or bosons.

3.1. Solutions to the two-dipole system

We solve the Schrödinger equation to obtain the wave function, \( \psi \), for the relative motion of the two dipoles in a box of size \( \phi \in [0: 100] \), with closed boundary conditions, that is \( \psi(0) = \psi(100) = 0 \). Since the dipole–dipole interaction is repulsive at short range the wave function must go to zero as the two particles coincide in space. We may therefore reduce the complexity of the problem and solve in the region \( \phi_1 > \phi_2 \) only (or vice versa). The full wave function can subsequently be found by extended to the opposite domain using continuity and considering the statistics of the particles (even function for bosons and uneven function for fermions). We start out by solving it for the case of \( \beta = 1 \) and \( \frac{h}{R} = 1 \). In figure 3, the wave functions of the four lowest eigenstates are shown. They all have a negative energy corresponding to bound states of two dipoles on a helix. The solid red curve is the ground state. It has a single maximum, at \( \phi \approx 2\pi \) corresponding to where the minimum in the two-dipole potential is located. The first excited state is the dashed green curve, it has a single node close to \( \phi = 10 \), between the first two minima of the two-dipole potential. The maximum is close to the second minimum in the potential corresponding to the two dipoles being separated by two windings on the helix. The short-dashed blue curve is the wavefunction of the second excited state. It has two nodes between the first three minima of the potential, and corresponding maxima at the first two minima, but because it has to be orthogonal to the two lower lying states it has a large part beyond the third minimum. The last curve in dotted purple is the wavefunction of the third excited state. As seen, the curvature at large \( \phi \) is negative, whereas the other three had a positive curvature. This is because of the boundary condition at \( \phi = 100 \) where the wavefunction is forced to be zero for our calculations. We
will return to this boundary effect below as it will also show up in our calculations of the case with three dipoles on the helix.

In the case of $\beta = 1$ shown in figure 3 there are three bound states. In figure 4 the energies of the four lowest states of two dipoles are shown. In the figure one can see that the number of (negative energy) bound states increases with the potential strength as expected. We find that one new bound state appears for $\beta$-values $\beta \approx 0.18, 0.44, 1.0$. Whether one bound state exists for all positive values of $\beta$ is not easily answered. Generally in one dimension, if the integral over the potential is negative, that is if $\int V(\phi) d\phi \leq 0$ then a bound state exists [38–40]. However, in our case the dipole potential diverges as $1/\phi^3$ at short distances, and a bound state could be found at larger distances. Furthermore, to be realistic we would need knowledge of the true short-range forces which are outside of the scope of this paper.

In figure 4 the ground state energy seems to be negative corresponding to strengths larger than $\beta \approx 0.04$. This may be an artefact of our already exceedingly large box of a maximum of $\phi = 1000$ corresponding to about 160 windings of the helix. For such a weak potential the wave function is running into the hard wall, and the forced boundary condition of zero would in itself increase the energy. An even larger box would then result in a lower energy. This would in turn push the threshold limit of bound state existence to a lower value than $\beta \approx 0.04$, which therefore only can be an upper limit. We shall elaborate on the sizes of the bound states in the next subsection.

3.2. The size of the bound states

In this section we explore how a ground state solution behaves, when the dipole moment changes. Changing the dipole moment corresponds to changing the dimensionless parameter $\beta$. By increasing the large dipole strength, $\beta$, the depths of the minima increase in the potential shown in figure 2. The ground state must consequently be increasingly more located in the deepest minimum, where $\phi = \phi_0$ and $V(\phi_0) = V_0$. We can then expand the potential around this minimum, or any of the other minima, up to inclusion of second order in $(\phi - \phi_0)$. This results in harmonic oscillator potentials of strength and energy shift, $V_0$, both proportional to $\beta$. The strength is also proportional to the square of the oscillator frequency, $\omega$.

The lowest energies of the oscillator spectrum, $E_{osc}(n) = V_0 + \hbar \omega (n + 1/2)$, would then be approached as $\beta$ increases. Both height and thickness of the barriers between minima would also increase with $\beta$, and decoupled oscillator solutions in different minima could be fairly accurate. The oscillator approximation would probably fail when $E_{osc}(n)$ is comparable to the lowest energy in the next minimum. However, for sufficiently large $\beta$ there is always room for decoupled states in the deepest minimum, since the energy difference also increases proportional to $\beta$.

The approximate oscillator solution then corresponds to the two dipoles oscillating about the distance where the potential is at a minimum. The size of the state can be calculated from the expectation value in the oscillator wave function, that is

$$\langle (\phi - \phi_0)^2 \rangle = \langle \phi^2 \rangle - 2 \langle \phi \rangle \phi_0 + \phi_0^2 \approx \langle \phi^2 \rangle - \phi_0^2 \propto 1/\omega \propto 1/\sqrt{\beta}. \quad (9)$$

Thus, we expect $\langle \phi^2 \rangle$ to scale with $\beta$ as

$$\langle \phi^2 \rangle = c_2 \frac{1}{\sqrt{\beta}} + c_1 \phi_0^2, \quad (10)$$

where $c_2$ should be 1 and $c_1$ could be obtained formally from the effective mass and the second derivatives of the potential.
However, we are not interested in their specific values, and instead we shall treat these constants as fitting parameters. We show the computed size of \( \langle \phi^2 \rangle \) for the ground state in figure 5 as a function of the strength, \( \beta \), where the solid green line is obtained as a fit to equation (10). In the limit of large \( \beta \) the fit reproduces the size very accurately which strongly indicate that the ground state in fact resembles that of a harmonic oscillator. This is consistent with \( c_2 \approx 1 \) and the resulting convergence of the green line to the value of \( \langle \phi^2 \rangle_0 \). However, in figure 5 we also notice some kind of divergence, or at least a strong increase, of the mean square value as \( \beta \) decreases towards smaller values. To understand this behavior we must investigate the opposite limit of asymptotically small \( \beta \)-values.

In the strict limit of \( \beta = 0 \) the eigenvalue solutions are planewaves in the relative angle with boundary conditions adjusted to fit inside the helix. When \( \beta \) is finite, but small and approaching zero we have in principle two different scenarios corresponding to either positive or negative ground state energies. It turns out, as we shall show, that it suffices to investigate the possibility of negative energy until \( \beta \) is too small to be of interest. If the ground state wave function can be located inside the helix, the large-angle behavior must accordingly be that of a bound state, that is \( \exp(-\kappa r) \) where \( \kappa = \sqrt{2E} \). This exponential fall-off is modified in the attractive region at smaller angle around \( \phi_0 \). We emphasize that the origin of binding leading to a state of negative energy is the dipole potential in equation (3), see figure 2. However, this does not imply that the major probability is found in the attractive region, which nevertheless is indispensable for providing the bound state.

The weak binding behavior in short-range interacting systems has been abundantly demonstrated by the occurrence of universal structures found in halo systems of both two- and three-body systems [4]. The mean square radius, \( \langle r^2 \rangle \), corresponding to an asymptotic large-distance \( s \)-wave reduced radial wave function, \( \exp(-\kappa r) \), is proportional to \( 1/\kappa^2 \propto 1/E \). This implies that the probability extends to extremely large distances for a very small energy. The question is now whether this behavior also is obtained in the weak binding limit of the dipole interacting two-body system confined to the helix. This dipole potential might lead to a different behavior due to the short-range strong repulsion and the localized attraction at finite angles, or distances.

The crucial qualitative features are reproduced by a schematic potential with infinite walls at zero, or small \( \phi \), and at a very large angle. The attraction is simulated by a square well potential at a relatively small \( \phi \)-value with adjustable depth and width. The complicated, but analytic, wave function increases as function of \( \phi \) from zero to a maximum around the square well attraction, and decreases then exponentially outside the well. For decreasing binding energies the amount of wave function increases at large distances. The probability at the inner parts become insignificantly small compared to the content in the much larger region of angles within the finite helix.

To test this anticipated behavior more quantitatively, we first assume that the exponential fall-off at large \( \phi \) also represents the wave function for small values both close to zero and around the minimum \( \phi_0 \). This is a valid assumption if the probability turns out to be insignificant in the small angle region, where the approximation is obviously wrong. The mean square value, \( \langle \phi^2 \rangle \), is then found to be

\[
\langle \phi^2 \rangle = \frac{\int_0^{\infty} \phi^2 e^{-2\kappa \phi} d\phi}{\int_0^{\infty} e^{-2\kappa \phi} d\phi} = \frac{1}{2\kappa^2}
\]

which is the general result derived in halo physics. It emphasizes that very weak binding leads to the specific \( 1/E \)-divergence of the mean square value. If present, the behavior can be exhibited very clearly by plotting the mean square value multiplied by the energy, where the expectation is an approach to a constant for decreasing energy.

The effect of the minimum at \( \phi_0 \) was seen in the strong interaction limit shown in figure 5. In the mean square results shown in figure 6 we therefore first subtract the value obtained for a structure localized in \( \phi_0 \). In this figure we first draw attention to the clean linear dependence of \( \langle \phi^2 \rangle \) with increasing \( |E| \). This is in direct contradiction to the behavior derived in equation (11). In addition, we observe the second important feature, that is a constant difference over a large energy interval between \( \langle \phi^2 \rangle \) and the same quantity for a structure localized at \( \phi_0 \).

This can perhaps be intuitively interpreted as revealing the usual halo structure translated to start from \( \phi_0 \) instead of zero. To test this possibility we use the line in figure 6 to derive a parametrization of two terms, \( \langle \phi^2 \rangle \approx \phi_0^2 + 0.75/|E| \). Unfortunately, the constant, 0.75, should have been 0.25 to match the halo explanation. However, we find numerically that the flat region continues essentially unchanged to the much larger energies with the results shown in figure 5. This connection becomes clear by using the harmonic oscillator structure around the minimum obtained for large binding, which leads to \( \langle (\phi - \phi_0)^2 \rangle = 1/\omega = 1/(2|E|) \). The full
calculation of this inverse energy dependence is found to be roughly the sum of halo and oscillator contributions, that is \(0.25 + 0.50 = 0.75\). This accounts for most of the low-energy behavior in figure 5.

The two terms, \(\phi_0^2\) and \(0.75/|E|\), are roughly equal when \(|E| \approx 0.02\). The inverse energy behavior derived in equation (11) can apparently only be reached for much smaller energies. This brings us to the third important feature in figure 6, that is the change of slope of \(\langle \phi^2 \rangle |E|\) from higher to lower energy. In the close-up where the logarithmic scale has been used for the smallest energies, the curve is more more flat and apparently approaching a constant. To be precise, the calculated size of \(\langle \phi^2 \rangle |E|\approx 0.3\) is obtained from \(\langle \phi^2 \rangle \approx 4.4 \times 10^4\) and the corresponding smallest binding energy of \(|E| \approx 7 \times 10^{-6}\). This constant is tantalizingly close to the halo estimate of 0.25 which from equation (11) is obtained for short-range potentials in the weak binding energy limit. The inset in figure 6 demonstrate the approach towards 0.25 for small \(|E|\). The logarithmic scale makes the preferred strict numerical conclusion of convergence towards the constant 0.25 difficult. The decrease might continue below 0.25 and in principle perhaps even down to zero. However, going below 0.25 would require a wave function that falls off in the non-classical region faster than the physical bound state wave function of the form \(e^{-k|z|}\). This would not be physically motivated. Pursuing the behavior to even smaller binding energies present computational accuracy problems as well as a requirement of larger helix sizes. Both obstacles can be overcome but improving them simultaneously would require a substantial additional numerical effort. Two orders of magnitude in energy obviously require two orders better accuracy as well as at least a ten times longer helix treated accurately at all distances. However, we believe the observed limiting behavior is quite convincing and completely consistent with the expectation of 0.25 derived rigorously from the physics of the problem. In any case this extreme limit would most likely be outside reach of experiments with finite helix sizes.

We emphasize that even for the lowest energy in figure 6 we have \(\phi_0 \ll \langle \phi^2 \rangle |E| \approx 200\) which is much smaller than the maximum angle of 1000 used in the numerical calculations. Thus, the boundary condition should only be able to influence the solutions marginally for all energies in figure 6. Pushing further to even weaker potentials can result in two different types of behavior. The first possibility would be a direct extrapolation of figure 6 until the helix size is reached or rather when we run out of numerical accuracy. The other option is that the short-range potential is too repulsive to support a bound state for an infinitely small strength. The latter possibility appears from our experience to be the least likely of the two, since we already have reached low-energy solutions located at large \(\phi \gg \phi_0\), although \(\phi < \phi_0\) are allowed as well.

4. The three-body problem

We now add a third dipole to the helix. It is of the same type as the other two, that is the same mass and dipole moment. They all interact through the two-dipole interaction in equation (8). The position of each of the dipoles is denoted \(\phi_1, \phi_2, \phi_3\), and we proceed as usual to separate out the center-of-mass motion by changing to relative and center-of-mass coordinates of the total three-body system. Again it is worth keeping in mind that we are confined to the helix corresponding to one-dimensional geometry [22, 37]. However, in our case of zero curvature and coordinate independent mass, this separation is easily seen as usual by adding the kinetic energy of the third particle in equation (4). For three equal masses we use the coordinate transformation

\[
x = \frac{1}{\sqrt{2}} (\phi_1 - \phi_2),
\]

\[
y = \frac{1}{\sqrt{6}} (\phi_1 + \phi_2) - \sqrt{\frac{2}{3}} \phi_3,
\]

\[
z = \frac{1}{\sqrt{3}} (\phi_1 + \phi_2 + \phi_3).
\]

In passing, we note that the three coordinates \(x, y,\) and \(z\) are atypical in the sense that they are built from angular variables and thus are intrinsically dimensionless. However, we could as well have used the proportional arc lengths as coordinates. With no external potential along the helix, the three body problem now reduces to a two-dimensional problem in the two relative coordinates \(x\) and \(y\), and a decoupled center-of-mass problem in the \(z\)-coordinate. The independent center-of-mass motion can be easily worked out. We use open boundary conditions on the helix and thus require the wave functions to vanish on the top and bottom of the helix which implies that the center-of-mass motion simply is as a particle in a box.
The two-dimensional Schrödinger equation that describes the relative motion of the three dipoles should contain five terms, two terms from the kinetic energy of the relative motion between the dipoles, and three potential terms from the pairwise dipole–dipole interaction

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + V(\sqrt{2x}) + \beta V\left(\frac{\sqrt{3}}{2}y - \frac{1}{\sqrt{2}}x\right) + \beta V\left(\frac{\sqrt{3}}{2}y + \frac{1}{\sqrt{2}}x\right).$$

(13)

Here $V$ is the two-dipole potential of equation (8). All terms are written in natural units using $\beta$ as in the case of two dipoles above. The Hamiltonian is also in units of $\mu_0 e^2/\hbar^2$ as in equation (6). Because the two-dipole potential is repulsive at short range, we use the same trick as for two dipoles to reduce the complexity of the system, we only solve it for $\phi_1 > \phi_2 > \phi_3$. And then depending on whether the dipoles are bosons or fermions, the full symmetric or antisymmetric wave function can be reconstructed for all values of $\phi_1, \phi_2, \phi_3$. The restriction to $\phi_1 > \phi_2 > \phi_3$ corresponds to a restriction on $x$ and $y$, namely that $y > \frac{1}{\sqrt{3}}x$. For definiteness, we will be working with a dipolar strength parameter of $\beta = 1$ when we plot the wave functions (below we will explore variations with $\beta$ and its effect on the relative distances within the ground state). In addition, we take $\hbar = R$, i.e. the pitch and the radius are the same. The two-dimensional wave equation is solved on a grid with $x \in [0: 160]$ and $y > \frac{1}{\sqrt{3}}x$. We observe the same behavior as for two dipoles with regards to the size of the states which also increases with decreasing $\beta$. From a practical point of view this means that for smaller $\beta$ the size of the grid has to be increased which slow down the numerical solution and reduces accuracy. We therefore restrict ourselves to the case of $\beta = 1$ for three dipoles.

4.1. Properties of the solutions

The ground state wave function of the three-body problem is shown in figure 7 in a three-dimensional level plot that includes a two-dimensional projection onto a contour plot for clarity. We only display the fraction of the coordinate space where $\phi_1 > \phi_2 > \phi_3$. Other parts may be constructed from assumptions of symmetry. The ground state displays a prominent single peak at around $x \sim 4.4$ and $y \sim 7.7$. This peak corresponds to a configuration where the three dipoles are placed directly above each other only separated by (approximately) one winding. More precisely, it corresponds to a configuration where $(\phi_1, \phi_2, \phi_3) \sim (4\pi, 2\pi, 0)$. We thus see a very nice consistency with respect to the case of two dipoles in which we also find a dominant configuration with the dipoles placed about one winding of the helix apart in order to exploit the attractive interaction in the head-to-tail setup.

We now consider the low-energy spectrum of three dipoles on a helix by representing the wave functions in contour plots as functions of $x$ and $y$ coordinates. This is shown in figure 8. As discussed above, the wave equation has been solved only for $\sqrt{3}y > x$. Solid (black) lines indicate where $x = \pm \sqrt{3}y$ in all the panels in figure 8. To extend the results to the full $(x, y)$-coordinate space, one needs to reflect the wave functions across the solid lines in the panels. Here we are assuming that the dipoles are identical bosons. This implies that the wave function must be symmetric in the exchange of any pair of particles, and thus we must reflect across the solid lines and keep a positive sign. In the case of fermionic dipoles, the solution would be the same except for a sign change across the diagonal.

The panels in figure 8 show the first four states in the spectrum. In the upper left corner, we have the ground state which is identical to the state shown in a different manner in figure 7. It is a state with three head-to-tail dipoles, here extended across the solid lines so it is really three copies of the central region (within the wedge traced by the solid lines containing the $y = 0$ axis). The first excited state in the top right corner has a much more detailed structure. It still contains a trace of the head-to-tail on successive windings structure of the ground state but now a lot of amplitude is move to larger values of $x$ in the central region around $y = 0$ (within the central wedge). This corresponds to configurations where the one of the outer dipoles from the head-to-tail configurations is now pushed one winding away from the two others (this can be done in two ways so we have $y \rightarrow -y$ symmetry here). Notice also the change in sign between the two regions with non-zero amplitudes. This is of course a result of the fact that higher excited states have additional nodes in the wave functions. We may relate this very directly to the physics we saw in the case of two dipoles in figure 3. There we see that the first excited two-body state (long dashed (green) line) has a small bit of amplitude around angles of $\phi \sim 2\pi$ but that most of its weight is around $\phi \sim 4\pi$ and thus
the two-body state has the dipoles sitting about two windings apart mainly. This is clearly also reflected in the contour plot of the first excited state for three dipoles seen in the top right panel of figure 8.

The second excited state of three dipoles is shown in the lower left panel in figure 8 and has a structure that can now be simply understood given the two lower states. Its amplitude is dominated by pairs of dipoles which are now about two winding apart. In comparison to the first excited state it has zero amplitude of the simple head-to-tail configuration seen in the ground state. It is a bit harder to compare this to the two-body case as the second excited state for two dipoles has them sitting really far apart (at the level of $\phi \sim 5\pi$, see figure 3), while the second excited state for three dipoles resembles more the physics in the first excited state in the two-body case only without the configurations where two of the dipoles are sitting one winding apart.

The third excited state seen in the lower right panel of figure 8 tells a similar story except that now the dipoles move even further apart as the amplitude is seen to move to larger values of $x$ and $y$. We also notice that a small bit of amplitude comes back to the ground state configuration in the region near the origin $(x, y) = (0, 0)$. However, the third excited state is not fully converged as one can see by the lack of symmetry (up to a sign) for $y \rightarrow -y$. It is the same sort of boundary effect that can be seen in figure 3 for the third excited state of the two-body system.

A numerically improved calculation for the third excited state would have to enlarge the box of discretization until the exponential fall off can take place within the box. The necessary increase of box size has to be substantial, and from figure 3 more precisely estimated to be twice as large as that of the second excited state. This implies roughly an $(x, y)$ box extending to $(40, 40)$ which increases the number of points by a factor of four which would increase the computer time by about an order of magnitude. With such an increase the fourth excited state would be far from converged and contained within the box. In spite of these numerical difficulties illustrate, the behavior the higher-lying excited states should now be clear. In higher excited states the dipoles are pushed further and further away from each other and is consistent with the picture that we have from the two-body case. A nice feature is that the ground state configuration with three dipoles head-to-tail on three successive windings does indeed seem to make an appearance in higher excited states also so we do see that the first minimum in the two-body potential in figure 2 plays a very dominant role in this geometry.

In order to further elucidate the configuration of the three dipoles of the helix we can consider the relative distances in angle between each pair of dipoles within the ground state. These distances are defined as $\phi_{ij} = \phi_i - \phi_j$ and we take the expectation value of this operator in the ground state. The results are shown in table 1 for different values of $\beta$ with $h = R$. The distances are calculated in units of $2\pi$. Because of the chosen ordering they are all positive, and $\phi_{13} = \phi_{12} + \phi_{23}$. As seen in the table, for larger values of $\beta$ the ground state has a clear interpretation as a ‘chain’ of three dipoles separated by one winding. This is seen to set in already for $\beta = 1$ and is accurate at the level of two decimal

| $\beta$ | $\langle \phi_{12}/2\pi \rangle$ | $\langle \phi_{23}/2\pi \rangle$ | $\langle \phi_{13}/2\pi \rangle$ |
|---------|-------------------------------|-------------------------------|-------------------------------|
| $\beta = 0.25$ | 0.50 | 0.44 | 0.94 |
| $\beta = 1$ | 1.01 | 1.01 | 2.03 |
| $\beta = 2$ | 1.00 | 1.00 | 2.00 |
places already for $\beta = 2$. For smaller values of $\beta$ we expect that kinetic terms will be more important and the dipoles would like to delocalize. In the table this is seen for a value of $\beta = 0.25$ where the expectation values of the distances are no longer close to $2\pi$, i.e. the dipoles tend to be sitting further than one winding apart on average. In this regime of weak dipolar interactions the dipoles will tend to spread out to minimize kinetic energy while at the same time being able to take advantage of the attraction from several of the pockets seen in figure 2.

5. Discussion and outlook

In the present paper we have considered the physics of dipolar particles that are confined to move on a one-dimensional helix. We first look at the dipole–dipole interaction on a helix, and how the interplay between the long range interaction and the peculiar geometry of the helix leads to a two particle potential with several minima of decreasing depth. These minima correspond to the attractive head-to-tail configuration and the decreasing depth of successive minima is a result of the dipoles being an increasing number of windings of the helix apart. Our main question concerns the formation of bound state in this non-trivial system. In particular, what type of bound states form with more dipoles. As our main focus we use the case of three dipoles.

In the strong interaction limit both two- and three-body bound states correspond to the dipoles being an integer number of windings apart in the quantum ground state of the system. However, for weaker interactions the bound states increase in size, and pairs of dipoles can no longer be said to be a certain number of windings apart as they become effectively delocalized across several windings of the helix. For three dipoles we show that for moderate dipole strengths they form a short yet well-defined chain of three dipoles sitting immediately underneath each other.

This affinity for chain formation was discussed previously in the limit of very strong interactions where classical crystal formation on the helix is expected [21]. There it was shown how the dipoles would form chains up the helix where each dipole was approximately one winding away from its neighbors on either side. In one dimension such long range orders are not possible in the quantum regime, and one would instead expect the formation of a Luttinger liquid in such a system as has been discussed in [17]. This should be more pronounced for smaller values of $\beta$ where kinetic terms are sizable and the particles will tend to delocalize, i.e. not merely stay approximately fixed in the minima provided by the attractive head-to-tail configuration. The formation of chains in related geometries in both two- [41, 42] and one-dimensional [43, 44] setups, and this chain formation is expected to persist and be in the many-body case also in the quantum regime [41, 45]. The strongly interacting regime can be explored by using harmonic approximations [46] to the full dipolar interaction for instance in the study of the thermodynamic properties of dipolar chains [47]. As we discussed above, a harmonic behavior is also seen in the helical geometry for large $\beta$ which is merely a reflection of the fact that the dipolar potential allows such an approximation for large dipole moments in any geometry where the head-to-tail configuration is possible. In future studies it would be interesting to extend the system to slightly longer chains and study the thermodynamics for instance using the harmonic approximation for strong interactions.

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