DISCRETE-TO-CONTINUUM LIMITS OF LONG-RANGE ELECTRICAL INTERACTIONS IN NANOSTRUCTURES*

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Abstract. We consider electrostatic interactions in two classes of nanostructures: (1) helical nanotubes, and (2) thin films with uniform bending (i.e., constant mean curvature). Starting from the atomic scale with a discrete distribution of dipoles, we obtain the continuum limit of the electrostatic energy; the continuum energy depends on the geometric parameters that define the nanostructure, such as the pitch and twist of the helical nanotubes and the curvature of the thin film. We find that the limiting energy is local in nature. This can be rationalized by noticing that the decay of the dipole kernel is sufficiently fast when the lattice sums run over one and two dimensions, and is also consistent with prior work on dimension reduction of continuum micromagnetic bodies to the thin film limit.

1. Introduction. Electrical and magnetic interactions are long-range; that is, a charge or dipole interacts with all the other charges and dipoles in the system, and the interactions cannot be truncated because the decay with distance is slow [Tou56, Bro63, JM94, MD14]. We consider such electrostatic interactions in nanostructures, specifically helical geometries and thin films with uniform bending. These geometries are ubiquitous in nanotechnology; while not periodic, their structure has significant symmetry that we exploit in this paper, using the framework of Objective Structures [Jam06]. We exploit this symmetry to adapt periodic calculations of the continuum energy to the setting of these nanostructures. Specifically, starting from a discrete atomic-scale description of the electrostatic energy, we find the limit energy when the discrete lengthscale of the nanostructures goes to zero.

For simplicity, we assume in this paper that the charge density can be approximated as composed of discrete dipoles. The electrostatic energy of such a system is the sum of all pairwise dipole-dipole interactions. Unlike short-range bonded atomic interactions that typically scale as r^{-6} with distance r, the dipole-dipole interactions decay slowly with distance as r^{-3} . Consequently, we cannot simply truncate after a few neighbors, and naive truncation can lead to qualitatively incorrect results in numerical calculations [MD14, GD20a, GD20b]. While we use the setting of discrete electrical dipoles, the setting of magnetic dipoles has an identical mathematical structure and physical interpretation [Bro63, JM94, MS02, SS09], and we borrow key ideas from that literature. Further, while discrete dipoles provide the simplest setting to illustrate the physics, it can be extended to the more realistic and general setting of a charge density field following ideas from [Xia05]. A key physical distinction between the electrical and magnetic situations is the possibility of electrical monopoles that does not exist for magnetic case, but we examine this elsewhere [SWB $^+$ 21] and assume here that there are no free charges.

We turn to the question of dealing with the non-periodic geometry of the nanostructures. While neither helices nor thin films with curvature are periodic, the framework of Objective Structures (OS) introduced in [Jam06] provides a powerful approach to deal with such geometries. In brief, OS provides a group-theoretic description of these nanostructures that enables a parallel to be made with periodic lattices. This parallel to periodic lattices has enabled the adaptation of various methods developed for lattices to the setting of helices and thin-films, e.g. [DJ07, HTJ12, ADE13a, ADE13b]. Our strategy in this work is to use the OS framework to adapt continuum limit calculations from the

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setting of periodic lattices to the setting of nanostructures.

Our work is focused on obtaining discrete-to-continuum limits of the energy. This multiscale approach has proven very powerful in enabling the systematic reduction of the very large number of degrees of freedom associated to the discrete problem to a much more tractable continuum problem. This overall idea has played an important role in developing models, often in conjunction with variational tools such as Γ -convergence, both for bulk crystals [BLBL02, BLBL07, Sch09] as well as for thin films [Sch06]. Further, these ideas have played a role in the development of numerical multiscale atomistic methods such as the quasicontinuum method [TOP96, MT02, TM11, KO01, LLO12, DLO10].

However, all the work in the previous paragraph is to restricted to the setting of short-range bonded atomic interactions. In the context of electrical and magnetic interactions, the calculation of continuum limit energies in the context of discrete-to-continuum has been examined both formally and rigorously using a discrete dipoles on a periodic 3-d lattice [Tou56, Bro63, JM94, MS02, SS09]. Further, this has been examined formally for periodic charge distributions, also in 3-d, [MD14]. All of these works show that the continuum limit energy consists of a local part and a nonlocal part. In contrast, in this work, we consider topologically low-dimensional structures: a 1-d helical nanotube and a 2-d thin film with constant bending curvature. In the limit that the discrete lengthscale characterizing the nanotube and thin film goes to 0, we find that the limit continuum energy is entirely local.

The absence of nonlocality in the limit can be rationalized by observing that the decay of the interactions as r^{-3} is sufficiently fast that we obtain a local limit if summed over a (topologically) 1-d or 2-d object. We highlight a complementary body of work that applies dimension reduction techniques to go from a 3-d continuum to a 2-d or 1-d continuum. In the context of electrical and magnetic interactions, [GJ97] and subsequent works [Car01, KS05, KSZ15] (for thin films) and [GH15, CH15] (for thin wires) find, as we do, that the limit energy is not nonlocal.

The techniques employed in this work are broadly based on the rigorous results provided in [JM94] on the continuum limit of magnetic dipole interactions on a 3-d lattice, with appropriate generalizations and modifications for our setting. The overall strategy of [JM94] is as follows. First, the operator that associates the discrete dipole lattice to the generated electric field is shown to be bounded for smooth test functions; next, the pointwise limit of the action of the operator on smooth test functions is obtained; and, finally, using the boundedness of the operator and the density of the test functions, the limit of the energy density is obtained. For the helical and thin film nanostructures considered in this work, we adapt this strategy to account for the fact that the lattice sites and dipoles are not related by a translation transformation, but by a more general isometric transformation.

The key results of this work are as follows. First, the limit energy is rigorously derived and found to be local. Second, the limiting energy density depends on the macroscopic geometric parameters, such as the pitch, radius and so on for the helical nanotube, and on the stretch and curvature for the thin film. These parameters can be related to macroscopic measures of deformation, and link the macroscopic deformation to the small-scale structure. Third, while the limiting energy is local, there are energetic contributions from both the normal and the tangential components of the dipole. This is in contrast to the result obtained by dimension reduction, and is due to the fact that we start with a single unit cell thickness in the normal direction and take the limit along the length (for the helix) or in the plane (for the thin film). In contrast, in dimension reduction approaches, there is no discreteness at all, and the limit is related to the ratio of the dimensions in and out of plane.

Organization. In section 2, we discuss prior work, primarily on dimension reduction from a 3-d continuum to a 2-d continuum, and highlight the local nature of the limiting energy. We then discuss heuristically the scaling of electrostatic interactions that lead to this locality generically for topologically low-dimensional nanostructures. In section 3, we present the main results for helical nanotubes and thin films with constant bending curvature. We prove various claims in section 4. In section 5, we summarize the results.

Notation. We denote the real line and set of integers by \mathbb{R} and \mathbb{Z} respectively; \mathbb{R}^d , \mathbb{Z}^d denote these in dimension d=1,2,3. For any $c,c_1,c_2\in\mathbb{R}$, $c\mathbb{Z}^d$ denotes the set $\{cz;z\in\mathbb{Z}^d\}$ and $c_1\mathbb{Z}\times c_2\mathbb{Z}$ denotes the set $\{(c_1z_1,c_2z_2);z_1,z_2\in\mathbb{Z}\}$. \mathcal{L} and \mathcal{U} denote the set of lattice sites and the lattice unit cell respectively; \mathcal{L}_λ and \mathcal{U}_λ denote these in the lattice scaled by λ , with $\mathcal{L}_1,\mathcal{U}_1$ denoting $\mathcal{L}_\lambda,\mathcal{U}_\lambda$ for $\lambda=1$. We use $\boldsymbol{x}=(x_1,x_2,x_3)\in\mathbb{R}^3$ to denote the point in space with components x_i in the orthonormal basis $\{e_1,e_2,e_3\}$ for \mathbb{R}^3 . We follow the standard notation wherein scalars are denoted by lowercase letters, vectors by bold lowercase letters, and second order tensors by bold uppercase

letters. $|m{x}| = \sqrt{\sum_{i=1}^n x_i^2}$ denotes the Euclidean norm of vector $m{x} \in \mathbb{R}^n$; $|m{A}| = \sqrt{m{A}:m{A}}$ denotes the

norm of tensor A; and $A:B=A_{ij}B_{ij}$ denotes the inner product of the two tensors. For any vector $a\in\mathbb{R}^n$ and tensor A, we have $|Aa|\leq |A||a|$. We use $|\Omega|$ to denote the Lebesgue measure of the set $\Omega\in\mathbb{R}^n$. We use $\chi_A=\chi_A(x)$ to denote the indicator function of set $A\subset\mathbb{R}^d$. We use $L^2(A,B)$ to denote the space of Lebesgue square-integrable functions $u\colon A\subset\mathbb{R}^n\to B\subset\mathbb{R}^m$; $(u,v)_{L^2(A,B)}$ for the inner product of functions $u,v\in L^2(A,B)$; and $||u||_{L^2(A,B)}$ the L^2 norm of $u\in L^2(A,B)$. When there is no ambiguity, we will suppress $L^2(A,B)$ and write (u,v) and ||u||. $C_0^\infty(\mathbb{R}^n,\mathbb{R}^m)$ denotes the space of infinitely differentiable test functions $u\colon\mathbb{R}^n\to\mathbb{R}^m$ with compact support in \mathbb{R}^n . $\mathcal{L}(V,W)$ is the space of bounded linear maps $T\colon V\to W$ where V,W are Hilbert spaces. The norm of the map $T\in\mathcal{L}(V,W)$ is denoted by $||T||_{\mathcal{L}(V,W)}$, and is given by the expression:

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$$||T||_{\mathcal{L}(V,W)} = \sup_{||f||_V \neq 0} \frac{||Tf||_W}{||f||_V}.$$

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We use $u_{\lambda} \xrightarrow{\lambda \to 0} u$ to denote the strong convergence of $u_{\lambda} \in V$ to $u \in V$ as $\lambda \to 0$, i.e., $||u_{\lambda} - u||_{V} \to 0$ as $\lambda \to 0$.

2. Prior Results on Dimension Reduction, and Dipole Interaction Scalings. We briefly revisit the results of [GJ97] and [CH15]. Respectively, they performed dimension reduction from the 3-d continuum to the 2-d thin film and 1-d thin wire limits for the magnetostatic energy.

Consider a material domain $\Omega_h = S \times [0, h]$, where $S \subset \mathbb{R}^2$ is a 2-d domain in the plane spanned by (e_1, e_2) , and h > 0 is the material thickness in the normal direction e_3 . Suppose $d: \Omega_h \to \mathbb{R}^3$, with d = 0 on $\mathbb{R}^3 \setminus \Omega_h$, is the dipole field in the material. The electrostatic energy density is given by

$$e_h(\boldsymbol{d}) = \frac{1}{|\Omega_h|} \int_{\Omega_h} \frac{1}{2} \nabla \phi(\boldsymbol{x}) \cdot \boldsymbol{d} \, d\boldsymbol{x},$$

where $|\Omega_h|$ is the volume of Ω_h , and ϕ is the electric potential that satisfies the electrostatic equation:

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$$(-\nabla \phi + \mathbf{d}) = 0$$
 on \mathbb{R}^3 , $|\nabla \phi(\mathbf{x})| \to \mathbf{0}$ as $|\mathbf{x}| \to \infty$

with $|\boldsymbol{d}|=d$. Let $\Omega_1=S\times[0,1]$, and $\boldsymbol{y}(\boldsymbol{x})=(x_1,x_2,x_3/h)\in\Omega_1$ for $\boldsymbol{x}\in\Omega_h$ is the map from Ω_h to Ω_1 . For fixed h>0, consider the dipole field $\boldsymbol{d}_h\colon\Omega_h\to\mathbb{R}^3$ and $\tilde{\boldsymbol{d}}_h\colon\Omega_1\to\mathbb{R}^3$ such that

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$$\tilde{\boldsymbol{d}}_h(\boldsymbol{y}(\boldsymbol{x})) = \boldsymbol{d}_h(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \Omega_h.$$

Let d_h be the sequence of dipole field for h > 0, and \tilde{d}_h is defined as above. Assume that dipole field \tilde{d}_h is such that, first, $\tilde{d}_h = 0$ on $\mathbb{R}^3 \setminus \Omega_1$, and second, it converges to \tilde{d}_0 in $L^2(\mathbb{R}^3)$; then the limit of the energy density $e_h = e_h(d_h)$ is [GJ97]:

$$e_h(\boldsymbol{d}_h) \to e_0(\tilde{\boldsymbol{d}}_0) = \frac{1}{2|\Omega_1|} \int_{\Omega_1} |\tilde{d}_{0_3}|^2 d\boldsymbol{x}$$

That is, the limiting energy e_0 is local, and only the normal component of the dipole moment appears 126 127 in the expression.

Next, consider a thin straight wire with axis along e_1 , denoted by $\Omega_h = (-1,1) \times B_2(\mathbf{0},h)$, where $B_2(\mathbf{0}, h)$ is a ball of size h centered at $\mathbf{0}$ in the plane spanned by (e_2, e_3) . The limiting energy density is [CH15]:

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$$\frac{1}{2|\Omega_1|} \int_{\Omega_1} \left(|\tilde{d}_{0_2}|^2 + |\tilde{d}_{0_3}|^2 \right) d\boldsymbol{x},$$

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where $\Omega_1 = (-1, 1) \times B_2(\mathbf{0}, 1)$ is the rescaled domain of Ω_h , and $\tilde{\mathbf{d}}_0$ is the limiting field. We notice 132 that the limiting energy is again local, and only the components of the dipole moment perpendicular 133 to the wire appear. 134

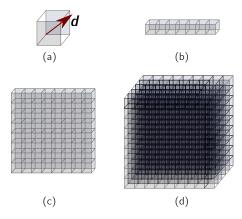


Fig. 2.1: A schematic of the unit cell with a dipole (a), and generic 1-d, 2-d, 3-d periodic lattices (b, c, d).

The absence of nonlocality in the limiting energy in the results above, as well as in our results 136 in section 3 below, can be physically understood through the fact that these structures are 1-d or 2-d topologically. To see this, we consider a system of discrete dipoles associated to the uniform 1-d, 2-d, and 3-d periodic lattices with the unit cell of size 1 (Figure 2.1). The energy of a lattice of dipoles is given by [Bro63, JM94]:

(2.1)
$$E = -\frac{1}{2} \sum_{i} \sum_{j,j \neq i} \mathbf{d}_i \cdot \mathbf{K}(\mathbf{x}_j - \mathbf{x}_i) \mathbf{d}_j = \sum_{i} |U_i| \left[-\frac{1}{|U_i|} \frac{1}{2} \sum_{j,j \neq i} \mathbf{d}_i \cdot \mathbf{K}(\mathbf{x}_j - \mathbf{x}_i) \mathbf{d}_j \right],$$

where the sum is over the cells in the lattice and the term inside square bracket denotes the energy 141 density of a cell i. d_i denotes the dipole in cell i, x_i denotes the coordinate of lattice site i, and K is the dipole field kernel defined as: 143

144 (2.2)
$$K(x) = -\frac{1}{4\pi |x|^3} \left(I - 3 \frac{x}{|x|} \otimes \frac{x}{|x|} \right), \quad x \neq 0.$$

We use these expressions to heuristically understand the scaling of the energy for systems with 145 different topological dimensions. For simplicity, we assume below that the volume of the unit cell 146 and the magnitude of the dipole are both 1, i.e., $|U_i| = 1$ and $|d_i| = 1$ for each i, and some constant 147 factors are neglected. 148

REMARK 2.1 (1-d lattice). We can estimate an upper bound on the energy density e of a typical unit cell as follows:

$$e \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times |\boldsymbol{d}| \times (\textit{number of dipoles at } r) \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times 1 \times 1 = \sum_{r=1}^{\infty} \frac{1}{r^3}.$$

We use that the total dipole moment at a distance r from a given unit cell is, at most, that of another dipole in the unit cell at a distance r. This sum is well-behaved and bounded.

Remark 2.2 (2-d lattice). As in the 1-d setting, we first bound the net dipole at a distance r from a given unit cell. Since the structure is a 2-d lattice, the number of unit cells at a distance r is of order $2\pi r$. Therefore, an upper bound on the energy density is:

$$e \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times |\boldsymbol{d}| \times (\textit{number of dipoles at } r) \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times 1 \times 2\pi r = 2\pi \sum_{r=1}^{\infty} \frac{1}{r^2}.$$

158 This sum is also well-behaved and bounded.

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Remark 2.3 (3-d lattice). Following the argument of the 2-d lattice, we now have that the net dipole at a distance r from a given unit cell is, at most, of the order $4\pi r^2$. Therefore, an upper bound on the energy density is:

$$e \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times |\boldsymbol{d}| \times (\textit{number of dipoles at } r) \leq \sum_{r=1}^{\infty} \frac{1}{r^3} \times 1 \times 4\pi r^2 = 4\pi \sum_{r=1}^{\infty} \frac{1}{r}.$$

This sum is divergent. However, through a more careful analysis that accounts for the signs – not just the magnitudes – of the dipole interactions, the energy density can be shown to be conditionally convergent [Tou56, JM94].

When the lattice sum is bounded and converges unconditionally, it is possible to truncate after a finite distance and obtain sufficient numerical accuracy. When the lattice sum is conditionally convergent, that can be physically related to nonlocality; specifically, the slow convergence does not allow for truncation, and the far-field values play an important role. [MD14] discusses this from a physical perspective.

- 3. Results on Continuum Limits of the Electrostatic Energy. We consider two classes of nanostructures: helical nanotubes and thin films, the latter allowing for a constant bending curvature (i.e., nonzero constant mean curvature and zero Gauss curvature), and obtain the corresponding continuum limit electrostatic energy. In both cases, we start with discrete dipoles, where the discreteness is parametrized by the scale $\lambda>0$, and examine the limit $\lambda\to0$. We show that the dipole-dipole interaction energy density per unit cross-sectional area in the case of nanotubes, and per unit thickness in the case of films converges to a local energy density in the limit.
- 3.1. Helical Nanotube. We consider a discrete helix with axis e_3 characterized by the angle θ and length δ . Suppose $x_0 \in \mathbb{R}^3$ is a point on the helix. Then, the other points on the helix are related by an isometric transformation of x_0 . Let $s \in \mathbb{R}$ be the parametric coordinate of a point on the helix. Then, the map $\bar{x} : \mathbb{R} \to \mathbb{R}^3$ that takes a point in the parametric space to a unique point on the helix can be expressed as

183 (3.1)
$$\bar{\boldsymbol{x}}(s) = \boldsymbol{Q}(s\theta)\boldsymbol{x}_0 + s\delta\boldsymbol{e}_3.$$

Here $Q(\theta)$ is the rotational tensor represented by the matrix in the orthonormal basis $\{e_1, e_2, e_3\}$ as:

185 (3.2)
$$Q(\theta) := \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

- We notice that these definitions imply that the pitch of the helix is $2\pi\delta/\theta$. 187
- Without loss of generality, we assume $x_0 = e_1$. The tangent vector to the helix at s is given by 188

189 (3.3)
$$t(s) = \frac{\mathrm{d}\bar{x}(s)}{\mathrm{d}s} = \theta Q'(s\theta)e_1 + \delta e_3.$$

- Let $\hat{t}(s) = t(s)/\sqrt{\theta^2 + \delta^2}$ denote the unit tangent vector. We define the second order projection 190
- tensors $P_{||} = P_{||}(s)$ and $P_{\perp} = P_{\perp}(s)$, for $s \in \mathbb{R}$, as follows

192 (3.4)
$$P_{||}(s) = \hat{t}(s) \otimes \hat{t}(s), \qquad P_{\perp}(s) = I - P_{||}(s).$$

For any vector \boldsymbol{a} and any $s \in \mathbb{R}$, we have 193

194 (3.5)
$$\mathbf{a} = \mathbf{P}_{\parallel}(s)\mathbf{a} + \mathbf{P}_{\perp}(s)\mathbf{a}, \quad \text{with} \quad \mathbf{P}_{\parallel}(s)\mathbf{a} \cdot \mathbf{P}_{\perp}(s)\mathbf{a} = 0.$$

3.1.1. Lattice Geometry and Dipole Moment. Let $\mathcal{L} = \mathbb{Z}$ denote the set of parametric coordi-195 nates of the points on helix. We consider a discrete system of dipole moments $d: \mathcal{L} \to \mathbb{R}^3$ associated 196 to the points on the helix given by \mathcal{L} , see Figure 3.1. The magnitudes of the dipoles at the lattice sites 197 are equal, but they are oriented differently; in particular, the orientations of dipoles at lattice sites 198 follow the relation: 199

200 (3.6)
$$d(s+1) = \mathbf{Q}(\theta)d(s), \quad s \in \mathcal{L}$$

We associate a unit cell to each lattice site. Let U(s) = [s, s+1) denote the unit cell in the parametric space at the site s, for $s \in \mathcal{L}$. Let $S(r), r \in \mathbb{R}$, be given by

$$S(r) = \{ \boldsymbol{x}; (\boldsymbol{x} - \bar{\boldsymbol{x}}(r)) \cdot \boldsymbol{t}(r) = 0, |\boldsymbol{x} - \bar{\boldsymbol{x}}(r)|^2 < R^2 \}.$$

- Note that $|S(r)| = |S(0)| = \pi R^2$. The unit cell in real space is defined by $\bar{U}(s) = \{x \in S(r); r \in U(s)\}$. 201
- We take, without loss of generality, $R^2 = 1/(\pi\sqrt{\theta^2 + \delta^2})$ so that $|\bar{U}(s)| = \text{area}(S) \times \text{length}(\{\bar{x}(r); r \in \mathbb{R}\})$
- U(s)) = $\pi R^2 \sqrt{\theta^2 + \delta^2} = 1$. 2.03

We now consider the setting in which the cells are of size $\lambda > 0$ so that as $\lambda \to 0$ the density 204 of cells in the helix increases. For $\lambda > 0$, suppose $\mathcal{L}_{\lambda} = \lambda \mathbb{Z}$ denotes the parametric coordinates 2.05

- of the sites in a scaled lattice, and $d_{\lambda} \colon \mathcal{L}_{\lambda} \to \mathbb{R}^{3}$ denotes the corresponding system of dipole moments. Associated to $s \in \mathcal{L}_{\lambda}$, let $U_{\lambda}(s) = [s, s + \lambda)$ denote the cell in the parametric space. 206 207
- The 3-d cell is given by $\bar{U}_{\lambda}(s) = \{ \boldsymbol{x} \in S_{\lambda}(r); r \in U_{\lambda}(s) \}$, where $S_{\lambda}(r) = \{ \boldsymbol{x}; (\boldsymbol{x} \bar{\boldsymbol{x}}(r)) \cdot \boldsymbol{t}(r) = 0, |\boldsymbol{x} \bar{\boldsymbol{x}}(r)|^2 < \lambda^2 R^2 \}$ is the scaled cross-section. Note that $\operatorname{area}(S_{\lambda}(r)) = \pi \lambda^2 R^2$ and
- $|\bar{U}_{\lambda}(s)| = \pi \lambda^2 R^2 \times \lambda \sqrt{\theta^2 + \delta^2} = \lambda^3$. Let $\tilde{d}_{\lambda} : \mathbb{R} \to \mathbb{R}^3$ be the piecewise constant extension of d_{λ}
- given by

212 (3.7)
$$\tilde{\boldsymbol{d}}_{\lambda}(s) = \frac{\boldsymbol{d}_{\lambda}(i)}{|\bar{U}_{\lambda}(s)|} = \frac{\boldsymbol{d}_{\lambda}(i)}{\lambda^{3}}, \quad \forall s \in U_{\lambda}(i), \quad \forall i \in \mathcal{L}_{\lambda}.$$

- To compute the limit of the dipole-dipole interaction energy as $\lambda \to 0$, we assume that dipole moment 213
- density field \tilde{d}_{λ} converges to some field $f \in L^2(\mathbb{R}, \mathbb{R}^3)$ in the L^2 norm. As in [JM94], instead of

working with d_{λ} , as defined above, we could assume that the dipole moment $d_{\lambda}(i)$, for $i \in \mathcal{L}_{\lambda}$, is due to the background dipole moment density field $f_{\lambda} \in L^2(\mathbb{R}, \mathbb{R}^3)$ such that 216

217 (3.8)
$$\boldsymbol{d}_{\lambda}(i) = \sqrt{\theta^2 + \delta^2} \int_{U_{\lambda}(i)} \int_{S_{\lambda}(r)} \boldsymbol{f}_{\lambda}(r) \, \mathrm{d}S_{\lambda}(r) \, \mathrm{d}r = \lambda^2 \int_{U_{\lambda}(i)} \boldsymbol{f}_{\lambda}(r) \, \mathrm{d}r,$$

- where $dS_{\lambda}(r)$ is the area measure for surface S_{λ} . We assumed that the background field is uniform 218 in $S_{\lambda}(r)$ for all $r \in \mathbb{R}$ and used $R^2 = 1/(\pi\sqrt{\theta^2 + \delta^2})$. The existence of one such background field 219 f_{λ} is evident: we can define $f_{\lambda} = \tilde{d}_{\lambda}$. The physical dimension of f_{λ} is dipole moment per unit 220 volume. We have the following lemma that relates the convergence of the background dipole moment 221 field and the piecewise constant extension. 222
- Lemma 3.1. Let f_{λ} , $\lambda > 0$, be the sequence of $L^2(\mathbb{R}, \mathbb{R}^3)$ functions and let $f \in L^2(\mathbb{R}, \mathbb{R}^3)$ such that $f_{\lambda} \to f$ in $L^2(\mathbb{R}, \mathbb{R}^3)$. Let $d_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ be given by (3.8) and let \tilde{d}_{λ} be a piecewise constant L^2 extension of d_{λ} given by (3.7). Then, $\tilde{d}_{\lambda} \to f$ in $L^2(\mathbb{R}, \mathbb{R}^3)$.

 On the other hand, if $d_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ is such that $\tilde{d}_{\lambda} \to f$ in $L^2(\mathbb{R}, \mathbb{R}^3)$, then there exists a background field $f_{\lambda} \in L^2(\mathbb{R}, \mathbb{R}^3)$ such that d_{λ} is given by (3.8). 223 224 225
- 226
- The proof is similar to the proof of Theorem 4.1 from [JM94]. 228
- Remark 3.1. Since the discrete dipole field d_{λ} has helical symmetry, from (3.8) we can see that 229 f will also have helical symmetry.

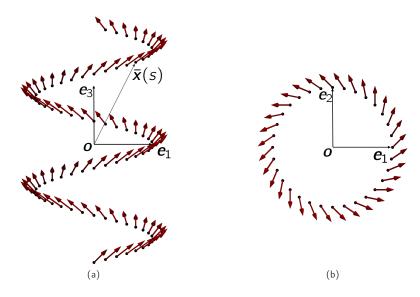


Fig. 3.1: Discrete dipole moments (red arrows) lying on the helix. (a) and (b) show the view in (e_1, e_3) and (e_1, e_2) planes respectively. The dipole moments corresponding to different sites are related by (3.6). For the parametric coordinate s, $\bar{x}(s)$ gives the coordinate of the point on the helix.

3.1.2. Electrostatic Energy. For $\lambda > 0$, the energy associated to the system of dipole moments 231 232 d_{λ} can be expressed as [Bro63, JM94]:

$$E_{\lambda} = -\frac{1}{2} \sum_{\substack{s,s' \in \mathcal{L}_{\lambda}, \\ s \neq s'}} \boldsymbol{d}_{\lambda}(s) \cdot \boldsymbol{K}(\bar{\boldsymbol{x}}(s') - \bar{\boldsymbol{x}}(s)) \boldsymbol{d}_{\lambda}(s') = |S_{\lambda}| e_{\lambda},$$

where e_{λ} is the energy per unit area given by

235 (3.9)
$$e_{\lambda} = -\frac{1}{2|S_{\lambda}|} \sum_{\substack{s,s' \in \mathcal{L}_{\lambda}, \\ s \neq s'}} \boldsymbol{d}_{\lambda}(s) \cdot \boldsymbol{K}(\bar{\boldsymbol{x}}(s') - \bar{\boldsymbol{x}}(s)) \boldsymbol{d}_{\lambda}(s').$$

Substituting (3.8) above and proceeding similar to Section 6 of [JM94], e_{λ} can be written as

$$(3.10) e_{\lambda} = (f_{\lambda}, T_{\lambda} f_{\lambda})_{L^{2}(\mathbb{R} \mathbb{R}^{3})},$$

where $T_{\lambda} \colon L^2(\mathbb{R}, \mathbb{R}^3) \to L^2(\mathbb{R}, \mathbb{R}^3)$ is the map given by

(3.11)
$$(T_{\lambda} \boldsymbol{f})(s) = \lambda^2 \int_{\mathbb{R}} \boldsymbol{K}_{\lambda}(s', s) \boldsymbol{f}(s') \, \mathrm{d}s'$$

and $K_{\lambda}(s',s)$, for $s,s'\in\mathbb{R}$, is the discrete dipole field kernel given by

$$\mathbf{K}_{\lambda}(s',s) = \sum_{\substack{u,v \in \mathcal{L}_{\lambda}, \\ u \neq v}} \chi_{U_{\lambda}(v)}(s') \mathbf{K}(\bar{\mathbf{x}}(v) - \bar{\mathbf{x}}(u)) \chi_{U_{\lambda}(u)}(s).$$

Scaling Property of K_{λ} . For any $a, b \in \mathbb{R}$, we have

$$\bar{\boldsymbol{x}}(\lambda a) - \bar{\boldsymbol{x}}(\lambda b) = \boldsymbol{Q}(\lambda a \theta) \boldsymbol{e}_1 + \delta \lambda a \boldsymbol{e}_3 - \boldsymbol{Q}(\lambda b \theta) \boldsymbol{e}_1 - \delta \lambda b \boldsymbol{e}_3$$

$$= \lambda \left(\bar{\boldsymbol{x}}(a) - \bar{\boldsymbol{x}}(b) + \underbrace{\left[\frac{\boldsymbol{Q}(\lambda a\theta) - \boldsymbol{Q}(\lambda b\theta) - (\lambda \boldsymbol{Q}(a\theta) - \lambda \boldsymbol{Q}(b\theta))}{\lambda} \right]}_{=:\boldsymbol{A}_{\lambda}(a,b)} \boldsymbol{e}_{1} \right).$$

Using the relation above, it is easy to show

$$\boldsymbol{K}_{\lambda}(s',s) = \frac{1}{\lambda^{3}} \sum_{\substack{u,v \in \mathcal{L}_{1}, \\ u \neq v}} \chi_{U_{1}(v)}(s'/\lambda) \boldsymbol{K}(\bar{\boldsymbol{x}}(v) - \bar{\boldsymbol{x}}(u) + \boldsymbol{A}_{\lambda}(v,u)\boldsymbol{e}_{1}) \chi_{U_{1}(u)}(s/\lambda),$$

- where we recall that $U_1(u) = [u, u+1), u \in \mathcal{L}_1$, is the lattice cell in the parametric space for $\lambda = 1$.
- 247 We define a discrete kernel $K_{1,\lambda}(s,s')$, for $s,s'\in\mathbb{R}$, as follows

248 (3.14)
$$\boldsymbol{K}_{1,\lambda}(s',s) = \sum_{\substack{u,v \in \mathcal{L}_1, \\ v \neq u}} \chi_{U_1(v)}(s') \boldsymbol{K}(\bar{\boldsymbol{x}}(v) - \bar{\boldsymbol{x}}(u) + \boldsymbol{A}_{\lambda}(v,u)\boldsymbol{e}_1) \chi_{U_1(u)}(s).$$

We then have

$$\boldsymbol{K}_{\lambda}(s',s) = \frac{1}{\lambda^3} \boldsymbol{K}_{1,\lambda}(s'/\lambda, s/\lambda).$$

- 3.1.3. Limit of Electrostatics Energy. In this section, we obtain the limit of the energy per
- unit surface area e_{λ} as $\lambda \to 0$ assuming that the background dipole field density (or equivalently the
- dipole moment density \tilde{d}_{λ}) f_{λ} converges to some density field f in L^2 . The idea is to first show that
- 254 the map T_{λ} in (3.11) is bounded and obtain its limit. With that, the limit of e_{λ} follows.

255 Limit of Discrete Electric Field. Let $T_{1,\lambda}$ be the map with kernel $K_{1,\lambda}$. For any function $f \in L^2(\mathbb{R}, \mathbb{R}^3)$, we have

$$(T_{1,\lambda}\mathbf{f})(s) = \int_{\mathbb{R}} \mathbf{K}_{1,\lambda}(s',s)\mathbf{f}(s') \, \mathrm{d}s'.$$

- We have the following main result on the map T_{λ} . 258
- Proposition 3.2. The map $T_{1,\lambda}$ and T_{λ} are bounded in $L^2(\mathbb{R},\mathbb{R}^3)$ for all $\lambda > 0$ and satisfy 259

260 (3.16)
$$||T_{\lambda}||_{\mathcal{L}(L^2, L^2)} = ||T_{1, \lambda}||_{\mathcal{L}(L^2, L^2)}.$$

Further, for $\mathbf{f} \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$, 261

$$(T_{\lambda}\boldsymbol{f})(s) \xrightarrow[\lambda \to 0]{} -h_0(\boldsymbol{I} - 3\boldsymbol{P}_{||}(s))\boldsymbol{f}(s) = -h_0(\boldsymbol{P}_{\perp}(s) - 2\boldsymbol{P}_{||}(s))\boldsymbol{f}(s)$$

pointwise, where $P_{\perp}(s)$ and $P_{\parallel}(s)$ are projection tensors that project onto the normal plane and 263 the tangent line to the helix respectively (see (3.4)). h_0 is a constant given by

265 (3.17)
$$h_0 = \sum_{v \in \mathbb{Z}_n} \frac{1}{4\pi |v|^3 (\theta^2 + \delta^2)^{3/2}}.$$

- We provide the proof of Proposition 3.2 in subsection 4.1. 266
- Limit of Energy. 267
- THEOREM 3.3. Let $\mathbf{f}_{\lambda} \in L^2(\mathbb{R}, \mathbb{R}^3)$ be a sequence of functions for $\lambda > 0$ with $\mathbf{f} \in L^2(\mathbb{R}, \mathbb{R}^3)$ such that $\mathbf{f}_{\lambda} \xrightarrow[\lambda \to 0]{} \mathbf{f}$ in L^2 . Let the system of dipole moments $\mathbf{d}_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ be given by (3.8). Then 268
- 269

$$e_{\lambda} \xrightarrow[\lambda \to 0]{} \frac{1}{2} h_0 \left[|| \boldsymbol{P}_{\perp} \boldsymbol{f} ||_{L^2(\mathbb{R}, \mathbb{R}^3)}^2 - 2 || \boldsymbol{P}_{||} \boldsymbol{f} ||_{L^2(\mathbb{R}, \mathbb{R}^3)}^2 \right],$$

- where h_0 is a constant defined in (3.17). 272
- *Proof.* Since T_{λ} is bounded and $f_{\lambda} \to f$, we have 273

$$\lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}_{\lambda}) = \lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}) + \lim_{\lambda \to 0} (T_{\lambda} (\boldsymbol{f}_{\lambda} - \boldsymbol{f})) = \lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}).$$

- We only need to analyze $T_{\lambda}f$ in the limit for $f \in L^2(\mathbb{R}, \mathbb{R}^3)$. Let $f^k \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$ be a sequence 275
- of functions such that $f^k \to f$. Using Proposition 3.2, we have

$$\lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}) = \lim_{k \to \infty} \lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}^{k}) + \lim_{k \to \infty} \lim_{\lambda \to 0} (T_{\lambda} (\boldsymbol{f} - \boldsymbol{f}^{k})) = \lim_{k \to \infty} \lim_{\lambda \to 0} (T_{\lambda} \boldsymbol{f}^{k})$$

$$= \lim_{k \to \infty} \left(\boldsymbol{H}_0 \boldsymbol{f}^k \right) = \boldsymbol{H}_0 \boldsymbol{f}.$$

Using the expression in (3.10) for e_{λ} , we have 280

281
$$e_{\lambda} = -\frac{1}{2} (\mathbf{f}_{\lambda}, T_{\lambda} \mathbf{f}_{\lambda})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} = -\frac{1}{2} \left[(\mathbf{f}_{\lambda} - \mathbf{f}, T_{\lambda} \mathbf{f}_{\lambda})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} + (\mathbf{f}, T_{\lambda} \mathbf{f}_{\lambda})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} \right]$$

$$= -\frac{1}{2} \left[(\mathbf{f}_{\lambda} - \mathbf{f}, T_{\lambda} \mathbf{f}_{\lambda})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} + (\mathbf{f}, T_{\lambda} \mathbf{f})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} + (\mathbf{f}, T_{\lambda} (\mathbf{f}_{\lambda} - \mathbf{f}))_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} \right].$$

- The first and third terms are zero in the limit. Taking the limit of the remaining term and using (3.18), 284

$$\lim_{\lambda \to 0} e_{\lambda} = \lim_{\lambda \to 0} -\frac{1}{2} (\mathbf{f}_{\lambda}, T_{\lambda} \mathbf{f}_{\lambda})_{L^{2}(\mathbb{R}, \mathbb{R}^{3})} = \frac{1}{2} h_{0} \left[||\mathbf{P}_{\perp} \mathbf{f}||_{L^{2}(\mathbb{R}, \mathbb{R}^{3})}^{2} - 2||\mathbf{P}_{||} \mathbf{f}||_{L^{2}(\mathbb{R}, \mathbb{R}^{3})}^{2} \right].$$

This completes the proof. 287

- Remark 3.2. The limiting energy only comprises of a local self-field energy. In the limit, any point on the helix sees the uniform 1-d system of dipole moments along the tangent line. Further, we see that both the normal components and the tangential component of the dipole moment contribute to the energy and electric field. This is in contrast to [CH15] where the thin wire limit of the magnetostatic energy has contribution only from the normal components.
- **3.2. Nanofilm with Constant Bending Curvature.** Let $\mathcal{S} = (-\bar{\theta}, \bar{\theta}) \times \mathbb{R}$ be the parametric 293 space for a surface with a constant bending curvature κ . The map that takes a point in the parametric 294 space to a unique point on the film is given by 295

296 (3.19)
$$\bar{x}(s_1, s_2) = \mathcal{R}Q(s_1)e_1 + s_2\delta e_3,$$

- where $\mathcal{R}=1/\kappa$ is the inverse of curvature, $\bar{\theta}>0$ is the angular size of the film, and δ is the spacing 297 in the flat direction. $\kappa, \delta, \bar{\theta}$ are fixed parameters for a given film. Here, $Q(\theta)$ is the rotational tensor 298 with the axis e_3 , see definition (3.2). The tangent vectors at $s := \{s_1, s_2\} \in S$ are 299

300 (3.20)
$$t_1(s) = \frac{\mathrm{d}\bar{x}}{\mathrm{d}s_1} = \mathcal{R} \mathbf{Q}'(s_1)\mathbf{e}_1, \qquad t_2(s) = \frac{\mathrm{d}\bar{x}}{\mathrm{d}s_2} = \delta \mathbf{e}_3$$

301 and the normal vector is

2.88 289

290

291

292

302 (3.21)
$$n(s) = Q(s_1)e_1.$$

3.2.1. Lattice Geometry and Dipole Moment. We consider a lattice embedded on the film \bar{x} . 303 304 We assume that the lattice is one lattice cell thick in the direction n normal to the film. Suppose $\mathcal{L} \subset \mathcal{S}$ is the set of parametric coordinates of the discrete lattice sites. Let \mathcal{L} and the lattice cell U305 (in the parametric space S) be given by 306

307
$$\mathcal{L} = \{ \boldsymbol{s} = (s_1, s_2) \in \mathcal{S}; \ s_1 = i\theta_l, s_2 = j, \ i, j \in \mathbb{Z} \} = (-\bar{\theta}, \bar{\theta}) \cap \theta_l \mathbb{Z} \times \mathbb{Z}$$
308 (3.22)
$$U(\boldsymbol{s}) = [s_1, s_1 + \theta_l) \times [s_2, s_2 + 1), \quad \forall \boldsymbol{s} \in \mathcal{L}.$$

- Here, θ_l is the angular width of the lattice cell. We assume that θ_l is such that the set of sites 310 in the angular direction, $(-\theta, \theta) \cap \theta_l \mathbb{Z}$, is not empty, and in fact is sufficiently large so that the 311 continuum limit approximation of the energy density is justified. We assume that the lattice has unit 312 thickness in the normal direction, and suppose that the film given by \bar{x} passes through the center of 313 the lattice in the normal direction. Then, the unit cell for a given site $s \in \mathcal{L}$ is $U(s) = \{x; x =$ 314 $\bar{x}(s) + tn(s), s \in U(s), t \in (-1/2, 1/2)$. On the lattice \mathcal{L} , we define a discrete system of dipole 315 moments $d: \mathcal{L} \to \mathbb{R}^3$. Similar to the case of the helical nanotube, the lattice cells in real space are 316 related by an isometric transformation, so the magnitudes of the dipoles at the lattice sites are equal, 317
- but they are oriented differently. In particular, we have 318

319 (3.23)
$$d(s+r) = Q(r_1)d(s), \quad s \in \mathcal{L},$$

- where $r = (r_1, r_2) \in \mathcal{L}$ such that $r + s \in \mathcal{L}$ (i.e. all the translations within \mathcal{L}). We see that the dipole orientation depends only on the angular (first) parameter and is invariant with respect to the 321 second parameter. 322
- We next consider the setting when the lattice is scaled by $\lambda > 0$. The scaled lattice \mathcal{L}_{λ} and the 323 associated lattice cell U_{λ} are defined by the natural scaling of \mathcal{L} and U as follows 324

325
$$\mathcal{L}_{\lambda} = \{ \mathbf{s} \in \mathcal{S}; \ s_1 = i\theta_l \lambda, s_2 = j\lambda, \ i, j \in \mathbb{Z} \} = (-\bar{\theta}, \bar{\theta}) \cap \lambda \theta_l \mathbb{Z} \times \lambda \mathbb{Z}$$
326 (3.24)
$$U_{\lambda}(\mathbf{s}) = [s_1, s_2 + \lambda \theta_1) \times [s_2, s_2 + \lambda \lambda] \quad \forall \mathbf{s} \in \mathcal{C}_{\lambda}$$

- $U_{\lambda}(s) = [s_1, s_1 + \lambda \theta_l) \times [s_2, s_2 + \lambda), \quad \forall s \in \mathcal{L}_{\lambda}.$ (3.24)339
- After scaling, the thickness of the lattice cell in the normal direction is λ and the unit cell for $s \in \mathcal{L}_{\lambda}$ 328
 - is $\{x \in \mathbb{R}^3; x = \bar{x}(s) + tn(s), s \in U_{\lambda}(s), t \in (-\lambda/2, \lambda/2)\}$. We can show that the unit cell in

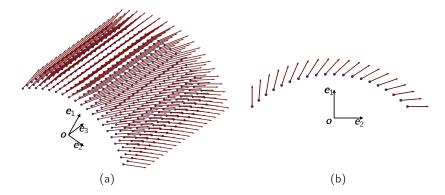


Fig. 3.2: Discrete dipole moments on a nanofilm with uniform bending curvature. (a) and (b) show the view from different perspectives.

the scaled lattice has volume $\lambda^3 \mathcal{R} \theta_l$. Suppose $\tilde{d}_{\lambda} : \mathcal{S} \to \mathbb{R}$ denotes the piecewise constant extension 330 of d_{λ} and is given by 331

332 (3.25)
$$\tilde{\boldsymbol{d}}_{\lambda}(\boldsymbol{s}) = \frac{\boldsymbol{d}_{\lambda}(\boldsymbol{a})}{\lambda^{3}\mathcal{R}\theta_{l}}, \quad \forall \boldsymbol{s} \in U_{\lambda}(\boldsymbol{a}), \, \forall \boldsymbol{a} \in \mathcal{L}_{\lambda}.$$

- We are interested in the limit of the energy when \tilde{d}_{λ} converges to f in $L^2(\mathcal{S}, \mathbb{R}^3)$. As in the case of 333
- the helix and following [JM94], we suppose that there exists a background dipole moment density 334
- field $f_{\lambda} \in L^2(\mathcal{S}, \mathbb{R}^3)$ such that the dipole moment at site $s \in \mathcal{L}_{\lambda}$ is given by 335

336 (3.26)
$$d_{\lambda}(s) = \int_{-\lambda/2}^{\lambda/2} \left[\int_{U_{\lambda}(s)} f_{\lambda}(t) \mathcal{R} dt_1 dt_2 \right] dt_3 = \mathcal{R} \lambda \int_{U_{\lambda}(s)} f_{\lambda}(t) dt,$$

- where $dt = dt_1 dt_2$ is the area measure (note that dt does not include \mathcal{R}). The existence of one 337
- such background field f_{λ} is evident: We can define $f_{\lambda} = \tilde{d}_{\lambda}$. Similar to the case of the helix, we 338
- have the following lemma that relates the convergence of the background dipole moment field and 339
- the piecewise constant extension. 340
- Lemma 3.4. Let f_{λ} , $\lambda > 0$, be a sequence of $L^2(\mathcal{S}, \mathbb{R}^3)$ functions and let $f \in L^2(\mathcal{S}, \mathbb{R}^3)$ be such that $f_{\lambda} \to f$ in $L^2(\mathcal{S}, \mathbb{R}^3)$. Let $d_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ be given by (3.26) and let \tilde{d}_{λ} be a piecewise constant L^2 extension of d_{λ} given by (3.25). Then, $\tilde{d}_{\lambda} \to f$ in $L^2(\mathcal{S}, \mathbb{R}^3)$.

 On the other hand, if $d_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ is such that $\tilde{d}_{\lambda} \to f$ in $L^2(\mathcal{S}, \mathbb{R}^3)$ then there exists a hardward field $f \in L^2(\mathcal{S}, \mathbb{R}^3)$. 341
- 342
- 343
- 344
- background field $\mathbf{f}_{\lambda} \in L^2(\mathcal{S}, \mathbb{R}^3)$ such that \mathbf{d}_{λ} is given by (3.26). 345
- The proof follows directly from the proof of Theorem 4.1 of [JM94]. 346
- REMARK 3.3. As different unit cells are related by isometric transformations, the dipole moments 347 in different unit cells are related by the rotational part of the isometric transformation. 348
- 3.2.2. Electrostatic Energy. As before, the energy associated to the system of dipole moments 349 d_{λ} , for $\lambda > 0$, is given by 350

351
$$E_{\lambda} = -\frac{1}{2} \sum_{\substack{\boldsymbol{s}, \boldsymbol{s}' \in \mathcal{L}_{\lambda}, \\ \boldsymbol{s} \neq \boldsymbol{s}'}} \boldsymbol{d}_{\lambda}(\boldsymbol{s}) \cdot \boldsymbol{K}(\bar{\boldsymbol{x}}(\boldsymbol{s}') - \bar{\boldsymbol{x}}(\boldsymbol{s})) \boldsymbol{d}_{\lambda}(\boldsymbol{s}') = |(-\lambda/2, \lambda/2)| \hat{e}_{\lambda},$$

- where $|(-\lambda/2, \lambda/2)| = \lambda$ is the thickness of the lattice in normal direction, and \hat{e}_{λ} is the energy per
- 353 unit length given by

354 (3.27)
$$\hat{e}_{\lambda} = -\frac{1}{2\lambda} \sum_{\substack{s,s' \in \mathcal{L}_{\lambda}, \\ s \neq s'}} d_{\lambda}(s) \cdot K(\bar{x}(s') - \bar{x}(s)) d_{\lambda}(s').$$

- For convenience, we normalize \hat{e}_{λ} by $\mathcal{R}\theta_l$, where $\mathcal{R}\theta_l$ is independent of λ and gives the size of
- original lattice in the angular direction. We let

357 (3.28)
$$e_{\lambda} = \frac{\hat{e}_{\lambda}}{\mathcal{R}\theta_{l}} \Rightarrow E_{\lambda} = \lambda(\mathcal{R}\theta_{l})e_{\lambda}.$$

Substituting (3.26) and proceeding similar to the case of the helix, we can express e_{λ} as

359 (3.29)
$$e_{\lambda} = (f_{\lambda}, T_{\lambda} f_{\lambda})_{L^{2}(S \mathbb{R}^{3})},$$

where $T_{\lambda} \colon L^2(\mathcal{S}, \mathbb{R}^3) \to L^2(\mathcal{S}, \mathbb{R}^3)$ is the map defined as

(3.30)
$$(T_{\lambda} \mathbf{f})(\mathbf{s}) = \frac{\mathcal{R}}{\theta_l} \lambda \int_{\mathcal{S}} \mathbf{K}_{\lambda}(\mathbf{s}', \mathbf{s}) \mathbf{f}(\mathbf{s}') \, d\mathbf{s}'$$

and $K_{\lambda}(s',s)$, for $s,s' \in \mathcal{S}$, is the discrete dipole field kernel given by

363 (3.31)
$$K_{\lambda}(s',s) = \sum_{\substack{\boldsymbol{u},\boldsymbol{v}\in\mathcal{L}_{\lambda},\\\boldsymbol{u}\neq\boldsymbol{v}}} \chi_{U_{\lambda}(\boldsymbol{v})}(s')K(\bar{\boldsymbol{x}}(\boldsymbol{v}) - \bar{\boldsymbol{x}}(\boldsymbol{u}))\chi_{U_{\lambda}(\boldsymbol{u})}(s).$$

- Scaling Property of K_{λ} . As in the case of the helix, it is convenient to first rescale the lattice
- 365 \mathcal{L}_{λ} such that the lattice cell size is independent of λ after rescaling, and define a new map on the
- 366 rescaled lattice. This is considered next.
- Let $S_{1,\lambda} = (-\bar{\theta}/\lambda, \bar{\theta}/\lambda) \times \mathbb{R}$ so that $s \in S$ implies $s/\lambda \in S_{1,\lambda}$. We define a rescaled lattice
- 368 $\mathcal{L}_{1,\lambda}$ such that $s \in \mathcal{L}_{\lambda}$ implies $s/\lambda \in \mathcal{L}_{1,\lambda}$. It is given by

369 (3.32)
$$\mathcal{L}_{1,\lambda} = \{ \mathbf{s} \in \mathcal{S}_{1,\lambda}; \, s_1 = i\theta_l, \, s_2 = j, \, i, j \in \mathbb{Z} \} = (-\bar{\theta}/\lambda, \bar{\theta}/\lambda) \cap \theta_l \mathbb{Z} \times \mathbb{Z}.$$

- The lattice cell for $s \in \mathcal{L}_{1,\lambda}$ is given by $U_1(s)$, where $U_1(s)$ is defined in (3.22) (using $\lambda = 1$ in U_{λ}).
- For $a, b \in S_{1,\lambda}$, we have

372 (3.33)
$$\bar{\boldsymbol{x}}(\lambda \boldsymbol{a}) - \bar{\boldsymbol{x}}(\lambda \boldsymbol{b}) = \lambda \left(\bar{\boldsymbol{x}}(\boldsymbol{a}) - \bar{\boldsymbol{x}}(\boldsymbol{b}) + \boldsymbol{A}_{\lambda}(\boldsymbol{a}, \boldsymbol{b}) \boldsymbol{e}_1 \right),$$

373 where

374 (3.34)
$$\mathbf{A}_{\lambda}(\mathbf{a}, \mathbf{b}) = \frac{\mathcal{R}}{\lambda} \left[\mathbf{Q}(\lambda a_1) - \mathbf{Q}(\lambda b_1) - \lambda \mathbf{Q}(a_1) + \lambda \mathbf{Q}(b_1) \right].$$

Keeping in mind these definitions, for $u \in \mathcal{L}_{1,\lambda}$, we also note

(3.35)

$$\chi_{U_{\lambda}(\lambda \boldsymbol{u})}(\boldsymbol{s}) = \begin{cases} 1 & \text{if } \boldsymbol{s} \in U_{\lambda}(\lambda \boldsymbol{u}), \\ 0 & \text{otherwise} \end{cases} = \begin{cases} 1 & \text{if } \boldsymbol{s}/\lambda \in U_{1}(\boldsymbol{u}), \\ 0 & \text{otherwise} \end{cases} = \chi_{U_{1}(\boldsymbol{u})}(\boldsymbol{s}/\lambda).$$

Using the above relation and (3.33), we can show, for any $s, s' \in \mathcal{S}$,

$$K_{\lambda}(s',s) = \frac{1}{\lambda^3} \sum_{\substack{\boldsymbol{u},\boldsymbol{v} \in \mathcal{L}_{1,\lambda},\\\boldsymbol{u} \neq \boldsymbol{v}}} \chi_{U_1(\boldsymbol{v})}(s'/\lambda) K(\bar{\boldsymbol{x}}(\boldsymbol{v}) - \bar{\boldsymbol{x}}(\boldsymbol{u}) + \boldsymbol{A}_{\lambda}(\boldsymbol{v},\boldsymbol{u})\boldsymbol{e}_1) \chi_{U_1(\boldsymbol{u})}(s/\lambda).$$

If we introduce the discrete dipole field kernel $K_{1,\lambda}(s',s)$, for $s,s'\in\mathcal{S}_{1,\lambda}$, defined on $\mathcal{L}_{1,\lambda}$ as:

381 (3.36)
$$K_{1,\lambda}(s',s) = \sum_{\substack{\boldsymbol{u},\boldsymbol{v}\in\mathcal{L}_{1,\lambda},\\\boldsymbol{u}\neq\boldsymbol{v}}} \chi_{U_1(\boldsymbol{v})}(s')K(\bar{\boldsymbol{x}}(\boldsymbol{v}) - \bar{\boldsymbol{x}}(\boldsymbol{u}) + \boldsymbol{A}_{\lambda}(\boldsymbol{v},\boldsymbol{u})\boldsymbol{e}_1)\chi_{U_1(\boldsymbol{u})}(s),$$

we have shown that:

383
$$K_{\lambda}(s',s) = \frac{1}{\lambda^3} K_{1,\lambda}(s'/\lambda,s/\lambda), \quad \forall s,s' \in \mathcal{S}.$$

- 3.2.3. Limit of Electrostatics Energy. In this section, we obtain the limit of the energy per unit length e_{λ} . The broad strategy is similar to the helical nanotube. We first show that the map T_{λ} is bounded and obtain its limit. The continuum limit of the energy density e_{λ} then follows easily.
- Limit of Discrete Electric Field. Let $T_{1,\lambda} : L^2(\mathcal{S}_{1,\lambda}, \mathbb{R}^3) \to L^2(\mathcal{S}_{1,\lambda}, \mathbb{R}^3)$ be the map with kernel $K_{1,\lambda}$. For any function $\mathbf{f} \in L^2(\mathcal{S}_{1,\lambda}, \mathbb{R}^3)$, we have

389 (3.37)
$$(T_{1,\lambda} \boldsymbol{f})(\boldsymbol{s}) = \frac{\mathcal{R}}{\theta_l} \int_{\mathcal{S}_{1,\lambda}} \boldsymbol{K}_{1,\lambda}(\boldsymbol{s}',\boldsymbol{s}) \boldsymbol{f}(\boldsymbol{s}') \, \mathrm{d}\boldsymbol{s}', \qquad \forall \boldsymbol{s} \in \mathcal{S}_{1,\lambda}.$$

Let $H_{\lambda} = H_{\lambda}(s)$ be the zeroth order moment (with respect to the first argument) of kernel K_{λ} given by

392 (3.38)
$$\boldsymbol{H}_{\lambda}(\boldsymbol{s}) = \frac{\mathcal{R}\lambda}{\theta_{l}} \int_{\boldsymbol{s}' \in \mathcal{S}} \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) \, \mathrm{d}\boldsymbol{s}', \quad \forall \boldsymbol{s} \in \mathcal{S}.$$

- We now state the limit result of T_{λ} .
- Proposition 3.5. Suppose $0 < \theta < \pi/4$. The maps $T_{1,\lambda}$ and T_{λ} are bounded in L^2 for all $\lambda > 0$ and satisfy

396
$$||T_{\lambda}||_{\mathcal{L}(L^{2}(\mathcal{S},\mathbb{R}^{3}),L^{2}(\mathcal{S},\mathbb{R}^{3}))} = ||T_{1,\lambda}||_{\mathcal{L}(L^{2}(\mathcal{S}_{1,\lambda},\mathbb{R}^{3}),L^{2}(\mathcal{S}_{1,\lambda},\mathbb{R}^{3}))}.$$

397 Further, for $\mathbf{f} \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$,

398
$$(T_{\lambda} f)(s) \xrightarrow[\lambda \to 0]{} H_0(s) f(s),$$

399 pointwise, where $H_0(s)$, for $s \in S$, is given by

$$H_0(s) = \lim_{\lambda \to 0} H_{\lambda}(s) = \mathcal{R} \sum_{\substack{u = (u_1, u_2) \in \theta_l \mathbb{Z} \times \mathbb{Z}, \\ u \neq 0}} K(u_1 t_1(s) + u_2 t_2(s)).$$

- 401 $t_i(s) = \frac{\mathrm{d}\bar{x}(s)}{\mathrm{d}s_i}$, i = 1, 2, are tangent vectors on the film.
- We provide the proof of Proposition 3.5 in subsection 4.2. Based on the proposition above, we state the main result for the thin film.
- 404 *Limit of Energy.*
- THEOREM 3.6. Let $f_{\lambda} \in L^2(\mathcal{S}, \mathbb{R}^3)$ be a sequence of functions for $\lambda > 0$ with $f \in L^2(\mathcal{S}, \mathbb{R}^3)$ such that $f_{\lambda} \to f$ in $L^2(\mathcal{S}, \mathbb{R}^3)$. Let the system of dipole moments $d_{\lambda} : \mathcal{L}_{\lambda} \to \mathbb{R}^3$ be given by (3.26).
- Let e_{λ} , given by (3.29), be the energy per unit length normalized by $\Re \theta_l$. Then

$$e_{\lambda} \xrightarrow[\lambda \to 0]{} -\frac{1}{2} (\boldsymbol{f}, \boldsymbol{H}_0 \boldsymbol{f})_{L^2(\mathcal{S}, \mathbb{R}^3)}.$$

409 $H_0 = H_0(s)$ is defined in Proposition 3.5.

- The proof of Theorem 3.6 follows from the proof of Theorem 3.3 and using Proposition 3.5.
- 411 Remark 3.4. Note that, for $s \in S$,

412 (3.39)
$$H_0(s) = Q(s_1)H_0(0)Q(-s_1).$$

- 413 Thus, if the limiting dipole moment field f is uniform in the e_3 direction, the electric field $H_0(s)f(s)$
- 414 will be independent of the e_3 -coordinate. It is easy to see from the expression of H_0 that both the
- 415 normal component and the tangential components of the dipole field contribute to the electric field
- and energy. This is in contrast to [GJ97] where the thin film limit of magnetostatic energy has
- 417 contribution only from the normal component.

4. Proof of Claims.

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- 4.1. **Helical Nanotube.** In this section, we prove Proposition 3.2. First, we collect some important results, and then show that T_{λ} is bounded and extends from $\mathbf{f} \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$ to $L^2(\mathbb{R}, \mathbb{R}^3)$.
- 421 We then obtain the limit of the map T_{λ} .
- Lemma 4.1. 1. For any $a, b \in \mathbb{R}$,

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$$\bar{\boldsymbol{x}}(b) - \bar{\boldsymbol{x}}(a) = \boldsymbol{Q}(a\theta)[(\boldsymbol{Q}((b-a)\theta) - \boldsymbol{I})\boldsymbol{e}_1 + \delta(b-a)\boldsymbol{e}_3],$$

- where \bar{x} is the map (3.1), Q is the rotational tensor (3.2), θ and δ define the helix.
- 425 2. For any $\theta \in (0, \pi)$,

426
$$\delta \leq \min_{a,b \in \mathcal{L}_1, a \neq b} |\bar{\boldsymbol{x}}(b) - \bar{\boldsymbol{x}}(a)|,$$

- where \mathcal{L}_1 is $\mathcal{L}_{\lambda} = \lambda \mathbb{Z}$ for $\lambda = 1$.
 - 3. For any $a, b \in \mathcal{L}_1$ and $\lambda > 0$,

429
$$\delta|a-b| < |\bar{x}(a) - \bar{x}(b) + A_{\lambda}(a,b)e_1|,$$

430 where $\mathbf{A}_{\lambda}(a,b)$ is given by

$$A_{\lambda}(a,b) = \frac{Q(\lambda a\theta) - Q(\lambda b\theta) - (\lambda Q(a\theta) - \lambda Q(b\theta))}{\lambda}.$$

- 432 4. For any $s, s' \in \mathbb{R}$ such that $|s s'| \ge 1$, suppose $a, b \in \mathcal{L}_1$ are such that $s \in [a, a + 1), s' \in [b, b + 1)$, then
- $\frac{|s s'|}{|a b|} < 3.$
- 435 *Proof.* 1. For any $\alpha, \beta \in \mathbb{R}$, we have the identities

436
$$(4.5) Q^{T}(\alpha) = Q(-\alpha), Q(\alpha)Q(\beta) = Q(\alpha+\beta), Q(\alpha)e_3 = e_3,$$

- where the last relation shows that e_3 is the axis of Q. By noting the definition of \bar{x} in (3.1) and using the identities above, (4.1) follows.
- 439 2. To show (4.2), we use (4.1) to get

$$|\bar{\boldsymbol{x}}(b) - \bar{\boldsymbol{x}}(a)|^2 = |(\boldsymbol{Q}((b-a)\theta) - \boldsymbol{I})\boldsymbol{e}_1|^2 + \delta^2|b-a|^2 \ge \delta^2|b-a|^2 \ge \delta^2,$$

where we used the fact that $|b-a| \ge 1$ for $a, b \in \mathcal{L}_1, a \ne b$.

3. To show (4.3), we substitute the definition of A_{λ} to get

(4.6)
$$\bar{\boldsymbol{x}}(a) - \bar{\boldsymbol{x}}(b) + \boldsymbol{A}_{\lambda}(a,b)\boldsymbol{e}_{1} = \frac{\boldsymbol{Q}(\lambda a\theta) - \boldsymbol{Q}(\lambda b\theta)}{\lambda}\boldsymbol{e}_{1} + (a-b)\delta\boldsymbol{e}_{3}.$$

Since $Q(\alpha)e_1$ is orthogonal to e_3 for any α , we have

$$|\bar{\boldsymbol{x}}(a) - \bar{\boldsymbol{x}}(b) + \boldsymbol{A}_{\lambda}(a,b)\boldsymbol{e}_1| \ge \delta|a-b|.$$

44. To show (4.4), we note that for $s,s'\in\mathbb{R}$ such that $|s-s'|\geq 1$ with $a,b\in\mathcal{L}_1$ and $s\in[a,a+1),s'\in[b,b+1)$, we can write $s=a+\Delta s$ and $s'=b+\Delta s'$ with $0\leq\Delta s,\Delta s'<1$. Thus

$$\frac{|s-s'|}{|a-b|} = \frac{|a-b+(\Delta s - \Delta s')|}{|a-b|} \le \frac{|a-b|+|\Delta s - \Delta s'|}{|a-b|} < 1 + \frac{2}{|a-b|} \le 3,$$

where in the last step we used the fact that $|a-b| \ge 1$ for $a, b \in \mathcal{L}_1, a \ne b$ (which is ensured when $|s-s'| \ge 1$).

This completes the proof.

- 453 **4.1.1. Boundedness.** We next show that T_{λ} is a bounded map. Let $S_{\lambda} \colon L^{2}(\mathbb{R}, \mathbb{R}^{3}) \to L^{2}(\mathbb{R}, \mathbb{R}^{3})$ be an isometry defined as
- $(S_{\lambda} \mathbf{f})(s) := \lambda^{1/2} \mathbf{f}(\lambda s).$
- It is easy to see that $||S_{\lambda}f||_{L^2} = ||f||_{L^2}$. The inverse of S_{λ} is given by

$$(S_{\lambda}^{-1} \mathbf{f})(s) = \lambda^{-1/2} \mathbf{f}(s/\lambda).$$

Using S_{λ} , we can show – noting the definition of T_{λ} in (3.11) – for $\mathbf{f} \in L^{2}(\mathbb{R}, \mathbb{R}^{3})$,

$$(T_{\lambda}\boldsymbol{f})(s) = \lambda^{2} \int_{\mathbb{R}} \boldsymbol{K}_{\lambda}(s',s)\boldsymbol{f}(s') \, ds' = \lambda^{2} \int_{\mathbb{R}} \frac{1}{\lambda^{3}} \boldsymbol{K}_{1,\lambda}(s'/\lambda,s/\lambda) \left(\lambda^{-1/2}(S_{\lambda}\boldsymbol{f})(s'/\lambda)\right) \, ds'$$

$$= \lambda^{-3/2} \int_{\mathbb{R}} \boldsymbol{K}_{1,\lambda}(s',s/\lambda)(S_{\lambda}\boldsymbol{f})(s')\lambda \, ds' = \lambda^{-1/2}(T_{1,\lambda}(S_{\lambda}\boldsymbol{f}))(s/\lambda)$$

$$= (S_{\lambda}^{-1}T_{1,\lambda}S_{\lambda}\boldsymbol{f})(s),$$

where we used a change of variable and the fact that $(S_{\lambda}^{-1}f)(s) = \lambda^{(-1/2)}f(s/\lambda)$. It follows from the above equation that

465
$$||T_{\lambda}||_{\mathcal{L}(L^{2},L^{2})} = \sup_{\|\boldsymbol{f}\|\neq 0} \frac{||T_{\lambda}\boldsymbol{f}||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}{||\boldsymbol{f}||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}} = \sup_{\|\boldsymbol{f}\|\neq 0} \frac{||S_{\lambda}^{-1}(T_{1,\lambda}S_{\lambda}\boldsymbol{f})||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}{||\boldsymbol{f}||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}$$

$$= \sup_{\|\boldsymbol{f}\|\neq 0} \frac{||T_{1,\lambda}(S_{\lambda}\boldsymbol{f})||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}{||\boldsymbol{f}||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}} = \sup_{\|S_{\lambda}\boldsymbol{f}\|\neq 0} \frac{||T_{1,\lambda}(S_{\lambda}\boldsymbol{f})||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}{||S_{\lambda}\boldsymbol{f}||_{L^{2}(\mathbb{R},\mathbb{R}^{3})}}$$

$$= ||T_{1,\lambda}||_{\mathcal{L}(L^{2},L^{2})}.$$

This completes the proof of (3.16) in Proposition 3.2. Next, we show that $T_{1,\lambda}$ is a bounded map to prove the boundedness of T_{λ} . We first analyze the discrete dipole field kernel $K_{1,\lambda}$, which is defined

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472 (4.7)
$$\boldsymbol{K}_{1,\lambda}(s',s) = \sum_{\substack{u,v \in \mathcal{L}_1, \\ v \neq u}} \chi_{U_1(v)}(s') \boldsymbol{K}(\bar{\boldsymbol{x}}(v) - \bar{\boldsymbol{x}}(u) + \boldsymbol{A}_{\lambda}(v,u)\boldsymbol{e}_1) \chi_{U_1(u)}(s),$$

- where $U_{\lambda}(s) = [s, s + \lambda)$ for $s \in \mathcal{L}_{\lambda}$, and $A_{\lambda}(a, b)$ is given by (3.13). 473
- Consider some typical $s, s' \in \mathbb{R}$ and the corresponding $a, b \in \mathcal{L}_1$ such that $s \in [a, a+1), s' \in \mathcal{L}_1$ 474
- [b, b+1). From (4.7), we have, for all $s, s' \in \mathbb{R}$ such that |s-s'| < 1, 475
 - If a = b, then $K_{1,\lambda}(s, s') = 0$.
 - If $a \neq b$, then from (4.2), we have

$$|\boldsymbol{K}_{1,\lambda}(s,s')| \le \sqrt{6}/(4\pi\delta^3)$$

using
$$|Aa| \leq |A||a|$$
 and $|I - 3(x/|x|) \otimes (x/|x|)| \leq \sqrt{6}, \forall x \neq 0$.

- Combining the two cases above, $|K_{1,\lambda}(s,s')| \leq \sqrt{6/(4\pi\delta^3)}$. 478
- We now consider a case when $|s-s'| \ge 1$. Noting that for this case, $a \ne b$. We proceed as 479 follows 480

$$|\boldsymbol{K}_{1,\lambda}(s,s')| \leq \frac{\sqrt{6}}{4\pi|s-s'|^3} \frac{|s-s'|^3}{|a-b|^3} \frac{|a-b|^3}{|\bar{\boldsymbol{x}}(a)-\bar{\boldsymbol{x}}(b)+\boldsymbol{A}_{\lambda}(a,b)\boldsymbol{e}_1|^3}$$

$$\leq \frac{\sqrt{6}}{4\pi|s-s'|^3} 3^3 \frac{|a-b|^3}{\delta^3|a-b|^3} = \frac{3^3\sqrt{6}}{4\pi\delta^3} \frac{1}{|s-s'|^3}$$

- where we used the bounds (4.3) and (4.4). Combining the above bound for $|s-s'| \geq 1$ with the 484
- bound for |s-s'| < 1, and renaming the constants, we can write 485

$$|\mathbf{K}_{1,\lambda}(s,s')| \le \frac{C_1}{C_2 + |s-s'|^3}.$$

Since the kernel $K_{1,\lambda}$ satisfies (4.8), we have 487

488 (4.9)
$$\int_{\mathbb{R}} |\mathbf{K}_{1,\lambda}(s',s)| \, \mathrm{d}s' \le C_3, \quad \int_{\mathbb{R}} |\mathbf{K}_{1,\lambda}(s',s)| \, \mathrm{d}s \le C_3,$$

- for some fixed $C_3 < \infty$ independent of λ . Using Young's inequality (e.g., Theorem 0.3.1 [Sog17]), 489
- we have 490

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491 (4.10)
$$||T_{1,\lambda}f||_{L^2(\mathbb{R},\mathbb{R}^3)} \le C_3||f||_{L^2(\mathbb{R},\mathbb{R}^3)}$$

- showing that $T_{1,\lambda}$ is a bounded linear map for all $\mathbf{f} \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$. Since $C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$ is dense in $L^2(\mathbb{R}, \mathbb{R}^3)$, it follows that T_{λ} is also bounded in $L^2(\mathbb{R}, \mathbb{R}^3)$, and extends as a bounded linear map 492
- 493
- from $C_0^{\infty}(\mathbb{R},\mathbb{R}^3)$ to $L^2(\mathbb{R},\mathbb{R}^3)$. 494
 - **4.1.2.** Limit of the Map T_{λ} . Let $f \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$. Write $T_{\lambda}f$ as:

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$$T_{\lambda}(\mathbf{f})(s) = \lambda^2 \int_{\mathbb{R}} \mathbf{K}_{\lambda}(s', s) \mathbf{f}(s') \, \mathrm{d}s'$$

497 (4.11)
$$= \underbrace{\left[\lambda^2 \int_{\mathbb{R}} \mathbf{K}_{\lambda}(s', s) \, \mathrm{d}s'\right]}_{=:\mathbf{H}_{\lambda}(s)} \mathbf{f}(s) + \lambda^2 \int_{\mathbb{R}} \mathbf{K}_{\lambda}(s', s) (\mathbf{f}(s') - \mathbf{f}(s)) \, \mathrm{d}s',$$

- The second term above is zero in the limit $\lambda \to 0$. To see this, consider any R > 0, and then using 499
- the bound on $K_{1,\lambda}$ in (4.8), we have 500

$$\frac{1}{\lambda} \int_{|s-s'| \ge R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \, \mathrm{d}s' \le \frac{1}{\lambda} \int_{|s-s'| \ge R\lambda} \frac{C_1}{C_2 + |s/\lambda - s'/\lambda|^3} \, \mathrm{d}s'$$

$$= \lambda^2 \int_{|s-s'| > R\lambda} \frac{C_1}{C_2 \lambda^3 + |s-s'|^3} \, \mathrm{d}s' = \lambda^2 \int_{|t| > R} \frac{C_1}{C_2 \lambda^3 + |\lambda t|^3} \lambda \, \mathrm{d}t$$

$$\int_{|t| \ge R} \frac{C_1}{C_2 + |t|^3} \, \mathrm{d}t,$$

In the intermediate step, we changed variables $t = (s' - s)/\lambda$. Thus, the upper bound on

$$\frac{1}{\lambda} \int_{|s-s'| \ge R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \, \mathrm{d}s'$$

is independent of λ , and goes to zero as $R \to \infty$. For the second term in (4.11), using that

506
$$m{K}_{\lambda}(s',s) = rac{1}{\lambda^3} m{K}_{1,\lambda}(s'/\lambda,s/\lambda)$$
, we get

$$\begin{vmatrix}
\lambda^{2} \int_{\mathbb{R}} \mathbf{K}_{\lambda}(s', s) (\mathbf{f}(s') - \mathbf{f}(s)) \, ds' \\
= \left| \frac{1}{\lambda} \int_{\mathbb{R}} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) (\mathbf{f}(s') - \mathbf{f}(s)) \, ds' \right| \\
= \left| \frac{1}{\lambda} \int_{|s-s'| \geq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \mathbf{f}(s') \, ds' - \frac{1}{\lambda} \int_{|s-s'| \geq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \, ds' \mathbf{f}(s) \right| \\
+ \frac{1}{\lambda} \int_{|s-s'| \leq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) (\mathbf{f}(s') - \mathbf{f}(s)) \, ds' \\
= \left| \frac{1}{\lambda} \int_{|s-s'| \geq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \mathbf{f}(s') \, ds' \right| + \left| \frac{1}{\lambda} \int_{|s-s'| \geq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) \, ds' \mathbf{f}(s) \right| \\
+ \left| \frac{1}{\lambda} \int_{|s-s'| \leq R\lambda} \mathbf{K}_{1,\lambda}(s'/\lambda, s/\lambda) (\mathbf{f}(s') - \mathbf{f}(s)) \, ds' \right|.$$

- We let $\lambda \to 0$ and then $R \to \infty$. In the limit $\lambda \to 0$, the third term above will go to zero, as 514
- $f \in C_0^{\infty}(\mathbb{R}, \mathbb{R}^3)$ and $K_{1,\lambda}$ is bounded. The first and second terms will go to zero using (4.12). Thus, 515
- we have from (4.11) that 516

$$\lim_{\lambda \to 0} T_{\lambda}(\mathbf{f})(s) = \left[\lim_{\lambda \to 0} \mathbf{H}_{\lambda}(s)\right] \mathbf{f}(s),$$

We next compute the limit of $\mathbf{H}_{\lambda}(s)$. Fix $s \in \mathbb{R}$ and suppose $a \in \mathcal{L}_{\lambda}$ such that $s \in U_{\lambda}(a)$. 518

Using the definition of $K_{\lambda}(s', s)$, we have 519

520
$$\boldsymbol{H}_{\lambda}(s) = \lambda^{2} \int_{\mathbb{R}} \boldsymbol{K}(s', s) \, ds' = \lambda^{2} \sum_{\substack{u \in \mathcal{L}_{1}, \\ u \neq a}} \boldsymbol{K}(\bar{\boldsymbol{x}}(u) - \bar{\boldsymbol{x}}(a)) \int_{U_{\lambda}(u)} \, dt$$
521
$$= \lambda^{3} \sum_{\substack{u \in \lambda \mathbb{Z}, \\ u \neq a}} \boldsymbol{K}(\bar{\boldsymbol{x}}(u) - \bar{\boldsymbol{x}}(a)).$$

From (4.5), we have $\bar{x}(u) - \bar{x}(a) = Q(a\theta)((Q((u-a)\theta) - I)e_1 + (u-a)\delta e_3)$. Using the identity $K(Qx) = QK(x)Q^T$ and $K(\lambda x) = K(x)/\lambda^3$, we get

524
$$K(Qx) = QK(x)Q^T$$
 and $K(\lambda x) = K(x)/\lambda^3$, we get

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$$\boldsymbol{H}_{\lambda}(s) = \boldsymbol{Q}(a\theta) \left[\sum_{u \in \lambda \mathbb{Z}, u \neq a} \boldsymbol{K}((\boldsymbol{Q}((u-a)\theta) - \boldsymbol{I})/\lambda \boldsymbol{e}_{1} + (u-a)\delta/\lambda \boldsymbol{e}_{3}) \right] \boldsymbol{Q}(-a\theta)$$
526
$$= \boldsymbol{Q}(a\theta) \left[\sum_{i \in \mathbb{Z}, i \neq 0} \boldsymbol{K}((\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I})/\lambda \boldsymbol{e}_{1} + i\delta \boldsymbol{e}_{3}) \right] \boldsymbol{Q}(-a\theta),$$
527

- where we changed variables $i=(u-a)/\lambda$. Note that $a\in\lambda\mathbb{Z}$, and, therefore, $(u-a)\in\lambda\mathbb{Z}$ for
- 529 $u \in \lambda \mathbb{Z}$, which implies $i \in \mathbb{Z}$. Since s is related to a by $s \in U_{\lambda}(a)$, we have $a \to s$ in the limit
- 530 $\lambda \to 0$. Therefore, we get

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$$\boldsymbol{H}_0(s) := \lim_{\lambda \to 0} \boldsymbol{H}_{\lambda}(s) = \boldsymbol{Q}(s\theta) \left[\lim_{\lambda \to 0} \sum_{i \in \mathbb{Z} - \{0\}} \boldsymbol{K}((\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I})/\lambda \boldsymbol{e}_1 + i\delta \boldsymbol{e}_3) \right] \boldsymbol{Q}(-s\theta).$$

To take the limit inside the summation, we show that the sum is absolutely convergent for all $\lambda > 0$

533 as follows:

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$$a_{\lambda} := \sum_{i \in \mathbb{Z} - \{0\}} |\boldsymbol{K} ((\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I})/\lambda \boldsymbol{e}_1 + i\delta \boldsymbol{e}_3)| \le \sum_{i \in \mathbb{Z} - \{0\}} \frac{c}{|(\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I})/\lambda \boldsymbol{e}_1 + i\delta \boldsymbol{e}_3)|^3}$$

$$= \sum_{i \in \mathbb{Z} - \{0\}} \frac{c}{(4\sin^2(i\lambda\theta/2)/\lambda^2 + i^2\delta^2)^{3/2}} \le \sum_{i \in \mathbb{Z} - \{0\}} \frac{c}{|i|^3} < \infty, \qquad \forall \lambda > 0.$$

Now, we can write

538
$$\boldsymbol{H}_0(s) = \boldsymbol{Q}(s\theta) \left[\sum_{i \in \mathbb{Z} - \{0\}} \lim_{\lambda \to 0} \boldsymbol{K} \left(\frac{\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I}}{i\lambda\theta} (i\theta\boldsymbol{e}_1) + i\delta\boldsymbol{e}_3 \right) \right] \boldsymbol{Q}(-s\theta).$$

Note that for a fixed $i \in \mathbb{Z}$

$$\lim_{\lambda \to 0} \frac{(\boldsymbol{Q}(i\lambda\theta) - \boldsymbol{I})}{i\lambda\theta} i\theta \boldsymbol{e}_1 + i\delta\boldsymbol{e}_3 = \lim_{h=i\lambda\theta \to 0} \frac{(\boldsymbol{Q}(h) - \boldsymbol{I})}{h} i\theta \boldsymbol{e}_1 + i\delta\boldsymbol{e}_3 = i\theta \boldsymbol{Q}'(0)\boldsymbol{e}_1 + i\delta\boldsymbol{e}_3,$$

- where $Q'(0) = d/dx Q(x)|_{x=0}$. Now, using the equation above, and the fact that K(x) is smooth
- away from x = 0 (which is ensured in the summation), we get

$$\mathbf{H}_0(s) = \mathbf{Q}(s\theta) \left[\sum_{i \in \mathbb{Z} - \{0\}} \mathbf{K} \left(i\theta \mathbf{Q}'(0) \mathbf{e}_1 + i\delta \mathbf{e}_3 \right) \right] \mathbf{Q}(-s\theta) = \mathbf{Q}(s\theta) \mathbf{H}_0(0) \mathbf{Q}(-s\theta).$$

544 Combining this with (4.13), we get

$$\lim_{\lambda \to 0} T_{\lambda}(\boldsymbol{f})(s) = \boldsymbol{H}_{0}(s)\boldsymbol{f}(s) = \boldsymbol{Q}(s\theta)\boldsymbol{H}_{0}(0)\boldsymbol{Q}(-s\theta)\boldsymbol{f}(s).$$

Next, we simplify $H_0(s)$. Using $QK(x)Q^T = K(Qx)$ and $Q(s\theta)Q'(0) = Q'(s\theta)$, we can show

$$\boldsymbol{H}_{0}(s) = \sum_{i \in \mathbb{Z}-0} \boldsymbol{K}(i\theta \boldsymbol{Q}'(s\theta)\boldsymbol{e}_{1} + i\delta\boldsymbol{e}_{3}) = \sum_{i \in \mathbb{Z}-0} \boldsymbol{K}\left(i|\boldsymbol{t}(s)|\,\hat{\boldsymbol{t}}(s)\right),$$

- where $t(s) = \theta Q'(s\theta)e_1 + \delta e_3$ is the tangent vector, and $\hat{t}(s) = t(s)/|t(s)|$ with $|t(s)| = \sqrt{\theta^2 + \delta^2}$.
- Using above and substituting the form of dipole field kernel K, it is easy to show that

550
$$\boldsymbol{H}_{0}(s) = -h_{0}\left[\boldsymbol{I} - 3\hat{\boldsymbol{t}}(s)\otimes\hat{\boldsymbol{t}}(s)\right] = -h_{0}\left[\boldsymbol{P}_{\perp}\boldsymbol{f}(s) - 2\boldsymbol{P}_{||}(s)\right],$$

551 with h_0 defined as

552 (4.14)
$$h_0 = \sum_{i \in \mathbb{Z}_{>0}} \frac{1}{4\pi |i|^3 (\theta^2 + \delta^2)^{3/2}}$$

and projection tensors $m{P}_{||}(s)=\hat{m{t}}(s)\otimes\hat{m{t}}(s)$ and $m{P}_{\perp}(s)=m{I}-m{P}_{||}(s)$.

- **4.2. Nanofilm with Uniform Bending.** In this section, we prove Proposition 3.5. The outline of the proof is similar to the case of the helix in subsection 4.1.
- LEMMA 4.2. 1. Suppose $s, s' \in \mathcal{S}_{1,\lambda} = (-\bar{\theta}/\lambda, \bar{\theta}/\lambda) \times \mathbb{R}$ such that $a, b \in \mathcal{L}_{1,\lambda} = (-\bar{\theta}/\lambda, \bar{\theta}/\lambda) \cap \theta_l \mathbb{Z} \times \mathbb{Z}$ with $s \in U_1(a) = [a_1, a_1 + \theta_l) \times [a_2, a_2 + 1), s' \in U_1(b)$. When
- $|s-s'| \ge \min\{\theta_l, 1\}$, we have $a \ne b$ and

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$$\frac{|s-s'|}{|a-b|} < 1 + \frac{\theta_l + 1}{\min\{\theta_l, 1\}} =: c_L.$$

560 2. For any $a, b \in \mathcal{L}_{1,\lambda}$, we have

$$(4.16) c_A|\boldsymbol{a}-\boldsymbol{b}| \leq |\bar{\boldsymbol{x}}(\boldsymbol{a}) - \bar{\boldsymbol{x}}(\boldsymbol{b}) + \boldsymbol{A}_{\lambda}(\boldsymbol{a},\boldsymbol{b})\boldsymbol{e}_1|,$$

where \bar{x} is given by (3.19) and $A_{\lambda}(a, b)$ is defined as

$$A_{\lambda}(\boldsymbol{a},\boldsymbol{b}) = \frac{\mathcal{R}}{\lambda} \left[\boldsymbol{Q}(\lambda a_1) - \boldsymbol{Q}(\lambda b_1) - \lambda \boldsymbol{Q}(a_1) + \lambda \boldsymbol{Q}(b_1) \right].$$

- Here $c_A = \min\{\delta, \mathcal{R}\sqrt{1-\bar{\theta}^2/3}\}$ is the constant independent of λ . Note that $c_A > 0$ for $0 < \bar{\theta} < \pi/2$.
- Proof. To show (4.15), we proceed as follows. For $s, s' \in \mathcal{S}_{1,\lambda}$ and corresponding $a, b \in \mathcal{L}_{1,\lambda}$, there exists $\Delta s, \Delta s'$ such that $s = a + \Delta s, s' = b + \Delta b$ with $0 \le \Delta s_1, \Delta s'_1 < \theta_l, 0 \le \Delta s_2, \Delta s'_2 < 1$.
- We have the bound

569 (4.17)
$$\frac{|s-s'|}{|a-b|} \le 1 + \frac{|\Delta s_1 - \Delta s_1'| + |\Delta s_2 - \Delta s_2'|}{|a-b|} < 1 + \frac{\theta_l + 1}{|a-b|} \le 1 + \frac{\theta_l + 1}{\min\{\theta_l, 1\}},$$

- 570 where in the last step we used the fact that any $a, b \in \mathcal{L}_{1,\lambda}$, satisfying $a \neq b$, are at least min $\{\theta_l, 1\}$
- 571 distance apart.
- 572 We next show (4.16). Using

$$\bar{\boldsymbol{x}}(\boldsymbol{a}) - \bar{\boldsymbol{x}}(\boldsymbol{b}) + \boldsymbol{A}_{\lambda}(\boldsymbol{a}, \boldsymbol{b})\boldsymbol{e}_{1} = \frac{\mathcal{R}}{\lambda}(\boldsymbol{Q}(\lambda a_{1}) - \boldsymbol{Q}(\lambda b_{1}))\boldsymbol{e}_{1} + \delta(a_{2} - b_{2})\boldsymbol{e}_{3}$$

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575
$$|(\boldsymbol{Q}(\theta_1) - \boldsymbol{Q}(\theta_2))\boldsymbol{e}_1|^2 = (\cos\theta_1 - \cos\theta_2)^2 + (\sin\theta_1 - \sin\theta_2)^2 = 2(1 - \cos(\theta_1 - \theta_2)),$$

576 we have that

577 (4.18)
$$|\bar{\boldsymbol{x}}(\boldsymbol{a}) - \bar{\boldsymbol{x}}(\boldsymbol{b}) + \boldsymbol{A}_{\lambda}(\boldsymbol{a}, \boldsymbol{b})\boldsymbol{e}_1|^2 = \delta^2 |a_2 - b_2|^2 + \frac{2\mathcal{R}^2}{\sqrt{2}} (1 - \cos(\lambda a_1 - \lambda b_1)).$$

Let $r=a_1-b_1$. Then, using a Taylor expansion and the mean value theorem, there exists ξ such that

$$1 - \cos(\lambda r) = \frac{1}{2}\lambda^2 r^2 - \frac{1}{24}\lambda^4 r^4 \cos(\xi).$$

Since $-1 \le \cos(\xi) \le 1$, it follows

$$1 - \cos(\lambda r \xi) \ge \frac{1}{2} \lambda^2 r^2 - \frac{1}{24} \lambda^4 r^4.$$

Substituting the relation above in (4.18), we get

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$$|\bar{\boldsymbol{x}}(\boldsymbol{a}) - \bar{\boldsymbol{x}}(\boldsymbol{b}) + \boldsymbol{A}_{\lambda}(\boldsymbol{a}, \boldsymbol{b})\boldsymbol{e}_{1}|^{2} \ge \delta^{2}|a_{2} - b_{2}|^{2} + \mathcal{R}^{2}r^{2}\left(1 - \frac{1}{12}\lambda^{2}r^{2}\right).$$

Since $a, b \in \mathcal{L}_{1,\lambda}$, we have $-2\bar{\theta} < \lambda r < 2\bar{\theta}$, and 584

$$1 - \frac{1}{12}\lambda^2 r^2 \ge 1 - \frac{1}{12}\bar{\theta}^2 4 = 1 - \frac{\bar{\theta}^2}{3}.$$

Using the two equations above and defining the constant c_A as in Lemma 4.2(2), (4.16) can be easily 586

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4.2.1. Boundedness. Let $S_{\lambda} : L^{2}(\mathcal{S}, \mathbb{R}^{3}) \to L^{2}(\mathcal{S}_{1,\lambda}, \mathbb{R}^{3})$ be a map such that, for any $f \in$ 588 $L^2(\mathcal{S}, \mathbb{R}^3),$ 589

$$(S_{\lambda} \mathbf{f})(\mathbf{s}) = \lambda \mathbf{f}(\lambda \mathbf{s}), \quad \forall \mathbf{s} \in \mathcal{S}_{1,\lambda}.$$

It is easy to see that S_{λ} is an isometry. The inverse of S_{λ} is given by

$$(S_{\lambda}^{-1} f)(s) = \lambda^{-1} f(s/\lambda), \quad \forall s \in \mathcal{S}.$$

593 Following the similar steps in subsubsection 4.1.1, we can show that

594
$$||T_{\lambda}||_{\mathcal{L}(L^{2},L^{2})} = ||T_{1,\lambda}||_{\mathcal{L}(L^{2},L^{2})}.$$

Thus, to show that T_{λ} is a bounded map, it is sufficient to show that $T_{1,\lambda}$ is bounded. Towards that 595

goal, we first establish that 596

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$$|\boldsymbol{K}_{1,\lambda}(\boldsymbol{s},\boldsymbol{s}')| \leq \frac{C_1}{C_2 + |\boldsymbol{s} - \boldsymbol{s}'|^3}, \qquad \forall \boldsymbol{s}', \boldsymbol{s} \in \mathcal{S}_{1,\lambda},$$

where C_1 , C_2 are constants that may depend on the parameters R, θ , δ defining the surface S and are 598 independent of λ . Similar to the case of the helix (subsubsection 4.1.1), we apply Theorem 0.3.1 599 of [Sog17] to show that, for any $\lambda > 0$, $T_{1,\lambda}$ is a bounded linear map on $C_0^{\infty}(\mathcal{S}_{1,\lambda},\mathbb{R}^3)$. Using the density of $C_0^{\infty}(\mathcal{S}_{1,\lambda},\mathbb{R}^3)$ in $L^2(\mathcal{S}_{1,\lambda},\mathbb{R}^3)$, $T_{1,\lambda}$ extends as a bounded linear map to $L^2(\mathcal{S}_{1,\lambda},\mathbb{R}^3)$. 600 601

It remains to show (4.19). We recall that $\bar{\theta}$ is the fixed angular extent of the film and satisfies the bound $0 < \bar{\theta} < \pi/2$ (in fact we restrict it such that $0 < \bar{\theta} < \pi/4$). Let $s, s' \in S_{1,\lambda}$ be any two generic points, and let $a, b \in \mathcal{L}_{1,\lambda}$ be such that $s \in U_1(a)$ and $s' \in U_1(b)$. We refer to subsubsection 3.2.1 and subsubsection 3.2.2 for the notation appearing in this section.

First, consider s, s' such that $|s - s'| \ge \min\{\theta_l, 1\}$. For this case, we have $a \ne b$. Noting that 606 $|I - 3(x/|x|) \otimes (x/|x|)| = \sqrt{6}, \forall x \neq 0$, we have

$$|K_{1,\lambda}(s,s')| \leq \frac{\sqrt{6}}{4\pi |\bar{x}(a) - \bar{x}(b) + A_{\lambda}(a,b)e_{1}|^{3}}$$

$$= \frac{\sqrt{6}}{4\pi |s - s'|^{3}} \frac{|s - s'|^{3}}{|a - b|^{3}} \frac{|a - b|^{3}}{|\bar{x}(a) - \bar{x}(b) + A_{\lambda}(a,b)e_{1}|^{3}}$$

$$\leq \frac{\sqrt{6}}{4\pi |s - s'|^{3}} c_{L}^{3} \frac{1}{c_{A}^{3}},$$
(4.20)

where we used the bounds (4.15) and (4.16). 612

Next, we consider the case when $|s-s'| < \min\{\theta_l, 1\}$. This can be further divided in two cases: 613

- Case 1: $\mathbf{a} = \mathbf{b}$ which implies $|\mathbf{K}_{1,\lambda}(\mathbf{s}',\mathbf{s})| = 0$.
- Case 2: $a \neq b$. For this case, we have 615

(4.21)
$$|K_{1,\lambda}(s,s')| \le \frac{\sqrt{6}}{4\pi |\bar{x}(a) - \bar{x}(b) + A_{\lambda}(a,b)e_1|^3} \le \frac{\sqrt{6}}{4\pi c_A^3 |a-b|^3}.$$

- Note that when $a \neq b$, we can have (A) $a_1 = b_1, a_2 = b_2 \pm 1$, or (B) $a_1 = b_1 \pm \theta_l, a_2 = b_2$,
- or (C) $a_1 = b_1 \pm \theta_l, a_2 = b_2 \pm 1$. For all the cases mentioned above, the denominator in
- (4.21) is bounded from below as follows $|a b| \ge \min\{\theta_l, 1\}$. Thus, we have

620
$$|K_{1,\lambda}(s,s')| \le \frac{\sqrt{6}}{4\pi c_A^3 (\min\{\theta_l,1\})^3}.$$

- In summary (4.22) holds for any s, s' such that $|s s'| < \min\{\theta_l, 1\}$.
- Combining the bound for the case $|s s'| < \min\{\theta_l, 1\}$ with the bound for the case $|s s'| \ge 1$
- 623 $\min\{\theta_l, 1\}$, we can write

624 (4.23)
$$|K_{1,\lambda}(s,s')| \le \frac{C_1}{C_2 + |s-s'|^3},$$

- where we have renamed the constants for convenience. This completes the proof of the boundedness
- of $T_{1,\lambda}$. We next obtain the limit of the map T_{λ} .
- **4.2.2.** Limit of Map T_{λ} . Let $f \in C_0^{\infty}(\mathcal{S}, \mathbb{R}^3)$. We write $T_{\lambda}f$ as follows

628
$$(T_{\lambda} \mathbf{f})(\mathbf{s}) = \frac{\mathcal{R}\lambda}{\theta_l} \int_{\mathcal{S}} \mathbf{K}_{\lambda}(\mathbf{s}', \mathbf{s}) \mathbf{f}(\mathbf{s}') \, d\mathbf{s}'$$

629 (4.24)
$$= \underbrace{\left[\frac{\mathcal{R}\lambda}{\theta_l}\int_{\mathcal{S}} K_{\lambda}(s',s) \, \mathrm{d}s'\right]}_{=:H_{\lambda}(s)} f(s) + \frac{\mathcal{R}\lambda}{\theta_l}\int_{\mathcal{S}} K_{\lambda}(s',s) (f(s') - f(s)) \, \mathrm{d}s',$$

- We next show that the second term in (4.24) is zero in the limit $\lambda \to 0$. Fix $\bar{R} > 0$, then using the
- relation $K_{\lambda}(s',s) = K_{1,\lambda}(s'/\lambda,s/\lambda)/\lambda^3$ and the bound on $K_{1,\lambda}$ in (4.23), we have

633
$$\left| \lambda \int_{\mathcal{S}} \chi_{|s-s'| \geq \bar{R}\lambda}(s') \boldsymbol{K}_{\lambda}(s',s) (\boldsymbol{f}(s') - \boldsymbol{f}(s)) \, \mathrm{d}s' \right| \leq \lambda \int_{\mathbb{R}^{2}} \chi_{|s-s'| \geq \bar{R}\lambda}(s') |\boldsymbol{K}_{\lambda}(s',s) (\boldsymbol{f}(s') - \boldsymbol{f}(s))| \, \mathrm{d}s'$$
(4.25)

$$634\atop 635 \le \frac{1}{\lambda^2} \int_{\mathbb{R}^2} \chi_{|\boldsymbol{s}-\boldsymbol{s}'| \ge \bar{R}\lambda}(\boldsymbol{s}') \frac{C_1}{C_2 + |\boldsymbol{s}/\lambda - \boldsymbol{s}'/\lambda|^3} \, \mathrm{d}\boldsymbol{s}'.$$

Using the change of variable $t'=s'/\lambda$ (so $ds'=\lambda^2 dt'$) and $t=s/\lambda$ to have

$$\begin{vmatrix}
4.26 \\
\delta_{37} \\
\delta_{38}
\end{vmatrix} \lambda \int_{\mathcal{S}} \chi_{|\boldsymbol{s}-\boldsymbol{s}'| \geq \bar{R}\lambda}(\boldsymbol{s}') \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) (\boldsymbol{f}(\boldsymbol{s}') - \boldsymbol{f}(\boldsymbol{s})) \, d\boldsymbol{s}' \\
\end{vmatrix} \leq \int_{\mathbb{R}^{2}} \chi_{|\boldsymbol{t}'-\boldsymbol{t}| \geq \bar{R}}(\boldsymbol{t}') \frac{C_{1}}{C_{2} + |\boldsymbol{t}'-\boldsymbol{t}|^{3}} \, d\boldsymbol{t}'.$$

639 From above, we have that

640 (4.27)
$$\lim_{\bar{R}\to\infty} \left[\lim_{\lambda\to 0} \left| \lambda \int_{S} \chi_{|s-s'|\geq \bar{R}\lambda}(s') K_{\lambda}(s',s) (f(s') - f(s)) \, \mathrm{d}s' \right| \right] = 0.$$

We bound the second term in (4.24) by splitting it into two parts as follows:

643
$$\left| \lambda \int_{\mathcal{S}} \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) (\boldsymbol{f}(\boldsymbol{s}') - \boldsymbol{f}(\boldsymbol{s})) \, d\boldsymbol{s}' \right| \leq \left| \lambda \int_{\mathcal{S}} \chi_{|\boldsymbol{s} - \boldsymbol{s}'| \geq \bar{R}\lambda}(\boldsymbol{s}') \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) (\boldsymbol{f}(\boldsymbol{s}') - \boldsymbol{f}(\boldsymbol{s})) \, d\boldsymbol{s}' \right| + \left| \lambda \int_{\mathcal{S}} \chi_{|\boldsymbol{s} - \boldsymbol{s}'| \leq \bar{R}\lambda}(\boldsymbol{s}') \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) (\boldsymbol{f}(\boldsymbol{s}') - \boldsymbol{f}(\boldsymbol{s})) \, d\boldsymbol{s}' \right|.$$
21

Since $|f(s') - f(s)| \le 2||f||_{L^{\infty}} < \infty$ and from (4.27), the first term in the equation above is zero in the limit $\bar{R} \to \infty$ following the limit $\lambda \to 0$. For the second term, we proceed as follows

646
$$\left| \lambda \int_{\mathcal{S}} \chi_{|\mathbf{s}-\mathbf{s}'| \leq \bar{R}\lambda}(\mathbf{s}') \mathbf{K}_{\lambda}(\mathbf{s}', \mathbf{s}) (\mathbf{f}(\mathbf{s}') - \mathbf{f}(\mathbf{s})) \, d\mathbf{s}' \right|$$
647
$$\leq \frac{1}{\lambda^{2}} \int_{\mathcal{S}} \chi_{|\mathbf{s}-\mathbf{s}'| \leq \bar{R}\lambda}(\mathbf{s}') |\mathbf{K}_{1,\lambda}(\mathbf{s}'/\lambda, \mathbf{s}/\lambda)| \, |\mathbf{f}(\mathbf{s}') - \mathbf{f}(\mathbf{s})| \, d\mathbf{s}'$$
648
$$\leq \frac{1}{\lambda^{2}} \int_{\mathbb{R}^{2}} \chi_{|\mathbf{s}-\mathbf{s}'| \leq \bar{R}\lambda}(\mathbf{s}') |\mathbf{K}_{1,\lambda}(\mathbf{s}'/\lambda, \mathbf{s}/\lambda)| \, |\mathbf{f}(\mathbf{s}') - \mathbf{f}(\mathbf{s})| \, d\mathbf{s}'.$$

650 Since $K_{1,\lambda}$ is bounded as $s' \to s$ (see (4.23)), $|\{s' \in \mathbb{R}^2; |s - s'| \leq \bar{R}\lambda\}| = \pi \bar{R}^2 \lambda^2$, and $\sup_{|s'-s| \leq \bar{R}\lambda} |f(s') - f(s)| \to 0 \text{ as } \lambda \to 0, \text{ we have}$

652 (4.29)
$$\lim_{\bar{R} \to \infty} \left[\lim_{\lambda \to 0} \left| \lambda \int_{S} \chi_{|s-s'| \le \bar{R}\lambda} K_{\lambda}(s', s) (f(s') - f(s)) \, \mathrm{d}s' \right| \right] = 0.$$

We have shown

654 (4.30)
$$\lim_{\lambda \to 0} \left| \lambda \int_{\mathcal{S}} \boldsymbol{K}_{\lambda}(\boldsymbol{s}', \boldsymbol{s}) (\boldsymbol{f}(\boldsymbol{s}') - \boldsymbol{f}(\boldsymbol{s})) \, \mathrm{d}\boldsymbol{s}' \right| = 0.$$

655 Thus, from (4.24), we have

656 (4.31)
$$\lim_{\lambda \to 0} (T_{\lambda} f)(s) = \left[\lim_{\lambda \to 0} H_{\lambda}(s)\right] f(s).$$

Limit of H_{λ} . Consider a typical $s \in S$ such that $s \in U_{\lambda}(a)$ where $a \in \mathcal{L}_{\lambda}$. Recall that \mathcal{L}_{λ} is

the lattice for $\lambda > 0$ and $U_{\lambda}(a) = [a_1, a_1 + \theta_l \lambda) \times [a_2, a_2 + \lambda)$ is the lattice cell. In the definition

of H_{λ} , we substitute K_{λ} , to get

660 (4.32)
$$\boldsymbol{H}_{\lambda}(\boldsymbol{s}) = \frac{\mathcal{R}\lambda}{\theta_l} \sum_{\boldsymbol{u} \in \mathcal{L}_{\lambda}, \boldsymbol{u} \neq \boldsymbol{a}} \boldsymbol{K}(\bar{\boldsymbol{x}}(\boldsymbol{u}) - \bar{\boldsymbol{x}}(\boldsymbol{a})) \int_{U_{\lambda}(\boldsymbol{u})} d\boldsymbol{s}' = \mathcal{R}\lambda^3 \sum_{\boldsymbol{u} \in \mathcal{L}_{\lambda}, \boldsymbol{u} \neq \boldsymbol{a}} \boldsymbol{K}(\bar{\boldsymbol{x}}(\boldsymbol{u}) - \bar{\boldsymbol{x}}(\boldsymbol{a})).$$

Substituting the definition of transformation \bar{x} in (3.19), we can show for $a, u \in \mathcal{L}_{\lambda}$ that

662
$$\bar{x}(u) - \bar{x}(a) = Q(a_1\theta) \left[\mathcal{R}(Q(u_1 - a_1) - I)e_1 + (u_2 - a_2)\delta e_3 \right].$$

Using the identities $K(Q(t)x) = Q(t)K(x)Q^{T}(t)$ and $K(\lambda x) = K(x)/\lambda^{3}$, from (4.32), we have (4.33)

664
$$\boldsymbol{H}_{\lambda}(\boldsymbol{s}) = \mathcal{R}\boldsymbol{Q}(a_1) \underbrace{\left[\sum_{\boldsymbol{u} \in \mathcal{L}_{\lambda}, \boldsymbol{u} \neq \boldsymbol{a}} \boldsymbol{K} \left(\mathcal{R}(\boldsymbol{Q}(u_1 - a_1) - \boldsymbol{I}) / \lambda \boldsymbol{e}_1 + (u_2 - a_2) \delta / \lambda \boldsymbol{e}_3 \right) \right]}_{=: \boldsymbol{H}_{\lambda}(\boldsymbol{s})} \boldsymbol{Q}(-a_1),$$

666 We analyze $ar{H}_{\lambda}$ as follows. First, we expand the sum $m{u} \in \mathcal{L}_{\lambda}$

667
$$\bar{\boldsymbol{H}}_{\lambda}(\boldsymbol{s}) = \sum_{u_{2} \in \lambda \mathbb{Z}} \left[\sum_{\substack{u_{1} \in \lambda \theta_{l} \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta}), \\ (u_{1}, u_{2}) \neq \boldsymbol{a}}} \boldsymbol{K} \left(\mathcal{R} \frac{\boldsymbol{Q}(u_{1} - a_{1}) - \boldsymbol{I}}{\lambda} \boldsymbol{e}_{1} + \delta \frac{u_{2} - a_{2}}{\lambda} \boldsymbol{e}_{3} \right) \right]$$

668 (4.34)
$$= \sum_{t_2' \in \mathbb{Z}} \left[\sum_{\substack{u_1 \in \lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta}), \\ (u_1, t_2') \neq (a_1, 0)}} \mathbf{K} \left(\mathcal{R} \frac{\mathbf{Q}(u_1 - a_1) - \mathbf{I}}{\lambda} \mathbf{e}_1 + \delta t_2' \mathbf{e}_3 \right) \right],$$

- where we introduced the new variable $t_2' = (u_2 a_2)/\lambda$. Since $u_2, a_2 \in \lambda \mathbb{Z}$, we have $t_2' \in \mathbb{Z}$. Using
- a Taylor expansion and the mean value theorem, we have an identity

$$Q(u_1 - a_1) - I = Q'(\xi)(u_1 - a_1),$$

- where $\xi = \xi(u_1 a_1) \in (-\bar{\theta}, \bar{\theta})$ depends on $u_1 a_1$. Based on the above observation, we decompose 674
- $m{H}_{\lambda}(s)$ 676

677
$$= \underbrace{\sum_{t_2' \in \mathbb{Z}} \left[\sum_{\substack{u_1 \in \lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta}), \\ (u_1, t_2') \neq (a_1, 0)}} K\left(\mathcal{R}Q'(0) \frac{u_1 - a_1}{\lambda} e_1 + \delta t_2' e_3\right) \right]}_{=: \bar{\boldsymbol{H}}_{\lambda}^{(1)}(\boldsymbol{s})}$$

$$(4.36)$$

$$+ \underbrace{\sum_{t_{2}' \in \mathbb{Z}} \left[\sum_{\substack{u_{1} \in \lambda \theta_{l} \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta}), \\ (u_{1}, t_{2}') \neq (a_{1}, 0)}} \left\{ K \left(\mathcal{R} \frac{\boldsymbol{Q}(u_{1} - a_{1}) - \boldsymbol{I}}{\lambda} \boldsymbol{e}_{1} + \delta t_{2}' \boldsymbol{e}_{3} \right) - K \left(\mathcal{R} \boldsymbol{Q}'(0) \frac{u_{1} - a_{1}}{\lambda} \boldsymbol{e}_{1} + \delta t_{2}' \boldsymbol{e}_{3} \right) \right\} \right]}_{=: \bar{\boldsymbol{H}}^{(2)}(\boldsymbol{s})}$$

- where two new terms are defined for convenience. 680
- **Step 1:** We show $\bar{\boldsymbol{H}}_{\lambda}^{(2)}$ goes to zero in the limit $\lambda \to 0$. Let 681

682 (4.37)
$$x_1 = \mathcal{R} \frac{Q(u_1 - a_1) - I}{\lambda} e_1, \quad x_2 = \mathcal{R} Q'(0) \frac{u_1 - a_1}{\lambda} e_1, \quad z = \delta t_2' e_3.$$

Consider a function $y: [0,1] \to \mathbb{R}^3$ defined as 683

684 (4.38)
$$y(r) = x_1 + r(x_2 - x_1).$$

Note that, since $(u_1, t_2') \neq (a_1, 0)$ and $t_2' \in \mathbb{Z}$, 685

(4.39)
$$|\boldsymbol{y}(r) + \boldsymbol{z}| \ge \min\{\delta, \min_{r \in [0,1], u_1 \in \lambda \theta_t \mathbb{Z} - \{a_1\} \cap (-\bar{\theta}, \bar{\theta})} |\boldsymbol{y}(r)| \}.$$

- $\min_{r \in [0,1], u_1 \in \lambda \theta_l \mathbb{Z} \{a_1\} \cap (-\bar{\theta}, \bar{\theta})} |\boldsymbol{y}(r)| > 0$ and the lower bound is independent of λ . 687
- For convenience, let $t = u_1 a_1$. Since $u_1, a_1 \in \lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta})$, and $u_1 \neq a_1$, we have $t \in$ 688
- $\lambda \theta_l \mathbb{Z} \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})$. The hypothesis of Proposition 3.5 restricts $\bar{\theta}$ such that 689

690 (4.40)
$$0 < \bar{\theta} < \pi/4 \quad \Rightarrow 1 > \cos(2\bar{\theta}) > 0.$$

With $t = u_1 - a_1$, writing out the action of $\mathbf{Q}(t)$ and $\mathbf{Q}'(0)$ on \mathbf{e}_1 , we get 691

692
$$x_1 = \mathcal{R}\frac{Q(t) - I}{\lambda}e_1 = \frac{\mathcal{R}}{\lambda}[(\cos(t) - 1)e_1 + \sin(t)e_2]$$

693 (4.41)
$$x_2 = \mathcal{R} Q'(0) \frac{t}{\lambda} e_1 = \frac{\mathcal{R} t}{\lambda} [-\sin(t) e_1 + \cos(t) e_2].$$

Through elementary calculations, we can show 695

696 (4.42)
$$|\boldsymbol{y}(r)|^2 = |\boldsymbol{x}_1 + r(\boldsymbol{x}_2 - \boldsymbol{x}_1)|^2 = \frac{\mathcal{R}^2}{\lambda^2} \left[2(1-r)^2(1-\cos(t)) + r^2t^2 + 2r(1-r)t\sin(t) \right].$$

Using a Taylor expansion and noting that $t \in \lambda \theta_l \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})$, there exists $\xi_1, \xi_2 \in (-2\bar{\theta}, 2\bar{\theta})$ with $\xi_1 = \xi_1(t), \xi_2 = \xi_2(t)$ such that

699 (4.43)
$$1 - \cos(t) = \cos(\xi_1)t^2/2, \quad \sin(t) = t\cos(\xi_2).$$

700 Thus

701
$$|\mathbf{y}(r)|^{2} = \frac{\mathcal{R}^{2}}{\lambda^{2}} \left[2(1-r)^{2} \cos(\xi_{1})t^{2}/2 + r^{2}t^{2} + 2r(1-r)t \cos(\xi_{2})t \right]$$
702
$$= \frac{\mathcal{R}^{2}t^{2}}{\lambda^{2}} \left[(1-r)^{2} \cos(\xi_{1}) + r^{2} + 2r(1-r) \cos(\xi_{2}) \right]$$
703
$$\geq \frac{\mathcal{R}^{2}t^{2}}{\lambda^{2}} \left[(1-r)^{2} \min_{\xi \in (-2\bar{\theta}, 2\bar{\theta})} \cos(\xi) + r^{2} + 2r(1-r) \min_{\xi \in (-2\bar{\theta}, 2\bar{\theta})} \cos(\xi) \right]$$
704
$$= \frac{\mathcal{R}^{2}t^{2}}{\lambda^{2}} \left[(1-r)^{2} \cos(2\bar{\theta}) + r^{2} + 2r(1-r) \cos(2\bar{\theta}) \right]$$
705
$$\geq \frac{\mathcal{R}^{2}t^{2}}{\lambda^{2}} \min_{r \in [0,1]} \left[(1-r)^{2} \cos(2\bar{\theta}) + r^{2} + 2r(1-r) \cos(2\bar{\theta}) \right]$$
706
$$(4.44) = \frac{\mathcal{R}^{2}t^{2}}{\lambda^{2}} \cos(2\bar{\theta}),$$

where we used the fact that $\min_{\xi \in (-2\bar{\theta}, 2\bar{\theta})} \cos(\xi) = \cos(2\bar{\theta})$ in the fourth equation, and $\cos(2\bar{\theta})$ is the minimum with respect to $r \in [0, 1]$ of the function in the square bracket in the fifth equation. Further, since $t \in \lambda \theta_l \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})$, we have

711 (4.45)
$$0 < C_y := \frac{\mathcal{R}^2 \lambda^2 \theta_l^2}{\lambda^2} \cos(2\bar{\theta}) = (\mathcal{R}\theta_l)^2 \cos(2\bar{\theta}) \le |\boldsymbol{y}(r)|^2,$$

for any $t \in \lambda \theta_l \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})$ and $r \in [0, 1]$. The lower bound on |y(r)| is independent of λ and r. Finally, combining (4.45) with (4.39) to get

714 (4.46)
$$0 < C_{yz} := \min\{\delta, \mathcal{R}\theta_l \sqrt{\cos(2\bar{\theta})}\} \le |y(r) + z|.$$

Proceeding further, we have, from the fundamental theorem of calculus,

716
$$K(\boldsymbol{x}_1 + \boldsymbol{z}) - K(\boldsymbol{x}_2 + \boldsymbol{z}) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}r} K(\boldsymbol{y}(r) + \boldsymbol{z}) \, \mathrm{d}r = \int_0^1 \nabla K(\boldsymbol{y}(r) + \boldsymbol{z}) \frac{\mathrm{d}}{\mathrm{d}r} \boldsymbol{y}(r) \, \mathrm{d}r$$
717
$$= \int_0^1 \nabla K(\boldsymbol{y}(r) + \boldsymbol{z}) (\boldsymbol{x}_2 - \boldsymbol{x}_1) \, \mathrm{d}r.$$
(4.47)

Note that because of (4.46), $\nabla K(y(r) + z)$ exists and is bounded. From the definition of $\bar{H}_{\lambda}^{(2)}$ in (4.36), a change of variable $t = u_1 - a_1$, the definition of x_1, x_2, z in (4.37) and (4.41), and noting

the identity (4.47), we have

722
$$|ar{m{H}}_{\lambda}^{(2)}(m{s})|$$

723
$$\leq \sum_{\substack{t_2' \in \mathbb{Z} \\ (u_1, t_2') \neq (a_1, 0)}} \left| K \left(\mathcal{R} \frac{\boldsymbol{Q}(u_1 - a_1) - \boldsymbol{I}}{\lambda} \boldsymbol{e}_1 + \delta t_2' \boldsymbol{e}_3 \right) - K \left(\mathcal{R} \boldsymbol{Q}'(0) \frac{u_1 - a_1}{\lambda} \boldsymbol{e}_1 + \delta t_2' \boldsymbol{e}_3 \right) \right|$$

724
$$\leq \sum_{t_{2}^{\prime} \in \mathbb{Z}} \left[\sum_{t \in \lambda \theta_{t} \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})} \left| \boldsymbol{K} \left(\boldsymbol{x}_{1} + \boldsymbol{z} \right) - \boldsymbol{K} \left(\boldsymbol{x}_{2} + \boldsymbol{z} \right) \right| \right]$$

725
$$\leq \sum_{t_2' \in \mathbb{Z}} \left[\sum_{t \in \lambda \theta_1 \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})} \int_0^1 |\nabla K(y(r) + z)| |x_2 - x_1| dr \right]$$

726
$$\leq \sum_{t_2' \in \mathbb{Z}} \left[\sum_{t \in \lambda \theta_l \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})} \int_0^1 \frac{C}{|\boldsymbol{y}(r) + \boldsymbol{z}|^4} |\boldsymbol{x}_2 - \boldsymbol{x}_1| dr \right]$$

(4.48)

727
$$= \sum_{t_2' \in \mathbb{Z}} \left[\sum_{t \in \lambda \theta_t \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})} \int_0^1 \frac{C}{(|\boldsymbol{y}(r)|^2 + |\boldsymbol{z}|^2)^2} |\boldsymbol{x}_2 - \boldsymbol{x}_1| \, dr \right],$$

where we utilized the bound on the gradient of K with constant C > 0 fixed.

Next, we get an upper bound on $|x_1 - x_2|$ in terms of t. From (4.41), we have

$$x_2 - x_1 = \frac{\mathcal{R}}{\lambda} \left[t \mathbf{Q}'(0) - \mathbf{Q}(t) + \mathbf{I} \right] \mathbf{e}_1.$$

730 By a Taylor expansion and the mean value theorem, we have ${m Q}(t) = {m I} + t {m Q}'(0) + (t^2/2) {m Q}''(\xi)$

where $\xi = \xi(t) \in (-2\bar{\theta}, 2\bar{\theta})$ depends on t. Substituting this and using the bound $|Q_{ij}''(\xi)| \le 1$ gives

732 (4.49)
$$|x_2 - x_1| = \frac{\mathcal{R}}{\lambda} \frac{|t|^2}{2} |Q''(\xi)| \le \frac{\mathcal{R}}{\lambda} \frac{|t|^2}{2}.$$

Combining the equation above with (4.48), we get

734
$$|\bar{\boldsymbol{H}}_{\lambda}^{(2)}(\boldsymbol{s})|$$
735
$$\leq \sum_{t'_{2} \in \mathbb{Z}} \left[\sum_{t \in \lambda \theta_{l} \mathbb{Z} - \{0\} \cap (-2\bar{\theta}, 2\bar{\theta})} \int_{0}^{1} \frac{C}{(|\boldsymbol{y}(r)|^{2} + |\boldsymbol{z}|^{2})^{2}} \frac{\mathcal{R}}{\lambda} \frac{|t|^{2}}{2} dr \right]$$
736
$$= \sum_{t'_{2} \in \mathbb{Z}} \left[\sum_{t' \in \theta_{l} \mathbb{Z} - \{0\} \cap (-2\bar{\theta}/\lambda, 2\bar{\theta}/\lambda)} \int_{0}^{1} \frac{C}{(|\boldsymbol{y}(r)|^{2} + |\boldsymbol{z}|^{2})^{2}} \frac{\mathcal{R}}{\lambda} \frac{\lambda^{2} |t'|^{2}}{2} dr \right]$$
737
$$\leq \lambda \left\{ \sum_{t'_{2} \in \mathbb{Z}} \left[\sum_{t' \in \theta_{l} \mathbb{Z} - \{0\} \cap (-2\bar{\theta}/\lambda, 2\bar{\theta}/\lambda)} \int_{0}^{1} \frac{C}{(|\boldsymbol{y}(r)|^{2} + |\boldsymbol{z}|^{2})^{2}} \frac{\mathcal{R}|t'|^{2}}{2} dr \right] \right\},$$
738

where in the third line we introduced the variable $t' = t/\lambda$. We only have to show that the term inside

the braces is bounded as $\lambda \to 0$ to conclude that $|\bar{H}_{\lambda}^{(2)}(s)| \to 0$ as $\lambda \to 0$. First, note from (4.44),

we have 741

742 (4.50)
$$|\mathbf{y}(r)|^2 \ge \frac{\mathcal{R}^2}{\lambda^2} |t|^2 \cos(2\bar{\theta}) = \mathcal{R}^2 |t'|^2 \cos(2\bar{\theta}).$$

Therefore, 743

744 (4.51)
$$\frac{C}{(|\boldsymbol{y}(r)|^2 + |\boldsymbol{z}|^2)^2} \le \frac{C}{(\mathcal{R}^2|t'|^2\cos(2\bar{\theta}) + |\boldsymbol{z}|^2)^2}.$$

Thus 745 (4.52)

$$|\bar{\boldsymbol{H}}_{\lambda}^{(2)}(\boldsymbol{s})| \leq \lambda \left\{ \sum_{t'_{2} \in \mathbb{Z}} \left[\sum_{t' \in \theta_{t} \mathbb{Z} - \{0\} \cap (-2\bar{\theta}/\lambda, 2\bar{\theta}/\lambda)} \int_{0}^{1} \frac{C}{(\mathcal{R}^{2}|t'|^{2} \cos(2\bar{\theta}) + |\boldsymbol{z}|^{2})^{2}} \frac{\mathcal{R}|t'|^{2}}{2} dr \right] \right\}.$$

- Note that the integrand is independent of r. Further, the numerator has $|t'|^2$ whereas the denominator 748
- has $(|t'|^2c+|z|^2)^2$, therefore, the sum inside the braces is absolutely convergent and finite. Hence, 749
- due to the factor λ , we have shown $\lim_{\lambda \to 0} |\bar{\boldsymbol{H}}_{\lambda}^{(2)}(s)| = 0.$ 750
- This completes the step 1. We next study $\bar{\boldsymbol{H}}_{\lambda}^{(1)}$ 751
- **Step 2:** We have from (4.36) 752

753
$$\bar{\boldsymbol{H}}_{\lambda}^{(1)}(\boldsymbol{s}) = \sum_{t_{2}' \in \mathbb{Z}} \left[\sum_{\substack{u_{1} \in \lambda \theta_{l} \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta}), \\ (u_{1}, t_{2}') \neq (a_{1}, 0)}} \boldsymbol{K} \left(\mathcal{R} \boldsymbol{Q}'(0) \frac{u_{1} - a_{1}}{\lambda} \boldsymbol{e}_{1} + \delta t_{2}' \boldsymbol{e}_{3} \right) \right]$$
754
$$= \sum_{t_{2}' \in \mathbb{Z}} \left[\sum_{\substack{u_{1} \in \lambda \theta_{l} \mathbb{Z}, \\ (u_{1}, t_{2}') \neq (a_{1}, 0)}} \boldsymbol{K} \left(\mathcal{R} \boldsymbol{Q}'(0) \frac{u_{1} - a_{1}}{\lambda} \boldsymbol{e}_{1} + \delta t_{2}' \boldsymbol{e}_{3} \right) \right]$$

755 (4.53)
$$- \underbrace{\sum_{t_2' \in \mathbb{Z}} \left[\sum_{\substack{u_1 \in [\lambda \theta_l \mathbb{Z}] - [\lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta})], \\ (u_1, t_2') \neq (a_1, 0)}}_{=:I_2} K \left(\mathcal{R} Q'(0) \frac{u_1 - a_1}{\lambda} e_1 + \delta t_2' e_3 \right) \right],$$

where we have used the notation $[\lambda \theta_l \mathbb{Z}] - [\lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta})]$ to denote the set $\{t \in \lambda \theta_l \mathbb{Z}; t \notin \theta_l \mathbb{Z}\}$ 757

 $\lambda \theta_l \mathbb{Z} \cap (-\theta, \theta)$. Using the decay property of the dipole field kernel K, we can show that $|I_2| \to 0$ 758

in the limit $\lambda \to 0$. Therefore, we have 759

760
$$\lim_{\lambda \to 0} \bar{\boldsymbol{H}}_{\lambda}^{(1)}(\boldsymbol{s}) = \lim_{\lambda \to 0} \sum_{t_2' \in \mathbb{Z}} \left[\sum_{\substack{u_1 \in \lambda \theta_1 \mathbb{Z}, \\ (u_1, t_2') \neq (a_1, 0)}} \boldsymbol{K} \left(\mathcal{R} \boldsymbol{Q}'(0) \frac{u_1 - a_1}{\lambda} \boldsymbol{e}_1 + \delta t_2' \boldsymbol{e}_3 \right) \right]$$

761
$$= \sum_{t_2' \in \mathbb{Z}} \left[\sum_{\substack{t_1' \in \theta_1 \mathbb{Z}, \\ (t_1', t_2') \neq (0, 0)}} \mathbf{K} \left(\mathcal{R} \mathbf{Q}'(0) t_1' \mathbf{e}_1 + \delta t_2' \mathbf{e}_3 \right) \right]$$

(4.54)763

where we introduced the new variable $t_1' = (u_1 - a_1)/\lambda$. Since $u_1 \in \lambda \theta_1 \mathbb{Z}$ and $a_1 \in \lambda \theta_l \mathbb{Z} \cap (-\bar{\theta}, \bar{\theta})$, we have $t_1' \in \theta_l \mathbb{Z}$. This completes step 2. Note that $\lim_{\lambda \to 0} \bar{H}_{\lambda}(s)$ is independent of $s \in \mathcal{S}$.

Upon substituting the limit of $\bar{H}_{\lambda}^{(1)}$ and $\bar{H}_{\lambda}^{(2)}$ in (4.36), we have shown

767 (4.55)
$$\lim_{\lambda \to 0} \bar{\boldsymbol{H}}_{\lambda}(\boldsymbol{s}) = \lim_{\lambda \to 0} \bar{\boldsymbol{H}}_{\lambda}(\boldsymbol{0}) = \sum_{\boldsymbol{u} = (u_1, u_2) \in \theta_l \mathbb{Z} \times \mathbb{Z}, \\ \boldsymbol{u} \neq \boldsymbol{0}} \boldsymbol{K} \left(\mathcal{R} \boldsymbol{Q}'(0) u_1 \boldsymbol{e}_1 + \delta u_2 \boldsymbol{e}_3 \right).$$

Recall that $s \in S$ was fixed such that $s \in U_{\lambda}(a)$, which implies that $a \to s$ as $\lambda \to 0$. With this observation and (4.55), we have from (4.33), (4.56)

770
$$\boldsymbol{H}_{0}(\boldsymbol{s}) = \lim_{\lambda \to 0} \boldsymbol{H}_{\lambda}(\boldsymbol{s}) = \mathcal{R}\boldsymbol{Q}(s_{1}) \left[\sum_{\substack{\boldsymbol{u} = (u_{1}, u_{2}) \in \theta_{l} \mathbb{Z} \times \mathbb{Z}, \\ \boldsymbol{u} \neq \boldsymbol{0}}} \boldsymbol{K} \left(\mathcal{R}\boldsymbol{Q}'(0) u_{1} \boldsymbol{e}_{1} + \delta u_{2} \boldsymbol{e}_{3} \right) \right] \boldsymbol{Q}(-s_{1}).$$

Next we simplify $H_0(s)$. Given the parametric map $\bar{x}=\bar{x}(s)$, the two tangent vectors at $s=(s_1,s_2)$ are

773 (4.57)
$$t_1(s) = \frac{\mathrm{d}\bar{x}}{\mathrm{d}s_1} = \mathcal{R}Q'(s_1)e_1, \qquad t_2(s) = \frac{\mathrm{d}\bar{x}}{\mathrm{d}s_2} = \delta e_3.$$

Using $QK(x)Q^T = K(Qx)$ and Q(r)Q'(0) = Q'(r), we write,

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$$\boldsymbol{H}_{0}(\boldsymbol{s}) = \sum_{\substack{\boldsymbol{u} = (u_{1}, u_{2}) \in \theta_{l} \mathbb{Z} \times \mathbb{Z}, \\ \boldsymbol{u} \neq \boldsymbol{0}}} \boldsymbol{K} \left(u_{1} \boldsymbol{t}_{1}(\boldsymbol{s}) + u_{2} \boldsymbol{t}_{2}(\boldsymbol{s}) \right).$$

This completes the proof of Proposition 3.5.

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5. Summary of Results. We have shown rigorously that certain low-dimensional nanostructures do not have long-range dipole-dipole interaction in the continuum limit. The energy density in the limit is entirely due to Maxwell-self field. In 1-d and 2-d lattices (in a 3-d ambient space), the dipole field kernel decay is sufficiently fast that long-range interactions do not contribute to the limit energy.

While our calculations show that the energy is local in the continuum limit for 1-d and 2-d discrete systems, in agreement with dimension reduction approaches that reduce a 3-d continuum to a 1-d or 2-d continuum (e.g., [GJ97, CH15] and others), we note an interesting difference. As shown in [GJ97] and other work following it, the thin film limit of the continuum electrostatic energy is due to the component of dipole moment field along the normal direction to the film. Similarly, the thin wire limit of the energy is due to components of dipole moment field in the plane normal to the wire, see [CH15]. This is different from the limit energy in the discrete-to-continuum limit: for the case of a helical nanotube, the limiting energy density is given by

$$h_0 \int_{\mathbb{D}} \left[|\boldsymbol{P}_{\perp} \boldsymbol{f}|^2 - 2|\boldsymbol{P}_{||} \boldsymbol{f}|^2 \right] ds,$$

where h_0 is a constant, and $P_{||}f$ and $P_{\perp}f$ are the projections of the dipole moment field f along the axis of the helix and in the plane normal to the axis of the helix respectively. Therefore, unlike the thin wire limit using dimension reduction, the discrete-to-continuum energy has contributions from both the normal and tangential components of the dipole moment field. For the case of a thin film with curvature, the limiting energy density is given by

$$-rac{1}{2}\int_{\mathcal{S}}oldsymbol{f}(oldsymbol{s})\cdotoldsymbol{H}_0(oldsymbol{s})oldsymbol{f}(oldsymbol{s})\,\mathrm{d}oldsymbol{s},$$

where 787

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$$\boldsymbol{H}_{0}(\boldsymbol{s}) = \mathcal{R} \sum_{\substack{\boldsymbol{u} = (u_{1}, u_{2}) \in \theta_{l} \mathbb{Z} \times \mathbb{Z}, \\ \boldsymbol{u} \neq \boldsymbol{0}}} \boldsymbol{K} \left(u_{1} \boldsymbol{t}_{1}(\boldsymbol{s}) + u_{2} \boldsymbol{t}_{2}(\boldsymbol{s}) \right).$$

Here, S is the parametric domain of the film, \mathcal{R} is the inverse of the curvature, θ_l is the angular width of the unit cell, and $t_i(s)$, i=1,2, are the tangent vectors at coordinate $s\in\mathcal{S}$. For simplicity, we fix 790 $s\in\mathcal{S}$ and assume $t_1=e_1$ and $t_2=e_2$; then the lattice sum above is over a 2-d lattice in (e_1,e_2) 791 plane. By substituting the form of K and computing $H_0(s)f(s)$, we can show that both the normal 792 and the tangential components of f are present in the final expression for the energy above. The difference between the dimension reduction approach on the one hand, and the discrete-to-continuum 794 limit on the other hand, is due to the fact that we assume that the discrete structures consist of a finite 795 unit cell in the thickness direction and do not take the limit in the thickness direction. 796

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