Formation of classical crystals of dipolar particles in a helical geometry

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Abstract
We consider crystal formation of particles with dipole–dipole interactions that are confined to move in a one-dimensional helical geometry with their dipole moments oriented along the symmetry axis of the confining helix. The stable classical lowest-energy configurations are found to be chain structures for a large range of pitch-to-radius ratios for a relatively low density of dipoles and a moderate total number of particles. The classical normal mode spectra support the chain interpretation through both structure and distinct degeneracies, depending discretely on the number of dipoles per revolution. A larger total number of dipoles leads to a clusterization where the dipolar chains move closer to each other. This implies a change in the local density and the emergence of two length scales, one for the cluster size and one for the inter-cluster distance along the helix. Starting from three dipoles per revolution, this implies a breaking of the initial periodicity to form a cluster of two chains close together and a third chain removed from the cluster. This is driven by the competition between in-chain and out-of-chain interactions, or alternatively by the side-by-side repulsion and the head-to-tail attraction in the system. The speed of sound propagates along the chains. It is independent of the number of chains, although it does depend on the geometry.

Keywords: dipolar molecules, collective dynamics, crystal formation

1. Introduction

A highly promising direction in cold-atom physics is the experimental realization and exploration of homo- and heteronuclear molecules at low temperatures [1–9]. The potential applications of such systems are wide-ranging within quantum simulation, information, computation, and metrology [10–13]. An important issue is the head-to-tail attraction that molecules with dipole moments have, which can severely limit experimental timescales due to strong losses [5, 14]. The suggested way forward has been to confine the molecules in low-dimensional setups where the head-to-tail attraction can be controllably reduced and losses can be suppressed. An experimental confirmation of this was recently achieved with a stack of two-dimensional planes [8] and in a three-dimensional optical lattice [9].

A great advantage of low-dimensional setups is that one can study the interplay of geometrical restrictions on dynamics in the presence of long-range interactions from the dipole–dipole forces. This is one of the main motivations of this paper. In the context of condensed-matter systems in low-dimensional systems, this interplay of range and geometry is a very active area of research (see [16] for an introduction). The geometry we will consider is that of a helix where we assume that the pitch and radius can be tuned experimentally. This can be realized in different ways. Laguerre-Gaussian beams with nonzero angular momentum are one possibility (bright [18–22] or dark [23, 24]). This method has some less desirable limitations on the maximum length of the uniform helix and the variational range of the parameters [15]. These restrictions can be dealt with by working instead with light guided by an optical nanofiber. Here it was recently shown that atoms can be trapped in the evanescent field surrounding the fiber waist [25–27]. A particularly interesting proposal concerns the generation of the double-helix potential known from DNA molecules [15].

Here we will explore the physics of a single-helix setup and assume that cold molecules are trapped on the helix. A few years ago, the same geometry was discussed as a possible example of a liquid–gas transition at zero temperature [28]. Furthermore, studies of the competition between dipolar particles and the external trapping potential have been done,
and linear to zig-zag transitions were found [29, 30]. This work builds on earlier findings of similar transitions in the case where the dipolar particles are replaced by charged ions [31, 32]. Helical structures have also been studied in spinor Bose–Einstein condensate with dipolar interactions, where they can appear as spin textures [33].

In our work, we assume that the helical trap is rigid and no movement can occur away from the helix, as has been the case in some recent studies of charged ions on a helix [34, 35]. This effectively means that we assume a tight trapping potential, and the cost of excitations in the transverse direction will thus be much larger than the interaction energies. We illustrate the geometry in figure 1 with different numbers of dipoles located on the helix. As we will see, they tend to form structures organized in chains depending on the density of the particles. The distance between the chains is not necessarily equidistant because the attractive and repulsive parts of the interaction strongly depend on dipole direction and distance. We are not aware of a previous discussion of the classical ground state phases in this setup with dipolar molecules.

In section 2, we provide energy expressions in a suitable coordinate system and focus on the simplest configurations as a function of geometric helix parameters and particle number. In sections 3 and 4, we discuss stability and normal modes, and the speed of sound in these 1D systems. Finally, section 5 contains a brief summary of the conclusions in addition to an outlook and perspectives related to experimental realizations.

2. Dipoles on a helix

We consider dipoles moving on the one-dimensional geometry of a helix. An experimental realization of this geometry is possible by applying counter-propagating laser beams to a tapered optical fiber [15] and trapping the dipoles in the evanescent field around the fiber. This is not strictly one dimensional, but by varying the laser power one can enter a one-dimensional regime. We first specify helix parameters, dipole coordinates, potentials, and energies; and second we calculate classically stable configurations.

2.1. Classical energy

A helix is described by two parameters, the height $h$ and the radius $R$. See figure 2 for a schematic drawing of a helix. The radius is the distance at which the helix revolves around a fixed axis, and the height is the vertical distance between two such revolutions. The position along the helix can be described by the arc length, $s$, along the helix or equivalently by the azimuthal angle, $\phi$, around the $z$-axis, $\phi = s/\alpha$, where $\alpha = (R^2 + (h/R)^2)^{1/2}$. We will use the angle $\phi$ where one circle is described by $\phi \in [0, 2\pi]$, and the following by $\phi$-values increasing beyond $2\pi$. The relationship to Cartesian coordinates is given by the following transformation:

$$ (x, y, z) = \left(R \sin \phi, R \cos \phi, h \frac{\phi}{2\pi}\right). \tag{1} $$

On the helix we place $N$ identical dipoles of mass $m$ and dipole moment $\boldsymbol{d}$, all aligned along the $z$-axis by an external field. The dipoles are then confined to move only on the helix, but they still interact through three-dimensional Cartesian space. The potential energy, $V$, of two dipoles at position $\mathbf{r}_i$ and $\mathbf{r}_j$ is

$$ V(\mathbf{r}_i, \mathbf{r}_j) = \frac{1}{4\pi\varepsilon_0} \frac{1}{r} \left| \mathbf{d} \cdot \mathbf{d} - 3 \left( \mathbf{d} \cdot \mathbf{\hat{r}} \right) (\mathbf{d} \cdot \mathbf{\hat{r}}) \right|, \tag{2} $$

where $r = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance between the dipoles and $\mathbf{\hat{r}} = (\mathbf{r}_i - \mathbf{r}_j)/r$ is the unit vector in the direction connecting the two dipoles. 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.

Using the transformation in equation (1), the potential energy of two dipoles positioned at angles $\phi_i$ and $\phi_j$ on the helix becomes

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

This effective potential scales as $R^{-3}$ and depends only on
The strongly damped oscillatory behavior reveals several minima with depths decreasing as $\phi^{-3}$, the same power as for interacting dipoles in three dimensions. The minima are crudely located at multiples of $2\pi$, that is, the first of them around 6, 12, and 18, as seen in figure 3. Thus, we have an effective 1D system with a long-range dipole-like interaction.

As seen from equation (3), the diverging repulsion for small $\phi$ with $h = R = 1$ turns into a diverging $\phi^{-3}$ attraction for sufficiently large $h/R$-values, that is, when $\frac{h}{R} > \pi \sqrt{2}$. The two dipoles would then prefer to be at the same point with infinite energy. In these cases, other short-range forces such as the van der Waals interaction become important. We want to avoid this regime, where chemistry rules, and hence we limit our investigations to cases where $\frac{h}{R} < \pi \sqrt{2}$.

The total potential energy, $E$, is obtained by adding the contributions from all pairs through equation (3) for any set of positions given by the coordinates $\{\phi_i\}$, that is,
\[
E\left(\{\phi_i\}\right) = \sum_{i<j}^N V(\phi_i, \phi_j). \tag{4}
\]

The stable crystal configurations can then be found as minima of the energy landscape providing equilibrium values for the positions $\{\phi_i\}$ for any given $N$ as a function of $h/R$.

2.2. Equilibrium configurations

Full coordinate variation of all positions implies minimization of an N-dimensional function. To simplify this problem, we impose constraints on the positions of the dipoles. We first assume that all the dipoles are equally spaced along the helix; that is, the angular distance, $\phi = |\phi_i - \phi_j|$, between neighboring particles is constant. A given total number of particles, $N$, then corresponds to varying the length of the helix. The resulting energy per dipole is shown in figure 4 as a function of $\phi$. For sufficiently large $N$, the energy per particle is independent of the length of the helix.

The oscillating functions in figure 4 are striking. The many minima at shorter and shorter angular distance correspond to an integer number of dipoles per winding of the helix. At larger separation, the oscillations continue but with cubic decrease of the depths occurring at approximately integer multiples of $2\pi$. The depths of the minima are roughly equal for large $\phi$ while decreasing toward smaller values of $\phi$.

To interpret these observations, it is useful to recall that head-to-tail vertical dipoles attract each other, while repulsion occurs between horizontal dipoles connected by a vector almost perpendicular to the dipole moments. The results in figure 3 thus suggest that the energy is dominated by the attraction between the dipoles in different windings because the dominating minimum is close to $2\pi$. The repulsion is much smaller between dipoles on the same winding, where $\phi$ differs from $2\pi$. Furthermore, the attractions between optimally placed dipoles on the same winding decrease with decreasing values of $h/R$; see figure 3. These conclusions emerge because the energy per dipole seems to be independent of the number of repulsions arising from dipoles on the same winding.

With this overall interpretation, we can look at more detailed features. The $h/R$ dependence of the positions of the minima is very weak, although visible. The minimum at the highest dipole separation, $\phi \approx 2\pi$, is in fact slightly less than $2\pi$. This means that each dipole in this case is not separated by exactly one winding, and thus the positions of the $N$ dipoles for such a chain rotate slowly around the axis of the helix. After about 75 layers, a full revolution of $2\pi$ is

![Figure 3](https://example.com/fig3.png)

**Figure 3.** The reduced potential, $4\pi R^3 \epsilon_0 V/d^2$, of two dipoles as a function of the relative angle, $\phi = \phi_i - \phi_j$, separating the particles on the helix. The helix parameters are chosen to be $h = R$ (blue) and $h = 1.6R$ (black).

![Figure 4](https://example.com/fig4.png)

**Figure 4.** The reduced energy per particle, $E/N$, in units of $d^2/(2\pi \varepsilon_0 R^3)$, as a function of the angular distance, $\phi$, between the particles. The different curves correspond to $h/R = 1.6, 1.0, 0.8,$ and $0.6$, with smaller well depths for decreasing $h/R$. The total particle number is $N = 100$. 

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completed. As seen in figure 4, the deviation from $2\pi$ remains essentially unchanged by a modest variation of $h/R$. The second highest minimum position at around $\pi$ in figure 4, corresponds to two dipoles per revolution. The configuration is then dipoles forming two chains on opposite sides of the helix, as illustrated in figure 1. Closer inspection reveals that each of the two chains is again slowly rotating around the helix axis.

The energy shown in figure 4 depends on the azimuthal angle and the ratio $h/R$, where the latter in principle can vary from 0 to $\pi\sqrt{2} \approx 4.4$. For two dipoles separated by $r$ in three dimensions, the energy scales as $r^{-3}$. For two dipoles separated by one winding, the three-dimensional distance scales as $h$, and according to equation (2), the energy per dipole must scale as $h^{-3}$. If this in-chain interaction is the dominating contribution, the energy per dipole should scale in this way. This is another way to investigate the aforementioned conclusion that the attraction between dipoles in different windings dominates the total energy, even for higher dipole density.

The expected scaling is tested in figure 5, where we show the product $\frac{k}{h \sqrt{2}} h^{-3}$, which should be constant under these assumptions of in-chain dominance. Over the range of $h/R$ from 0.2 to 1.8, the deviations from an average constant are less than 10%. This change is due mostly to the slight rotation of equilibrium angle with each revolution, i.e., dependency on both $h/R$ and the angle. The in-chain dominance would be violated by even larger values of $h$, where out-of-chain and in-chain distances become comparable. However, configurations with too-large $h$-values are unstable and hence uninteresting.

The opposite limit of $h \to 0$ would also violate the distinction between particles in different chains, as evident from the geometry where all particles would be on a circle and all repelling each other by an $h$-independent interaction. The equilibrium structure then necessarily must be equidistant spacing around the resultant ring for all particle numbers. The chain structure has disappeared. However, this structure is reached in only the extreme limit of $h \to 0$, whereas the chain structure is maintained for any finite, even infinitesimally small, value of $h/R$. The current calculations assume equidistant angular spacing, which implies that the in-chain particles approach each other in head-to-tail attractive configurations, and simultaneously all out-of-chain interactions become repulsive. Thus the energy scaling of these rather unstable configurations approaches $h^{-3}$.

The understanding of equilibrium configurations as effective chain structures has some interesting consequences for the spectrum of normal modes.

### 3. Normal modes

Vibrations around equilibrium configurations reveal intrinsic properties of the vibrating structures. The corresponding uncoupled motion of orthogonal modes can be found by expansion of the energy in equation (4) to the second order in coordinate deviations from the set of their equilibrium values $\{\phi_{i}^{(0)}\}$. Then we have

$$E - E_0 \approx \frac{1}{2} \sum_{i,j} K_{i,j} \left( \phi_i^{(0)} \phi_j^{(0)} - \phi_i^{(0)} \phi_j^{(0)} \right),$$

where $E_0$ is the energy of the equilibrium configuration. Both the vanishing first derivatives (omitted) and the second derivatives ($K$) are taken at the equilibrium. The variable change corresponding to diagonalizing the matrix $K$ in equation (6) provides a set of eigenvalues defined by $\frac{1}{2} \omega_n^2 r^2$. The resulting frequencies $\omega_n^2$ are all positive if the equilibrium configuration is stable. Conversely, if one or more eigenvalues $\omega_n^2$ are negative, then the system is unstable toward coordinate deviations in the corresponding directions.

#### 3.1. Stability

We calculate the elements of the $K$-matrix in equation (5) analytically from the expression in equation (3). We subsequently diagonalize this matrix and obtain the eigenvalues expressed as eigenfrequencies. The corresponding eigenvectors include all the $N$ angular coordinates, in contrast with the energy calculations in the preceding section, where constant differences between neighboring particles were maintained. This extension of configuration space implies that the computed eigenfrequencies can show instability corresponding to vibrational modes different from vibrations where the nearest-neighbor distances are maintained.

We emphasize that a near (first-order) miss of the minimum due to a too-restricted (constant-difference) variational space does not jeopardize the stability condition because the second derivatives remain unchanged by moving from approximate to true (close-lying) minimum. A conclusion of stability (all $\omega_n^2$ are positive) of the calculated restricted solution then means that the marginally deviating true solution also is stable. On the other hand, instability of the restricted solution implies that the true solution may deviate substantially.

It turns out that the restricted configurations (constant angular separation) are not always stable and that the stability depends on both the geometry of the helix ($\frac{h}{R}$) and the total
number of dipoles $N$. The configuration with one dipole per winding is always stable as long as the short-range interaction is repulsive, that is, $\frac{h}{R} < \frac{\pi}{2}$. For two, three, and more dipoles per winding, the picture becomes more complicated.

It is tempting to believe that distances corresponding to the minima in figure 4 are good candidates for stable configurations. We therefore place the dipoles at these points with equidistant separation such that two, three, and four dipoles are at $\phi \approx \pi$, $\phi \approx 2\pi/3$, and $\phi \approx \pi/2$, respectively. We then increase the total number of particles, $N$, or equivalently the extension of the helix, and observe when, or possibly if, these configurations become unstable. Obviously, an unstable configuration must require another structure of lower energy. However, finding those structures for increasing $N$ quickly becomes a complicated many-body problem. These solutions are generally beyond the scope of this paper.

In figure 6 the critical number of dipoles $N_{crit}$ is shown as a function of $\frac{h}{R}$. Values of $N$ smaller (larger) than $N_{crit}$ are then stable (unstable). If there is no point for a particular value of $\frac{h}{R}$ it is because the system is stable up to at least our maximum total number, $N = 1600$. Two dipoles per winding are stable in the equidistant configuration when $\frac{h}{R} < 0.65$, at least up to $N = 1600$. For $\frac{h}{R} > 0.65$, the system becomes unstable at much smaller values of $N$, decreasing from about 550 toward zero as $\frac{h}{R}$ increases. In contrast, for three dipoles per winding, the critical value of $N$, decreases from about 1600 to about 500 when $\frac{h}{R}$ increases from 0.5 to 0.9. For $\frac{h}{R} > 0.9$, the equidistant configuration is stable for three dipoles per winding for all $N < 1200$.

The stability behavior for three and four dipoles per winding is similar, but stability already arises for values larger than $h/R \approx 0.6$. This smaller threshold of $h$-instability has to arise from the presence of the fourth particle. Roughly in the interval $0.2 < h/R < 0.6$, the four equidistantly placed dipoles become unstable only for a relatively large dipole number, as shown in figure 6. For small $h/R$-values, the behavior is similar to that of our three cases in figure 6. The apparent extra stability of four chains is due to strong repulsion between neighboring dipoles in the same circle. If possible, they lock each other in the minima seen in figure 4.

When $h/R$ decreases below about 0.2, the equidistant four-particle system again becomes stable, but now due to the overwhelmingly dominating in-chain head-to-tail attraction. This configuration is reached by decreasing $h$ toward zero for equidistant angular distances. The stability in at least a local minimum is guaranteed for any particle number per winding by strong in-chain attraction and a comparably much smaller out-of-chain repulsion. The stability behavior for different dipole numbers is a sobering illustration of the possible many-body complexity of even the current one-dimensional system. The detailed structure changes responsible for these instabilities are investigated in the next subsection.

### 3.2. Chain structure

To understand the computed properties, we first return to the two-chain structure illustrated in figure 1 for two dipoles per winding. We focus on the two nearest-neighbour dipoles belonging to different chains. When $\frac{h}{R}$ increases for a given $N$, their interaction changes from repulsive to attractive, and therefore it becomes energetically unfavorable to maintain the configuration of equal angular spacing. It is advantageous to move the two chains closer to each other. For example, for $N \approx 600$ the stable configuration for small $\frac{h}{R}$ becomes unstable when $\frac{h}{R}$ increases above 0.75.

This result can be understood by extending the helix by adding one pair at a time. Each of these extra dipoles at the end of the helix repels the neighbor in the opposite chain in the circle beneath. In contrast, the interaction with dipoles on circles far away will be attractive because such pairs approach the head-to-tail attractive configurations. The larger the $N$, the greater the number of these attractions, which eventually will dominate over the repulsion between nearest neighbors. This is directly related to the two-body potential shown in figure 3, where the attraction already appears for $\phi > 2\pi$.

This explanation is tested by varying the distance between the two chains in figure 1. The resulting energy per dipole is shown in figure 7, where the equidistant configuration corresponds to the angle close to $\pi$. The corresponding maximum demonstrates, instability, and the two minima at about 1.8 and 4.3 strongly suggest an equilibrium configuration where the two chains remain, but at a smaller distance. The two minima are equivalent because each chain can be
chains are separated by a third chain of dipoles between two other chains: the third is measured from the first. This is done from top to bottom for \(N = 500\) (black circles), \(N = 700\) (red triangles), and \(N = 1000\) (blue squares), dipoles and \(\phi = 0.6\). The resulting energies are shown in figure 8 for three different total numbers of particles. For \(N = 500\), we see the minimum at \(\phi = \frac{1}{3}2\pi\), that is, directly between the two first chains corresponding to the equidistant configuration, and consistent with \(N < N_{\text{crit}} \approx 900\). For \(N = 700\), it is difficult to extract an accurate value for the position of the minimum; but increasing further to \(N = 1000\), two separate minima appear on the opposite site of the value for the (now unstable) equidistant configuration.

This interpretation is again supported by the observation that the structure of the first unstable normal mode with imaginary frequency corresponds to the two nearest chains vibrating against each other, whereas all other normal modes are stable. All these properties show that even when the equidistant configuration becomes unstable, the chain structure can still be considered the basic constituent. This means that the attraction of two dipoles above each other in a chain dominates over the interaction between dipoles in different chains.

### 3.3. Small systems

The long-distance interaction is responsible for many properties. In particular, it provides the attraction between particles on windings far apart, leading to collapse of the system for sufficiently large \(N\). By the same token, small \(N\) leads to stable systems with equidistant spacing of the dipoles for moderate values of \(h/R\); see figure 6. In addition, small \(N\) allows faster computations. We can exploit this fact to study generic properties such as structures of low-lying normal modes.

We choose \(N = 12\) because this number of dipoles is divisible by 2, 3, and 4 dipoles per winding. This match is expected to provide more binding and very clean vibrational normal modes. We show the lowest frequencies in figure 9 for 2, 3, and 4 dipoles per winding. It is striking that the spectra are almost two-, three-, and four-fold degenerate. This is caused by the commensurability to the number of particles per winding and implies that the eigenvalues appear either pairwise, as triples, or as quadruplets. The degeneracies become less pronounced as the frequency increases.

These properties are signals of the chain structures discussed in the preceding subsections. The computed

\[\text{Figure 8. Reduced energy per dipole, } \frac{E}{R}, \text{ as a function of the position of a third chain of dipoles between two other chains: the first two chains are separated by } \phi = \frac{1}{2}2\pi \text{ radians, and the position of the third is measured from the first. This is done from top to bottom for } N = 500 \text{ (black circles), } N = 700 \text{ (red triangles), and } N = 1000 \text{ (blue squares), dipoles and } \phi = 0.6.\]

\[\text{Figure 9. (top) The spectrum of squared frequencies for 12 dipoles, with two (blue squares), three (red circles), and four (black triangles) dipoles per revolution. (bottom) The amplitudes of the normal modes for the lowest nearly degenerate eigenvalues. On the left are eigenmode number 3 (blue squares) and 4 (red circles) for two and three dipoles per winding respectively. In the middle are eigenmode number 4 (blue squares) and 5 (red circles) for two and three dipoles per winding. On the right is eigenmode number 6 (red circles) for three dipoles per winding.}\]
The degenerate normal modes correspond, for two dipoles per winding, to the two chains moving either exactly in phase, preserving the same particle distances, or to chains moving against each other exactly in opposite phase. In general, we characterize each of the normal mode oscillations by a set of relative amplitudes, where each describes the maximum deviation from equilibrium along the helix of the corresponding dipole. The amplitudes of these oscillations are also shown in figure 9. The same degeneracies at higher frequencies correspond to the same vibrational relationship between chains but now with additional nodes along the chains.

For two particles per winding, the amplitudes for eigenmode number 3 (bottom left in figure 9) show alternating direction for neighboring dipoles. This means that the two chains oscillate against each other. For three particles per winding, eigenmodes 4, 5, and 6 are shown from left to right in the bottom panel of figure 9. The left side shows two chains moving against the third, as seen by two almost equal neighboring amplitudes and one amplitude of about twice the size in the opposite direction. Similarly, in the middle are the three chains in phase, as the three neighboring amplitudes are equal. On the right, we again see two chains moving against the third.

For four particles per winding (not shown in figures), the four normal modes are similarly related to chains moving in phase, pairs moving against each other, or triples against a single chain. The degeneracies and the normal mode structure are effects of the next-nearest-neighbor interaction, and the small differences within the almost degenerate frequencies are due to small nearest-neighbor corrections to the vibration-dominating next-nearest interaction.

These simple structures arise so purely because an integer number of particles can precisely fit into one winding. If this is not the case, the degeneracies are broken and the spectra move towards another type of degeneracy. A non-integer ratio between particle number and particles per winding must destroy the picture of chain structures, simply because identical chains cannot be formed. However, the lowest energy from the strongest attraction arises by adding the odd particles at the ends of the chains. These features are illustrated by the example of \( N = 13 \) shown in figure 10, where the top panel exhibits frequencies for 2, 3, or 4 dipoles per winding, with the additional dipole placed at the end of one of the chains.

The degeneracies compared with \( N = 12 \) are now lifted, although traces can be detected. However, the modes exhibited in figure 9 still come in pairs for two dipoles per winding, even though their frequencies differ. The same features of normal mode similarity between systems with \( N = 12 \) and \( N = 13 \) are also seen for the energies of three and four particles per winding. The amplitudes for two modes of two dipoles per winding at the bottom of figure 9 show that one of the chains is essentially not moving, whereas the other is undergoing an odd parity oscillation. The interpretation is generally that the slightly different chains still vibrate against each other. These boundary layer effects would decrease as the total number of particles increases.

4. Speed of sound

The speed of sound in a crystal is a fundamental property that plays an important role in many physical processes. The sound is mediated by particle motion, and normal modes carry the necessary information about the correlated small-amplitude vibrations that form the sound waves. The length of our one-dimensional regular crystal is \( N(\Delta \phi)_0 \), where \( (\Delta \phi)_0 = \phi_{i+1} - \phi_i \) is the distance between equally spaced neighboring dipoles along the helix. The corresponding wave numbers are \( k_n = \frac{2\pi n}{NR(\Delta \phi)_0} \), where \( n \) is an integer. The speed of sound is then given by \( c = \omega_n/k_n \) in the limit of small \( k_n \) when \( \omega_n \) is the \( n \)th normal mode frequency. Because small \( k_n \) requires large \( N \), we have to find normal modes for large systems.

4.1. Simple models

The restoring force is obtained in general from the energy in equation (5) for arbitrary, independent displacements of the individual dipoles. The stable configurations are equidistantly distributed dipoles along the helix for a modest density per revolution and perhaps also only for a finite total number of particles. For this structure, we search for small-amplitude vibrations around equilibrium, which allows sufficiently accurate energy calculation by using the second order, as in equation (5). Large \( N \) is expected to eliminate dependence on specific choices of end-point configurations. We will explore consequences of these approximations while staying within the validity ranges found in the preceding sections.
The equal spacing condition for a very long sequence of dipoles has several consequences that we must take into account. First, the same translation of all dipoles does not change any of the relative distances, and the total energy must remain unchanged as well. Second, all two-body properties depend only on the relative distance between the particles. In particular, the value of \( K_{ij} \) is thus the same as \( K_{k+i+k+j} \) for any value of \( k \). The double sum in equation (5) can then be performed in a different order, where the summation indices are along a constant sum, \( k \), and a constant difference, \( l \). However, only relative distances produce any energy variation. Let us measure deviations from equilibrium positions for the individual variables, that is, using the coordinates \( \phi_i = \phi_j - \phi_j^{(0)} \). In addition, we assume that the energy to the second order in distances from equilibrium is independent of which particle is used as the reference position. These assumptions lead to

\[
E - E_0 = \sum_{l>0}^1 \frac{1}{2} K_{k+1,k-1} (\phi_{k+1} - \phi_{k+1}^{(0)}) (\phi_{k-1} - \phi_{k-1}^{(0)}).
\]

where we measure relative to particle \( k \). Equation (7) is then independent of \( k \) and the curvature depends only on \( l \).

The classical force on particle \( n \) is minus the gradient of the potential energy given in equation (7), which, according to Newton’s second law, equals mass times acceleration given as the second derivative of the equation of motion becomes

\[
m \frac{\partial^2 \phi_i}{\partial t^2} = \frac{1}{2} \sum_{l>0}^1 K_l (\phi_{k+l} + \phi_{k-l} - 2 \phi_k).
\]

where we use the definitions \( K_l = K_{k+1,k-1} \). We now search for periodic motion, \( \phi_j = A_j \cos(\omega \tau + a_j) \), around the \( j \) equilibrium positions. The time dependence is canceled on both sides of equation (8) if and only if the amplitudes are identical, that is, \( A_j = A_0 \), and simultaneously the average phase \( (a_k + a_{k+j})/2 \) equals \( a_0 \) for all \( l \). The latter condition immediately implies a linear dependence of the phases, that is, \( a_j = a_0 + jb_j \). With these definitions, we arrive at the frequency given by

\[
ma^2 = \sum_{l>0}^1 K_l (1 - \cos(lb_1))
\]

These frequencies with the corresponding eigen phases given by \( b_1 \) characterize the \( N \)-independent periodic solutions. The spectrum is continuous because any value of \( b_1 \) between 0 and \( 2\pi \) provides a frequency through equation (9). An appropriate discretization can for example be found by assuming the same phase, apart from a multiple of \( 2\pi \), for the end-point dipoles. This means that \( a_0 = a_N + n2\pi \), which is equivalent to \( b_1 = 2\pi n/N \) for any integer value \( n \). This can be obtained by bending the helix to let the two end points meet. Now the \( N \)-independent solutions, \( a_n \), result from equation (9).

The size of \( K_l \) decreases strongly with \( l \) because the overall energy scale is obtained from a cubic decrease with distance. The largest \( K_l \) is then usually by far the lowest \( l \), that is \( l = 1 \). By using only the lowest order in an expansion of equation (9), we find the lowest frequencies to be approximately given by

\[
\omega_n \approx \frac{2\pi n}{N} \sqrt{\sum_{l>0}^1 K_l / m}.
\]

The speed of sound, \( c \), is then obtained as the ratio between \( \omega_n \) and the wave number \( k_n \), where the latter is found by equating the total length of the helix with the wave length. Thus, \( RN(\Delta \phi)_0 = 2\pi n/k_n \), where \( (\Delta \phi)_0 \) is the angular distance between the equidistantly placed dipoles. We then finally get

\[
c = \frac{\omega_n}{k_n} \approx R(\Delta \phi)_0 \sqrt{\sum_{l>0}^1 K_l / m},
\]

which is the result for a periodic structure of particles located on a ring [17]. Thus, we get the same \( c \) independent of which of the lowest modes of \( n = 1, 2, 3 \) we used. Furthermore, \( c \) is also roughly independent of the number of dipoles per winding. This is seen from equation (9) when the \( K_l \)-summation is dominated by the first in-chain contribution for \( l = l_0 \), giving \( c = R(\Delta \phi)_0 \sqrt{K_{l_0} / m} \). We then obtain the same \( c \) because both \( K_{l_0} \) and \( (\Delta \phi)_0 \) are independent of \( l_0 \) or equivalent dipole density.

### 4.2. Numerical results

We calculate all \( N \) eigenfrequencies, \( \omega_n \), as functions of \( N \) for \( 1, 2, 3, \) and 4 dipoles per revolution in the equidistant stable configurations. We first show the ordered frequencies for \( N = 20, 50, \) and 100 and for \( h = R \) in figure 11. The x-axis is scaled with the different numbers of dipoles. The details are not meant to be visible on this figure, where the striking features are that all eigenfrequencies, after scaling, essentially follow the same curve, varying from zero to a maximum value of about 50 for the largest frequency.

This behavior is evident from equation (9), where the discretization of \( b_1 \) is considered to vary from 0 to \( 2\pi \). These two end-point values of \( b_1 \) result in the maximum value of the cosine function and a limiting largest value obtained as the sum of all the curvatures. This sum is essentially independent...
of \( N \) because \( K_I \) decreases very fast with the distance between the dipoles, as parameterized by the index \( l \). Thus, only the smallest values of \( l \) then contribute in the summation. Values of \( b_1 \) around \( \pi \) produce alternating signs of the cosine function and give the small frequencies.

We now focus on the lowest frequencies, which, according to equation (9), are expected to vanish as \( n/N \) for increasing \( N \). We therefore show the frequencies multiplied by \( N/n \) in figure 12 as functions of \( N \) for the preceding case of a few dipoles per revolution. The linear dependence is quickly reached for most of the stable systems. This arises from the allowed lowest-order substitution of the argument in the sine function of equation (9). Here \( 2\pi n/N \ll 1 \) or equivalently \( N \) must considerably exceed \( 6n = 6, 12, 18 \), which should easily be fulfilled for our cases. Also, an increase proportional to \( n \) is seen in all cases.

An exception in figure 12 is seen for two dipoles per revolution, where the small \( N \) increase is followed by a maximum and a subsequent decrease. This behavior reflects the transition towards instability of the configuration of equidistant spacing. Another exception appears for three particles per revolution. The constant values approached by the second and third lowest frequencies occur apparently for much larger values of \( N \), that is, about 500 and 1500. The latter anomaly can be explained by starting with a very small \( N \), where we know that a near-three-fold degeneracy appears. By increasing \( N \), the two lowest frequencies increase, whereas the third stabilizes and remains at this constant value when \( N \) passes 500. The other two, initially lowest, frequencies continue to increase until about 1500, where a new stabilization takes place due to the crossing of an initially much higher-lying mode.

The stability of \( \text{Neoh} \) for large \( N \) reflects the appearance of acoustic modes, which, as we will discuss now, correspond to in-chain dipole oscillations. The frequency crossings of these modes by lower-lying modes for small \( N \) reflect that out-of-chain oscillations are more favorable for small chains.

The features discussed here are exemplified by \( h = R \) results. However, the general behavior for other helix parameters can be understood with the same ingredients. The curvatures change and accordingly also the frequencies. The only other differences are that the stabilities depend rather strongly on \( h/R \) and the large \( N \)-limit and that the resultant linear dependence on \( 1/N \) may sometimes not be reached for the equidistant configurations.

We now proceed to calculate the speed of sound by dividing the frequencies by the wave number, as in equation (11). This means multiplying the numbers in figure 12 by \( R(\Delta \phi)_{10}/(2\pi n) \), where \( n = 1, 2, \) and 3. The results are shown in figure 13 for \( n = 1 \) as a function of \( h/R \). A smooth curve for one dipole per revolution is found for a large range of helix parameters. The speed of sound decreases roughly by \( (h/R)^3 \) with increasing \( h/R \). This is almost the same scaling as observed for energy; see figure 5. These results are calculated from the lowest frequency, but essentially the same curve appears by use of the second and third frequencies, corresponding to \( n = 2, 3 \). The proportionality in \( n \) from equation (11) is canceled by that in \( k_w \).

More dipoles per revolution also lead to a series of points in figure 5. However, instability at large \( N \) before stabilization prevents calculation of the speed of sound, and fewer points can be obtained. It is striking that all available points appear essentially on the same curve as the one-chain result. The equidistant equilibrium spacing, \( (\Delta \phi)_{10} \), decreases with the number of dipoles per revolution. The factor of \( L \) inside the square root in equation (11) can compensate for this when a single value of \( K_I \) dominates the speed of sound. This happens in the chain picture. Here \( K_I \) will be small for \( l \) less than the number of chains, \( l_0 \). However, \( K_{l_0} \) will be the term describing the interaction with the nearest neighbor within a single chain. The \( K_I \) terms for \( l < l_0 \) are interactions with particles in different chains. In summary, we have a chain-dominated dynamics where we can use an in-chain nearest-neighbor approximation for any number of chains. Thus, the sound waves travel within each chain, and the perturbations of the waves within a single chain from neighboring chains are minimal.

Finally, we investigate the consequences of the instability of some of the configurations. For \( h = R \), we know that the chains prefer specific distances for sufficiently large \( N \), as exemplified in figures 7 and 8. We therefore calculate the normal mode spectra for the non-equidistant equilibrium configurations of two dipoles per winding. The resulting points for an average value, \( (\Delta \phi)_{10} \), fall on the common curve.
in figure 13 found for the equidistant configurations. This again supports the interpretation in terms of the foregoing chain structures.

5. Discussion and outlook

The classical potential energy is calculated for a total large number, \( N \), of dipoles placed on a helix and uniformly distributed with a density corresponding to 2, 3, and 4 dipoles per winding. The dependence on the ratio of the two helix lengths, pitch-to-radius \((h/R)\), is investigated. The unit of energy is given by dipole moment squared divided by the cubic power of the radius. These parameters enter only as a scale, without influence on the geometric structures providing stability. The one-dimensional confinement implies that the dipoles prefer to be located at specific angular distances from each other along the helix. This is due to the strong attraction between head-to-tail configurations combined with equally strong side-by-side repulsion. The system collapses into strings of infinite energy when \( h > R \pi \sqrt{2} \), which therefore is a limit we do not exceed.

The stable structures for relatively small densities can be characterized as a number of chains formed by dipoles almost head-to-tail along the helix. The stable chain structures are equidistantly distributed when \( h/R \) is larger than about 1 and \( N \) is relatively small. Increasing \( N \) for these \( h/R \) values leads to instability. For decreasing \( h/R \), stability is maintained for larger \( N \) but eventually lost for all densities. The structures with lower energy that cause this instability in the case with a few dipoles per winding are clusterized states where chains of dipoles cluster. These modes of instability are investigated through the classical normal modes. An abrupt change in the chain structures occurs when \( h/R \) is only marginally varied. This is analogous to spontaneous symmetry breaking of a symmetric minimum by conversion into a maximum and two asymmetric minima. A main finding is that both initial and final structures can be characterized as chains, and thus the change is really in the local density due to clusterization.

By increasing the density, the preferred configuration changes from one to more chains. For densities corresponding to fewer than five dipoles per winding, the equidistant spacing around the circles is broken for a sufficiently extended helix. The more chains that are imposed, the greater the stability because the short-range repulsion between neighboring dipoles on the circles locks all dipoles in positions on average as far away from each other as possible. This is classical crystal formation.

Detailed investigations are also carried out for smaller \( N \), where we find signals of preferred geometries in degeneracies, or lack thereof, in the normal mode frequencies. For example, \( N = 12 \) allows very symmetric structures of 2, 3, and 4 chains with corresponding normal mode degeneracies of 2, 3, and 4. The normal mode amplitudes reflect preference for chains as inert units vibrating against each other. The degeneracies are broken by addition of one more dipole at the end of one chain. However, the chains still prefer to vibrate in the same way as inert entities. Finally we calculate the speed of sound whenever we find stable structures for sufficiently large \( N \). We find the same behavior of the speed of sound as a function of \( h/R \) for 2, 3, and 4 chains in the system. This confirms the chain picture because it shows that sound waves propagate along the chains.

In this paper, we investigated a finite number of dipoles on a finite helix. Boundary conditions corresponding to densities of a non-integer average number of dipoles per winding were discussed for only a few small systems. For larger systems, the optimum configurations would be chains found by dividing the dipole number by the number of windings and rounding up to the nearest integer. This leaves room for adding the non-matching dipoles at the outer circle. They would each prefer to be located in continuation of one of the chains. For very large systems, these end-point structures are not expected to influence the bulk structures.

In future studies, we want to consider the quantum effects on the system from both the few-body and the many-body point of view. For few-body quantum bound states, previous studies have considered dipolar particles in one-dimensional tubes and on rings [36–40]. Dipolar interactions can be addressed using harmonic approximations [41–43], stochastic variational methods [44], and exact diagonalization [45–47]. All of these methods should be adaptable to helical geometry. For treatment of larger particle numbers, we imagine that a combination of Luttinger approaches with dipolar particles [28, 48–54] and matrix product states [55] or density matrix renormalization group methods [56, 57] are possible approaches. Some recent examples of the numerical methods applied to dipolar particles can be found in [58–61].

As discussed briefly in the introduction, we expect that the most straightforward experimental realization of helical geometries will be in systems where light is guided by an optical nanofiber with a diameter that is smaller than the wavelength of the light such that an evanescent wave builds that can be used as an atomic trap. This has been done by the Rauschenbeutel group in Vienna [25–27]. The same group suggested the creation of helical traps in a recent paper [15]. At the moment, these proposals involve trapping of non-polar rubidium atoms, and thus one would need to extend the technique either to polar molecules or to atoms with large intrinsic magnetic dipolar moments. Given the added complications in producing cold polar molecules, it may be easier to use magnetic dipoles.

Our study here concerns a single helix. An obvious extension is to the double-helix DNA geometry proposed in [15]. Based on the current finding, one might expect that this would be merely a doubled version of the single-helix ground states. However, due to long-range interactions, one could imagine that more involved states would be allowed. In terms of quantum mechanical few- and many-body states, this should be directly addressable using the techniques previously discussed. An interesting recent proposal concerns a generalization to a system where there are three intertwined helical traps corresponding to the geometry of three-stranded DNA molecules. In this case, it has been suggested that three-body bound states across the strands could occur in the case where no two-body bound states across any two out of the
three strands are possible [62, 63]. This could connect such systems to the Efimov physics studied in few-body nuclear and atomic physics [64]. Again, the foregoing methods would be able to address such ideas.

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