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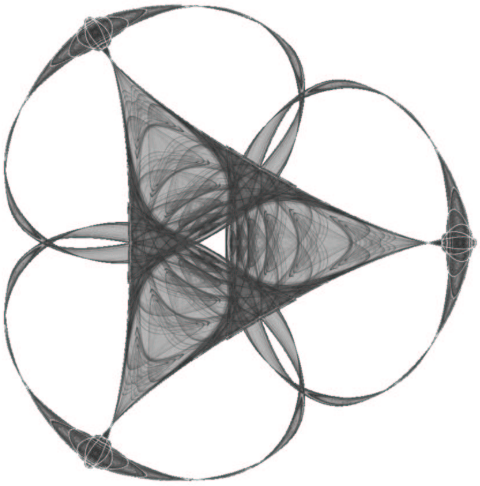

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DISCRETE NETWORK APPROXIMATION FOR HIGHLY-PACKED COMPOSITES WITH IRREGULAR GEOMETRY IN THREE DIMENSIONS

LEONID BERLYAND *, YULIYA GORB †, AND ALEXEI NOVIKOV ‡

Abstract. We introduce a discrete network approximation to the problem of the effective conductivity of the high contrast, highly packed composites in three dimensions. The inclusions are irregularly (randomly) distributed in a hosting medium, so that a significant fraction of them may not participate in the conducting spanning cluster. For this class of spacial arrays of inclusions we derive a discrete network approximation and obtain its a priori error estimate. We obtained an explicit dependence of the network approximation and its error on the irregular geometry of the inclusions' array. We use variational techniques to provide rigorous mathematical justification for the approximation and its error estimate.

Key words. effective conductivity, discrete network, error estimate, variational bounds.

AMS subject classifications. 74Q05, 35Q72, 94C05.

1. Introduction. We are interested in high–contrast two–phase composites, when the geometry of distribution of phases significantly affects their effective properties. In this work we study the effective conductivity of particulate composites, where highly conducting spherical inclusions are densely packed into a homogeneous matrix.

Periodic lattices of highly conducting inclusions were first analyzed by [9] (for other references see e.g. [4]). In the case of irregularly distributed inclusions, the main difficulty is that when the concentration of the inclusions is high, the geometric connectivity patterns in the whole composite (percolation effects) become important. This issue was addressed in [4], where a discrete network approximation for effective conductivity was developed for irregularly distributed 2D disks (see e.g. [5] for references on other discrete network models). The main result of a subsequent work [5] was error estimates of the discrete network approximation, which are valid in the homogenization limit as R, radius of the disks, tends to zero. The key ingredient of the construction of the error estimates [5] is the $\delta - N$ close packing condition, which loosely speaking allows for "holes of size N in the conducting spanning cluster".

In this work we investigate how the discrete network approach [4, 5] can be applied to study the effective conductivity $\widehat{A}$ in three dimensions, where the geometry of the connectivity patterns in much more complex than in two dimensions. We develop the discrete network with the energy $\mathcal{I}$, and study its approximation error

$$\text{Error} = |\widehat{A} - \mathcal{I}|.$$

There are two main results of this work. The first result is asymptotic. In theorem 4.4 we show that the effective conductivity $\widehat{A}$ and the energy of the discrete network I satisfy

$$\widehat{A} = \mathcal{I} + O(1), \quad \mathcal{I} = O(\ln \delta), \tag{1.1}$$

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where the *relative interparticle distance* [5] δ is, loosely speaking, a dimensionless characteristic distance between inclusions in the conducting spanning cluster. The second result is concerned with the relative error estimates of the discrete network approximation which hold in the limit $R \to 0$. In theorem 4.5 we prove that

$$\frac{\widehat{A} - \mathcal{I}}{\mathcal{I}} \leq \frac{C(\mathcal{D})}{\ln \delta}. \tag{1.2}$$

for $\delta - \mathcal{D}$ connected distributions of inclusions, where $\mathcal{D}$ is, loosely speaking, "the diameter of the holes" in the composite.

Our main tool is the construction of the variational upper and lower bounds. The key ingredient of this construction is our *central projection partition*, an effective and elegant algorithm that automatically accounts for geometric distribution of disks. We introduce this partition because it decomposes the matrix into simple geometric figures: tetrahedra, prisms and hoses, and consequently allows to construct "good" trial fields for the lower and upper bounds.

The paper is organized as follows. In Section 2 we present a mathematical formulation of the problem under consideration. The variational bounds for the effective conductivity $\widehat{A}$ are also given there. In Section 3 we construct our discrete network. In particular, the central projection partition is introduced in Subsection 3.2 and the δ-$\mathcal{D}$ connectedness property of the discrete network is defined in Subsection 3.4. The variational error estimates for the effective conductivity $\widehat{A}$ are given Section 4. The trial functions for the lower and upper variational bounds are constructed in Subsections 4.1 and 4.2, respectively. The main results (1.1) and (1.2) are proved in Subsection 4.3. In Appendices some intermediate and additional calculations can be found.

2. Formulation of the problem. Consider a three-dimensional model of a two-phase composite that consists of a matrix of finite conductivity in which a large number of perfectly conducting inclusions are randomly distributed. The composite is modelled by a parallelepiped $Y = [-L_1, L_1] \times [-L_2, L_2] \times [-1, 1]$. The inclusions are modelled by identical non-overlapping balls B_i of radius R, $i = 1, \dots N$, where N is the number of inclusions. The distribution of the balls is high, that is, the characteristic distance between two neighboring balls is much smaller than their radius. Then the perforated domain

$$Q = Y \setminus \bigcup_{i=1}^{N} B_i \tag{2.1}$$

models the matrix of the composite. Let $Q^{\pm} = \{\boldsymbol{x} = (x, y, z) \in \mathbb{R}^3 : z = \pm 1\}$ be the upper/lower boundary of the domain Q and $Q_{lat} = \partial Y \setminus (Q^- \cup Q^+)$ the lateral boundary of Q.

Let the potential $u(\boldsymbol{x}) = u(x, y, z)$, $\boldsymbol{x} \in \mathbb{R}^3$ be a function from $H^1(Q)$. Introduce the space:

$$V = \{u \in H^1(Q) : u(\boldsymbol{x}) = t_i \text{ on } \partial B_i, u(\boldsymbol{x}) = \pm 1 \text{ on } Q^{\pm}\} \tag{2.2}$$

and define a functional:

$$I[u] = \frac{1}{8L_1 L_2} \int_Q |\nabla u|^2 d\boldsymbol{x}, \quad u \in H^1(Q). \tag{2.3}$$

Suppose the function u solves of the variational minimization problem:

$$\min_{\widetilde{u}\in V} I[\widetilde{u}] =: I[u]. \tag{2.4}$$

Then the potential u inside the matrix Q satisfies the Euler-Lagrange equation of (2.4):

$$\begin{array}{lll}
(a) & \triangle u = 0 & \text{in } Q \\
(b) & u(\boldsymbol{x}) = t_i & \text{on } \partial B_i, \;\; i = 1, \dots, N \\
(c) & u(\boldsymbol{x}) = \pm 1 & \text{on } Q^{\pm} \\
(d) & \displaystyle\int_{\partial B_i} \frac{\partial u}{\partial \boldsymbol{n}} d\boldsymbol{x} = 0, & i = 1, \dots, N \\
(e) & \displaystyle\frac{\partial u}{\partial \boldsymbol{n}} = 0 & \text{on } Q_{lat}.
\end{array} \tag{2.5}$$

The effective conductivity $\widehat{A}$ of the composite is defined as the minimum of the functional (2.3), (2.4), over the class V given by (2.2):

$$\widehat{A} = I[u] = \frac{1}{8L_1L_2}\int_Q |\nabla u|^2 d\boldsymbol{x}. \tag{2.6}$$

(see e.g. [2, 3, 8, 10]).

Applying the Green's formula to (2.3) and taking into account (2.5a) we obtain that $\widehat{A}$ can also be defined as the total flux per unit length through a horizontal cross-section of the domain. By the integration by parts of $\int_Q \triangle u \, d\boldsymbol{x}$ and (2.5a) we have that the *total fluxes* through the horizontal boundaries Q^- and Q^+ are equal:

$$\int_{Q^+} \frac{\partial u}{\partial \boldsymbol{n}} d\boldsymbol{x} = -\int_{Q^-} \frac{\partial u}{\partial \boldsymbol{n}} d\boldsymbol{x}. \tag{2.7}$$

Therefore for an equivalent definition of the effective conductivity we can take, for example, the total flux through the boundary Q^+ per unit length defined by

$$\widehat{A} = \frac{1}{8L_1L_2}\int_{Q^+} \frac{\partial u}{\partial \boldsymbol{n}} d\boldsymbol{x} = \frac{1}{8L_1L_2}\int_{Q^+} \frac{\partial u}{\partial z} d\boldsymbol{x}. \tag{2.8}$$

Our goal is to use variational approach to investigate $\widehat{A}$ when inclusions are close to touching. Besides the direct variational problem (2.3), (2.4), (2.2) we consider a dual variational problem in which $\widehat{A}$ is equivalently defined [7] as a maximum of the functional J:

$$\widehat{A} = \max_{\widetilde{\boldsymbol{v}}\in W} J[\widetilde{\boldsymbol{v}}] =: J[\boldsymbol{v}], \tag{2.9}$$

where

$$J[\boldsymbol{v}] = -\frac{1}{2}\int_Q \boldsymbol{v}^2 d\boldsymbol{x} + \frac{1}{2}\int_{Q^+} \boldsymbol{v}\cdot\boldsymbol{n}\, d\boldsymbol{x} - \frac{1}{2}\int_{Q^-} \boldsymbol{v}\cdot\boldsymbol{n}\, d\boldsymbol{x}, \tag{2.10}$$

and the class of all fluxes W is given by:

$$W = \left\{ \boldsymbol{v} \in \boldsymbol{L}^2(Q) : \; \boldsymbol{v}(\boldsymbol{x})\cdot\boldsymbol{n} = 0 \text{ on } Q_{lat}, \; \int_{\partial B_i} \boldsymbol{v}\cdot\boldsymbol{n}\, d\boldsymbol{x} = 0, \;\; \operatorname{div} \boldsymbol{v} = 0 \right\}. \tag{2.11}$$

The details of the derivation of (2.9), (2.10) and (2.11) can be found e.g. in [7].

Thus, for any $u \in V$ and $\boldsymbol{v} \in W$ we obtain the following bounds on the effective conductivity $\widehat{A}$:

$$\frac{1}{2}\int_{Q} \boldsymbol{v}^2 d\boldsymbol{x} + \frac{1}{2}\int_{Q^+} \boldsymbol{v}\cdot\boldsymbol{n}\, d\boldsymbol{x} - \frac{1}{2}\int_{Q^-} \boldsymbol{v}\cdot\boldsymbol{n}\, d\boldsymbol{x} \leq \widehat{A} \leq \frac{1}{8L_1L_2}\int_{Q} |\nabla u|^2 d\boldsymbol{x}. \tag{2.12}$$

The equality is achieved when $\boldsymbol{v} = \nabla u$.

3. Discrete Network. In this section we construct a discrete network (graph) approximating the continuum problem (2.8). We use here the Keller's observation [9] that the dominant contribution to the effective conductivity comes from the thin gaps (*hoses*) between closely spaced neighboring inclusions, so that the flux outside of these gaps does not change asymptotics of $\widehat{A}$. We define notions of neighboring balls and hoses, connecting them, in subsection 3.1. Next we define an algebraic quadratic form:

$$\mathcal{I} = \frac{1}{8L_1L_2}\sum_{i,j} g_{ij}(t_i - t_j)^2, \tag{3.1}$$

where t_i is the value of the potential in the ball B_i, $(i = 1,\dots,N)$ and the number g_{ij} is a *specific flux* defined in subsection 3.3. The quadratic form (3.1) is our discrete network approximation to effective conductivity (2.6): $\widehat{A} \sim \mathcal{I}$.

In order to determine t_i, $i = 1,\dots,N$ in (3.1) we set up a *discrete minimization problem* supplemented with appropriate boundary conditions. The obtained minimization problem amounts to solving a simple system of linear algebraic equations, what makes it attractive for numerical implementations.

Our error estimates of the discrete network rely on the variational bounds (2.12). Upper and lower trial fields for (2.12) are constructed using our decomposition of the domain Q into simple geometric regions. This decomposition is obtained by the *central projection partition* which we introduce in Section 3.2. Finally, we give useful properties of the discrete network approximation in subsection 3.4.

3.1. Construction of the Network. Neighbors and necks of the discrete network can be defined using the notion of the *Voronoi diagram* [1] of the domain Q. For the centers of the balls B_i:

$$P = \{\boldsymbol{x}_i \in \mathbb{R}^3,\ i = 1,\dots,N\}, \tag{3.2}$$

the Voronoi diagram is the partition of the domain Q into non-overlapping *Voronoi cells* $V(\boldsymbol{x}_i)$. Each $V(\boldsymbol{x}_i)$ is the set of all points in $\mathbb{R}^3$ that are closer to $\boldsymbol{x}_i$ than to any other site from P.

The Voronoi diagram in $\mathbb{R}^3$ can also be defined as follows. Introduce the bisector of two sites $\boldsymbol{x}_i$, $\boldsymbol{x}_j \in P$, which is the perpendicular plane through the midpoint of the line segment $\boldsymbol{x}_i\boldsymbol{x}_j$. The region $V(\boldsymbol{x}_i)$ of a site $\boldsymbol{x}_i \in P$ is the intersection of half-spaces bounded by bisectors, therefore it is a 3-dimensional convex polyhedron (Figure 3.1). The boundary of $V(x_i)$ consists of *faces*, which are the convex polygons, *edges*, which are the intersections of the faces, and *vertices*, intersections of the edges.

Without loss of generality, hereafter we assume that P is in *general position* [1], that is, no 5 points lie on a common sphere and no 4 points are cocircular and on a common plane. This assumption implies that each face/edge/vertex is shared by exactly two/three/four Voronoi cells, respectively.

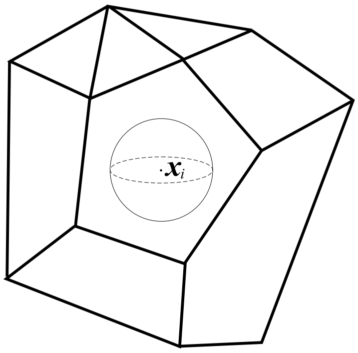


FIG. 3.1. *The Voronoi cell* $V(\boldsymbol{x}_i)$

Neighbors are defined to be the balls centered at sites whose Voronoi cells share a common face.

For a given array of the balls B_i centered at $\boldsymbol{x}_i$, $i = 1, \ldots, N$, the discrete network is the (Delaunay) graph $\mathcal{G} = (X, E)$, with vertices $X = \{\boldsymbol{x}_i : i = 1, \ldots, K, \ K \geq N\}$ and edges $E = \{e_{ij} : i, j = 1, \ldots, K\}$, connecting each pair of *neighbors* (see Figure 3.2). In addition, if one of the Voronoi faces of some site $\boldsymbol{x}_k$ lies on the boundary of the domain Q, then we connect $\boldsymbol{x}_k$ with this boundary by perpendicular line segment $e_{kk''}$, obtaining new vertex $\boldsymbol{x}_{k''}$ on the boundary.

Note that $K \geq N$, where N is the number of inclusions, since the graph $\mathcal{G}$ contains extra vertices $\boldsymbol{x}_{k''}$.

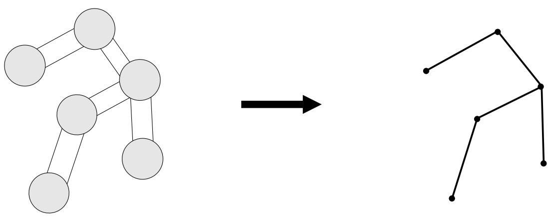


FIG. 3.2. *Balls and hoses are identified with the graph* $\mathcal{G}$

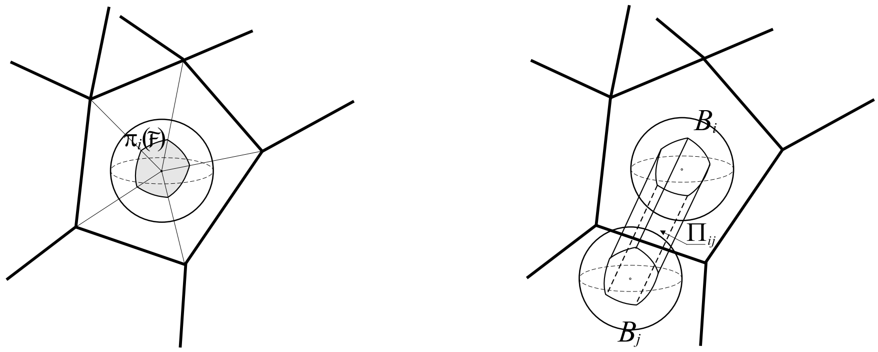
3.2. Central Projection Partition. The *central projection partition* is an elegant algorithm to decompose the domain Q into three types of solids: *hoses, prisms and tetrahedra*.

DEFINITION 3.1. *The central projection is the collection* $\{\pi_i, \, i = 1, \ldots, N\}$ *of maps* $\pi_i : \partial V(\boldsymbol{x}_i) \to \partial B_i$ *given by*

$$\pi_i(\boldsymbol{x}) = R \frac{\boldsymbol{x} - \boldsymbol{x}_i}{|\boldsymbol{x} - \boldsymbol{x}_i|}.$$

Every projection π_i partitions the sphere ∂B_i into non-overlapping curvilinear polygons $\{\pi_i(\mathcal{F})\}$, where $\mathcal{F}$ is a face of the Voronoi cell $V(\boldsymbol{x}_i)$.

For each Voronoi face $\mathcal{F}$ there are two projections $\pi_i(\mathcal{F})$ and $\pi_j(\mathcal{F})$ (one of them is depicted in Figure 3.3(a)) onto neighboring spheres ∂B_i and ∂B_j, respectively. These projections $\pi_i(\mathcal{F})$ and $\pi_j(\mathcal{F})$ are the (nonflat) bases of a *hose* Π_{ij} (Figure 3.3(b)), a (generalized) cylinder.

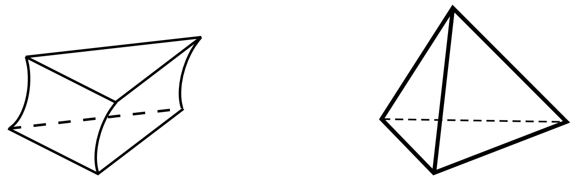


(a) $\pi_i(\mathcal{F})$, the projection of the Voronoi face $\mathcal{F}$

(b) The hose Π_{ij}

FIG. 3.3.

Similarly, the central projections of Voronoi edges and Voronoi vertices give rise to prisms and tetrahedra, respectively.



(a) the prism

(b) the tetrahedron

FIG. 3.4.

More specifically, for every Voronoi edge $\mathcal{E}$ there are three projections $\pi_i(\mathcal{E})$, $\pi_j(\mathcal{E})$ and $\pi_k(\mathcal{E})$, which are arcs on the spheres ∂B_i, ∂B_j and ∂B_k, respectively. Connecting the endpoints of the corresponding arcs, we obtain a figure, referred to as a *prism*, shown in Figure 3.4(a).

For every Voronoi vertex $\mathcal{V}$ there are four projections $\pi_i(\mathcal{V})$, $\pi_j(\mathcal{V})$, $\pi_k(\mathcal{V})$ and $\pi_m(\mathcal{V})$, which are four points on spheres ∂B_i, ∂B_j, ∂B_k and ∂B_m, respectively. These points being connected yield a *tetrahedron* (Figure 3.4(b)).

The introduced *central projection partition* of Q can alternatively be constructed using four pairwise neighbors. We give this alternative construction in Appendix 5.1.

For consistency of the presentation, we introduce a notion of a *quasi-ball*, when we construct the discrete network at the boundary. Suppose that three balls B_m, B_n, B_q, centered at $\boldsymbol{x}_m$, $\boldsymbol{x}_n$ and $\boldsymbol{x}_q$, respectively, lie near the upper boundary Q^+ (see Figure 3.5). In order to construct a hose connecting, for example, the ball B_m with Q^+, we consider the reflection $B_{m'}$, centered at $\boldsymbol{x}_{m'}$, of the ball B_m along the plane containing Q^+ and repeat the central projection construction for 4 neighbors B_m, B_n, B_q and $B_{m'}$. The intersection of the hose $\Pi_{mm'}$, connecting the balls B_m and $B_{m'}$, with the upper boundary Q^+ is a curvilinear polygon on Q^+, referred to as a *quasi-ball*. The quasi-ball is centered at the intersection of the line segment $e_{mm'}$, connecting $\boldsymbol{x}_m$ and $\boldsymbol{x}_{m'}$, and denoted by $\boldsymbol{x}_{m''}$. We assume that the quasi-ball has the radius equal to infinity. We assign $+1$ as the value of the potential on this quasi-ball,

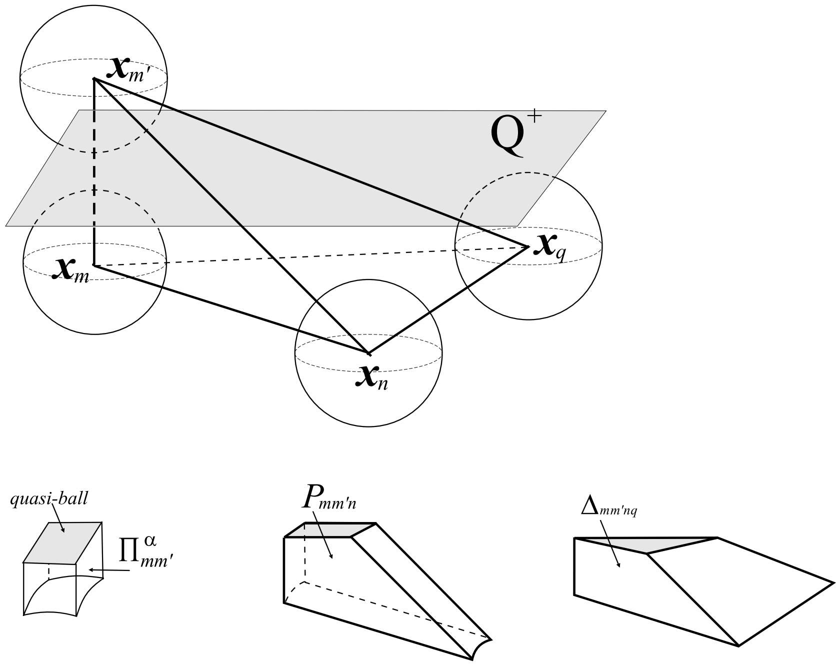


FIG. 3.5. *Construction near the upper boundary of Q*

because it lies on the upper boundary of the composite Q. Prisms $P_{mnm'}$, $P_{m'mq}$, $P_{m'nq}$ and tetrahedron $\Delta_{m'mnq}$ intersected with Q^+ yield the truncated prisms and tetrahedron (which can be obtained by an auxiliary constriction [5]), that we still call the prisms and tetrahedron respectively, with the values +1 of the potential on their upper boundaries (such a tetrahedron and one of the prisms are shown in Figure 3.5). The constructions of the quasi-balls on other boundaries of Q are analogous.

3.3. Discrete minimization problem. Using the central projection partition of the matrix Q, it is possible to decompose the value of $\widehat{A}$ (2.6) into the sum of the Dirichlet's integrals over hoses, prisms and tetrahedra, that is

$$\widehat{A} = \frac{1}{8L_1L_2}\left(\sum_{\Pi_{ij}}\int_{\Pi_{ij}}|\nabla u|^2 d\mathbf{x} + \sum_{P_{ijk}}\int_{P_{ijk}}|\nabla u|^2 d\mathbf{x} + \sum_{\Delta_{ijkm}}\int_{\Delta_{ijkm}}|\nabla u|^2 d\mathbf{x}\right).$$

The asymptotic derivation of the discrete minimization problem consists of three main observations.

First, since [4, 5]:

$$\begin{aligned} \sum_{P_{ijk}}\int_{P_{ijk}}|\nabla u|^2 d\mathbf{x} &\ll \sum_{\Pi_{ij}}\int_{\Pi_{ij}}|\nabla u|^2 d\mathbf{x}, \\ \sum_{\Delta_{ijkm}}\int_{\Delta_{ijkm}}|\nabla u|^2 d\mathbf{x} &\ll \sum_{\Pi_{ij}}\int_{\Pi_{ij}}|\nabla u|^2 d\mathbf{x}, \end{aligned} \tag{3.3}$$

then the total Dirichlet integral is approximately integral over the hoses:

$$\widehat{A} \sim \frac{1}{8L_1L_2}\sum_{\Pi_{ij}}\int_{\Pi_{ij}}|\nabla u|^2 d\mathbf{x}. \tag{3.4}$$

Second, inside the hoses the potential u is well approximated by the linear interpolation [4, 5, 9] between the values of the potentials on the neighboring balls B_i and B_j. Therefore the local flux in the hose Π_{ij} is

$$\nabla u = \left(0,\ 0,\ \frac{t_i - t_j}{H_{ij}(x,\, y)}\right), \tag{3.5}$$

where

$$H_{ij}(x,\, y) = \begin{cases} |\boldsymbol{x}_i - \boldsymbol{x}_j| - 2\sqrt{R^2 - x^2 - y^2}, & \text{when both } \boldsymbol{x}_i \text{ and } \boldsymbol{x}_j \text{ is a ball,} \\ |\boldsymbol{x}_i - \boldsymbol{x}_j| - \sqrt{R^2 - x^2 - y^2}, & \text{one of } \boldsymbol{x}_i,\ \boldsymbol{x}_j \text{ is a quasi-ball,} \end{cases} \tag{3.6}$$

is the distance between the inclusions and $|\boldsymbol{x}_i - \boldsymbol{x}_j|$ is the Euclidean distance between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. Hence,

$$\int_{\Pi_{ij}} |\nabla u|^2 d\mathbf{x} = (t_i - t_j)^2 \int_{\Pi_{ij}} \frac{d\mathbf{x}}{H_{ij}^2} = g_{ij}(t_i - t_j)^2, \tag{3.7}$$

where the specific flux g_{ij} in the hose Π_{ij} is defined by

$$g_{ij} = \int_{\Pi_{ij}} \frac{d\mathbf{x}}{H_{ij}^2} = \int_{\pi_i(\mathcal{F})} \frac{dxdy}{H_{ij}(x,\, y)}, \tag{3.8}$$

and $\pi_i(\mathcal{F})$ is the base of the common Voronoi face of two sites $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ lying on the sphere ∂B_i (shown in Figure 3.3).

Finally, the specific fluxes g_{ij} are asymptotically large [9] when inclusions B_i and B_j are close to touching:

$$g_{ij} = -\pi R \ln \delta_{ij} + O(1), \quad \text{as} \quad \delta_{ij} \to 0, \tag{3.9}$$

where the *relative interparticle distance* is a dimensionless parameter given by

$$\delta_{ij} = \begin{cases} \frac{|\boldsymbol{x}_i - \boldsymbol{x}_j|}{R} - 2, & \text{when both } \boldsymbol{x}_i \text{ and } \boldsymbol{x}_j \text{ is a center of the ball,} \\ \frac{|\boldsymbol{x}_i - \boldsymbol{x}_j|}{R} - 1, & \text{one of } \boldsymbol{x}_i,\ \boldsymbol{x}_j \text{ is a quasi-ball.} \end{cases} \tag{3.10}$$

Combining (3.3), (3.7), (3.8), (3.9) we have

$$\widehat{A} \sim \frac{1}{8L_1L_2} \sum_{\Pi_{ij}} g_{ij}(t_i - t_j)^2.$$

This asymptotic derivation, however, does not imply

$$\widehat{A}\ \sim\ \frac{1}{8L_1L_2} \min_{(\tilde{t}_1,\ldots,\tilde{t}_N)} \sum_{\Pi_{ij}} g_{ij}(\tilde{t}_i - \tilde{t}_j)^2, \tag{3.11}$$

because $\bar{\mathbf{t}} = (\bar{t_1}, \ldots, \bar{t_N})$, the minimizer of the quadratic form

$$\mathcal{I}(\tilde{\mathbf{t}}) = \frac{1}{8L_1L_2} \sum_{\Pi_{ij}} g_{ij}(\tilde{t}_i - \tilde{t}_j)^2 \tag{3.12}$$

with $\tilde{\mathbf{t}} = (\tilde{t}_1, ..., \tilde{t}_N)$ and appropriate boundary conditions (defined below), may be different from the values $t_1, \ldots, t_N$ of the potentials on the balls $B_1, \ldots, B_N$, defined by (2.5). The value of $\mathcal{I}(\bar{\mathbf{t}})$ (3.12), defined on the minimizer $\bar{\mathbf{t}} = (\bar{t}_1, ..., \bar{t}_N)$,

$$\mathcal{I}(\bar{\mathbf{t}}) = \min_{\tilde{\mathbf{t}}} \mathcal{I}(\tilde{\mathbf{t}}) \tag{3.13}$$

is called [4, 5] the *energy of the discrete system.*

To prescribe the boundary condition for the discrete network approximation on the horizontal boundaries we consider sets $S^{\pm}$ of the centers of the balls that cross or touch boundaries $Q^{\pm}$ and quasi-balls lying on $Q^{\pm}$. Then we define the values of the discrete potentials $\widetilde{t}_i$ on $S^{\pm}$ by

$$\widetilde{t}_i = \pm 1, \quad \text{when } \boldsymbol{x}_i \in S^{\pm}. \tag{3.14}$$

Then the set $\mathbb{I}$ of the "interior" sites of the discrete system is defined by $\mathbb{I} = \{\boldsymbol{x}_i,\ i = 1, \dots N\} \setminus \{S^+ \cup S^-\}$.

If $\boldsymbol{x}_{i''} \notin \mathbb{I} \cup (S^- \cup S^+)$, then it is a center of a quasi-ball that lies on the lateral boundary Q_{lat}. The set of such vertices is denoted by S_{lat}. For $\boldsymbol{x}_{i''} \in S_{lat}$ we assign the value of the discrete potential equal to the potential of the site $\boldsymbol{x}_i$ connected with $\boldsymbol{x}_{i''}$ by the edge $e_{i''i}$:

$$\widetilde{t}_{i''} = \widetilde{t}_i, \quad \text{for } \boldsymbol{x}_{i''} \in S_{lat},\ \boldsymbol{x}_i \in \mathbb{I}. \tag{3.15}$$

We comment that the potentials $t_{i''}$ for $\boldsymbol{x}_{i''} \in S_{lat}$ do not participate in (3.11) and can be found after the solving the problem by using the equality (3.15). Note that the lateral boundary condition (2.5e) for the discrete network can be interpreted as follows:

$$\sum_{\Pi_{i''j}, i''\, fixed} g_{i''j}(t_{i''} - t_j) = g_{i''i}(t_{i''} - t_i) = 0, \quad \text{for } \boldsymbol{x}_i \in S_{lat}. \tag{3.16}$$

Let us define the discrete fluxes through the boundaries S^+ and S^- in the following way:

$$P^+ = \sum_{\Pi_{ij},\ \boldsymbol{x}_i \in S^+} g_{ij}(t_i - t_j); \quad P^- = \sum_{\Pi_{ij},\ \boldsymbol{x}_i \in S^-} g_{ij}(t_i - t_j). \tag{3.17}$$

Then similarly to (2.8) we have

$$\mathcal{I}(\mathbf{t}) = \frac{1}{8L_1L_2} \sum_{\Pi_{ij}} g_{ij}(t_i - t_j)^2 = \frac{1}{8L_1L_2} \left(P^+ - P^- \right). \tag{3.18}$$

The derivation of (3.18) is similar to the one in the planar case in [5].

3.4. Properties of the Discrete Network. Here we collect some properties of the discrete network approximation, which we use for our variational error estimates. Since the effective conductivity $\widehat{A}$ is approximated by the fluxes in the hoses between closely spaced inclusions (3.4), we define a notion of a δ-subgraph that corresponds to some collection of the densely packed balls in the composite. Then we introduce a so-called *δ-$\mathcal{D}$ partition* $\{\Lambda_\delta\}$ of Q into polyhedra with δ-short edges and triangles as faces. The error estimates of our discrete network approximation are determined in terms of these characteristic parameters δ and $\mathcal{D}$.

The discrete minimization problem (3.13)-(3.15) amounts to solving a linear algebraic system whose solutions are the discrete potentials t_i at the interior vertices as indicated in the following lemma.

LEMMA 3.2. *There is a unique solution* $\mathbf{t} = \{t_i : \boldsymbol{x}_i \in \mathbb{I}\}$ *to the discrete minimization problem* (3.13)-(3.15)*, which satisfies the discrete Euler-Lagrange equations:*

$$\sum_{\Pi_{ij}, i\, fixed} g_{ij}(t_i - t_j) = 0, \quad \textit{for fixed } \boldsymbol{x}_i \in \mathbb{I}. \tag{3.19}$$

For any graph $\mathcal{G}$ and $\delta > 0$ we obtain the *δ-subgraph* $\mathcal{G}_\delta$ by discarding edges e_{ij} if the corresponding $\delta_{ij} > \delta$. For given $\delta > 0$ consider the set of *small* triangles such that *all* their edges belong to the δ-subgraph $\mathcal{G}_\delta$:

$$\{\text{ triangle } \boldsymbol{x}_i \boldsymbol{x}_j \boldsymbol{x}_k : e_{ij}, e_{jk}, e_{ki}, \in \mathcal{G}_\delta \} \tag{3.20}$$

We say that δ-subgraph $\mathcal{G}_\delta$ induces δ-$\mathcal{D}$ partition $\{\Lambda_\delta\}$ of Y if for any two vertices $\boldsymbol{x}_i, \boldsymbol{x}_j \in \mathcal{G}$, satisfying $|\boldsymbol{x}_i - \boldsymbol{x}_j| > \mathcal{D}R$, any path in $\mathcal{G}$ connecting them contains at least one vertex of the subgraph $\mathcal{G}_\delta$. The partition $\{\Lambda_\delta\}$ is the set of non-overlapping δ-polyhedra Λ_δ which are three dimension solids, whose boundary consists of small triangles (3.20). Loosely speaking, the number $\mathcal{D}$ is the *relative diameter* of "holes" in the composite.

Definition 3.3. *The distribution of balls is δ-$\mathcal{D}$ connected if there exists the δ-$\mathcal{D}$ partition $\{\Lambda_\delta\}$ of Y.*

The main use of the δ-$\mathcal{D}$ partition is the following maximum principle.

Lemma 3.4. *(The Discrete Maximum Principle).*
Suppose $\mathbf{t} = \{t_1, t_2, \ldots, t_M\}$ is the solution to the discrete problem (3.19). Denote by

$$t_{max} = \max_{\boldsymbol{x}_i \in \partial\Lambda_\delta} t_i, \quad t_{min} = \min_{\boldsymbol{x}_i \in \partial\Lambda_\delta} t_i \tag{3.21}$$

are the maximal and minimal values of the potential on the boundary of any δ-polyhedron Λ_δ. Then the value of the potential t_k at any vertex $\boldsymbol{x}_k$ in the interior of this δ-polyhedron: $\boldsymbol{x}_k \in \Lambda_\delta$, is bounded as

$$t_{min} \le t_k \le t_{max}.$$

The proofs of Lemmas 3.2 and 3.4 are identical to 2D case [5].

An immediate consequence of the maximum principle is a bound on the potential difference of the vertices inside Λ_δ in terms of the potentials of the vertices on $\partial\Lambda_\delta$.

Lemma 3.5. *Suppose Λ_δ is any δ-polyhedron of the δ-$\mathcal{D}$ partition. For any vertices $\boldsymbol{x}_k, \boldsymbol{x}_l \in Int\Lambda_\delta$ the values of the potential on them are bounded as follows:*

$$(t_k - t_l)^2 \le \frac{\mathcal{D}^3}{4} \sum_{\Pi_{ij} \in \partial\Lambda_\delta} (t_i - t_j)^2. \tag{3.22}$$

Proof. The formula (3.22) can be proved by applying the discrete maximum principle (3.21) and the triangle inequality for the values t_i on $\boldsymbol{x}_i \in \Lambda_\delta$:

$$(t_k - t_l)^2 \le (t_{max} - t_{min})^2 \le n \sum_{\Pi_{ij} \in \partial\Lambda_\delta} (t_i - t_j)^2,$$

where n is the number of the vertices of $\partial\Lambda_\delta$. This number is less than the number M of balls of radius R that can be placed inside the sphere of radius $\mathcal{D}R$. The number M is bounded by $M \le \dfrac{\mathcal{D}^3}{4}$. Hence, we obtain (3.22). □

The numbers of the hoses, prisms and tetrahedra inside any Λ_δ of δ-$\mathcal{D}$ partition of Y can be bounded in terms of the parameter $\mathcal{D}$ as follows.

Lemma 3.6. *For any Λ_δ of the δ-$\mathcal{D}$ partition of Y the number of tetrahedra $\#\triangle_{\Lambda_\delta}$, the number of prisms $\#P_{\Lambda_\delta}$, the number of hoses $\#\Pi_{\Lambda_\delta}$ in Λ_δ satisfy:*

$$\begin{aligned} (a) &\quad \#\triangle_{\Lambda_\delta} \le K_1 \mathcal{D}^3, \\ (b) &\quad \#P_{\Lambda_\delta} \le K_2 \mathcal{D}^3, \\ (c) &\quad \#\Pi_{\Lambda_\delta} \le K_3 \mathcal{D}^3. \end{aligned} \tag{3.23}$$

where constants K_i, $i = 1, 2, 3$, *are universal.*

The derivation of (3.23) and the values of the corresponding constants can be found in Appendix 5.2.

4. Variational Error Estimates. Our approach to variational error estimates is to construct trial fields for (2.12), that give rise to tight upper and lower bounds (constructed in subsections 4.1 and 4.2, respectively), when inclusions are close to touching. For both lower and upper bounds in (2.12) the trial functions $u \in V$ and $\boldsymbol{v} \in W$ are constructed in the hoses, prisms and tetrahedra determined by the central projection partition of the matrix Q. The piecewise-differentiable trial function $u \in V$ is chosen so that it takes values ± 1 on $Q^{\pm}$, linear in the hose, by the linear interpolation in the tetrahedron, and by linear interpolation for every cross-section of the prism. The trial field $\boldsymbol{v} \in W$ is chosen so that it is equal to the zero everywhere except in the hoses. In the hoses it is equal to the local flux defined by (3.5), where t_i are determined as solutions of the discrete minimization problem (3.13)-(3.15).

Our goal is to investigate when the discrete energy $\mathcal{I}$ (3.13) is a *good* approximation for $\widehat{A}$. For this purpose in the subsection 4.3 the difference between upper and lower bounds is estimated in terms of the parameters δ, $\mathcal{D}$ and $\mathcal{I}$, and the error is obtained.

4.1. Lower Bound. The construction, derivation and justification of the lower bound is identical to [5], where the technical details of this construction can be found.

THEOREM 4.1. *The lower bound on the effective conductivity* $\widehat{A}$ *is given by*

$$\mathcal{I}(\mathbf{t}) \leq \widehat{A} \tag{4.1}$$

where $\mathcal{I}(\mathbf{t})$ *is defined by* (3.13), $\mathbf{t} = (t_1, \dots t_N)$ *are the solutions of the minimization problem* (3.13)-(3.15) *(or equivalently* (3.19)*) and the specific fluxes* g_{ij} *are defined by* (3.8).

Proof. Consider two neighboring balls B_i and B_j centered at $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$, and values of the potentials t_i and t_j, respectively. The hose Π_{ij} connects them. We choose

$$\boldsymbol{v} = \boldsymbol{v}_{ij} = \begin{cases} \left(0, \, 0, \, \frac{t_i - t_j}{H_{ij}(x, y)}\right), & \text{in } \Pi_{ij}; \\ (0, \, 0, \, 0), & \text{otherwise,} \end{cases} \tag{4.2}$$

where the distance between two neighboring balls $H_{ij}(x, y)$ is defined by (3.6). Note that this function is divergence-free since its normal components match along the discontinuity. The potentials t_i and t_j on the balls B_i and B_j satisfy the linear system (3.19). Then the integral condition $\displaystyle\int_{\partial B_i} \boldsymbol{v} \cdot \boldsymbol{n} \, d\boldsymbol{x} = 0$, in the definition of the class W, satisfied. So $\boldsymbol{v} \in W$.

Now we calculate $J[\boldsymbol{v}]$ defined by (2.10). First, evaluate the integral

$$-\frac{1}{2} \int_Q \boldsymbol{v}^2 d\boldsymbol{x} = \sum_{\Pi_{ij}} g_{ij} (t_i - t_j)^2$$

by the definition of the specific flux g_{ij} and by the choice of the function $\boldsymbol{v}$. Also we note that the fluxes through the boundaries $\{z = \pm 1\}$ are equal to the discrete fluxes $P^{\pm}$ defined by (3.17). Then

$$J[\boldsymbol{v}] = \frac{1}{8L_1L_2} \left(-\frac{1}{2} \int_Q \boldsymbol{v}^2 d\boldsymbol{x} + \frac{1}{2} \int_{\{z=1\}} \boldsymbol{v} \cdot \boldsymbol{n} \, d\mathbf{x} - \frac{1}{2} \int_{\{z=-1\}} \boldsymbol{v} \cdot \boldsymbol{n} \, d\mathbf{x} \right)$$

$$= \frac{1}{8L_1L_2}\sum_{\Pi_{ij}} g_{ij}(t_i-t_j)^2 + \frac{1}{4L_1L_2}(P^+ - P^-) = \mathcal{I}(\mathbf{t}).$$

Then from (2.12) we obtain (4.1). □

4.2. Upper Bound. The upper bound on the effective conductivity is given by the following theorem.

THEOREM 4.2. *For any* δ-$\mathcal{D}$ *connected distribution of the balls the upper bound on the effective conductivity* $\widehat{A}$ *is*

$$\widehat{A} \le \mathcal{I}(\mathbf{t}) + \boldsymbol{C}R\sum_{\Pi_{ij}}(t_i-t_j)^2 \tag{4.3}$$

where $\mathbf{t} = (t_1, \ldots, t_N)$ *is the solution to the discrete minimization problem* (3.13)-(3.15)*, and the constant* $\boldsymbol{C}$ *depends on the relative diameter* $\mathcal{D}$ *only:*

$$\boldsymbol{C} \le C_0\mathcal{D}^3.$$

The proof of this theorem relies on the following more general variational upper bound given by Lemma 4.3. In Finite Element Methods [11] for a given distributions of points $\boldsymbol{x}_i$ and the Delaunay tetrahedralization $\{T\}$ the quotient $\frac{\rho}{l}$, where ρ is the circumradius and l is the length of the shortest edge of the tetrahedron T is called a mesh quality measure. We use here a parameter

$$\gamma = \max_{T\in\{T\}} \frac{\rho}{l} \tag{4.4}$$

to measure the regularity of our (Delaunay) graph $\mathcal{G}$ or, equivalently, the Delaunay tetrahedralization $\{T\}$ induced by $\mathcal{G}$.

LEMMA 4.3. *For any distribution of the balls the upper bound on the effective conductivity* $\widehat{A}$ *is*

$$\widehat{A} \le \frac{1}{8L_1L_2}\sum_{T\subset Y}\Bigg(\sum_{\Pi_{ij}\subset T}\left[g_{ij} + 2\pi R\ln 2\gamma + 4\pi R\left(1-\frac{1}{2\gamma}\right)\right](t_i-t_j)^2 + \sum_{P_{ijk}\subset T} 4R\gamma\left\{(t_i-t_j)^2+(t_i-t_k)^2\right\} + \sum_{\triangle_{ijkm}\subset T}\frac{1}{2}\pi^2\gamma^3\rho R\left\{(t_i-t_m)^2+(t_j-t_m)^2+(t_k-t_m)^2\right\}\Bigg) \tag{4.5}$$

where γ *is the the measure of regularity of* $\mathcal{G}$*, given by* (4.4)*, and* ρ *is the circumradius of the tetrahedron* T.

Note that inside every tetrahedron $T \subset Y$ there are four hoses, three prisms and one tetrahedron (that is, the last sum in (4.3) contains only one term).

Estimates in the prisms and tetrahedra near boundary require an auxiliary construction [5]. For clarity of presentation we omit this construction here.

Proof of Lemma 4.3. The trial function $u \in V$ is piecewise differentiable. Its construction will be done in the hose Π_{ij}, prism P_{ijk} and tetrahedron $\triangle_{ijkm}$.

First, let us consider the hose Π_{ij}. We choose the local coordinate system so the z-axis is directed along the edge connecting two neighbors, as shown in Figure 4.1

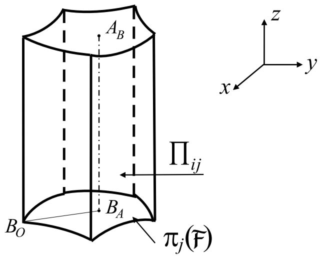


FIG. 4.1. *The hose* Π_{ij}

(points A_B and B_A are the points of the intersection of the line segment connecting two centers $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ with the spheres ∂B_i and ∂B_j, respectively).

We take a trial function u in Π_{ij} to be linear in z, inversely proportional the distance $H_{ij}(x, y)$, defined by (3.6), so that u takes values t_i and t_j on the spheres ∂B_i and ∂B_j, respectively. Then in the hose Π_{ij}

$$u(\boldsymbol{x}) = u(x, y, z) = \frac{t_i - t_j}{H_{ij}(x, y)} z + \frac{t_i + t_j}{2}, \quad z \in \left(-\frac{H_{ij}(x, y)}{2}, \frac{H_{ij}(x, y)}{2} \right) \tag{4.6}$$

Then the Dirichlet integral of the function u defined by (4.6) over the hose Π_{ij} is bounded (see details in Appendix 5.3, Lemma 5.2) as follows:

$$\int_{\Pi_{ij}} |\nabla u|^2 d\boldsymbol{x} \leq \left\{ g_{ij} + \left(-2\pi R \ln \left(\frac{l}{2\rho} \right) + 4\pi R \left(1 - \frac{l}{2\rho} \right) \right) \right\} (t_i - t_j)^2, \tag{4.7}$$

where ρ is the circumradius, l is the length of the shortest edge of T and $\dfrac{\rho}{l} = \gamma$.

Next we construct the trial function u in the prism P_{ijk}. Consider the prism $P_{ijk} = A'B'C'C''B''A''$ shown in Figure 4.2. We choose the local coordinate system so that the triangle $\triangle A'B'C'$ lies on the xz plane and the y-axis is directed along the altitude of this prism (Figure 4.2).

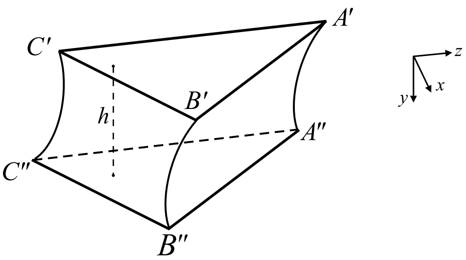


FIG. 4.2. *The prism* $P_{ijk} = A'B'C'C''B''A''$

The trial function u is linear between triangles $\triangle A'B'C'$ and $\triangle A''B''C''$, taking values t_i, t_j, t_k on arcs $A'A''$, $B'B''$, $C'C''$, respectively. Let h be the length of the altitude of the prism $A'B'C'C''B''A''$: $h \leq 2R$. Note that for such a choice of the coordinate system for some $y = y_0 \in (0, h)$: $u(x, y_0, z_1) = u(x_2, y_0, z_2)$, $\forall x_1, x_2, z_1, z_2$. Then

$$\int_{P_{ijk}} |\nabla u|^2 d\boldsymbol{x} \leq \int_0^h dy \int_{\triangle A'B'C'} |\nabla u|^2 \, dxdz \leq 2R \int_{\triangle A'B'C'} |\nabla u|^2 \, dxdz \tag{4.8}$$

For construction of the gradient of u in the triangle $\triangle A'B'C'$ we use the procedure offered in [5], which yields the following bound:

$$\int_{P_{ijk}} |\nabla u|^2 d\boldsymbol{x} \leq \frac{2R}{\sin\theta}\left\{(t_i - t_j)^2 + (t_i - t_k)^2\right\}, \tag{4.9}$$

where $\theta = \angle BAC$ is the smallest angle in the triangle $\triangle A'B'C'$ $\left(\theta \leq \frac{\pi}{3}\right)$.

The right hand side of the formula (4.9) can be expressed in terms of the quotient $\frac{\rho}{l}$ as follows:

$$\sin\theta \geq \frac{l}{2\rho}. \tag{4.10}$$

(see details in Appendix 5.4).

Now from (4.9) and (4.10) we obtain the following estimation in the prism P_{ijk}:

$$\int_{P_{ijk}} |\nabla u|^2 d\boldsymbol{x} \leq 4R\frac{\rho}{l}\left\{(t_i - t_j)^2 + (t_i - t_k)^2\right\}. \tag{4.11}$$

Finally, we construct the trial function u in the tetrahedron $\triangle_{ijkm} = A'B'C'D'$. Inside of the tetrahedron the trial function u is a linear function, taking values t_i, t_j, t_k and t_m at the points A', B', C' and D' respectively. The Dirichlet integral of such a function over $\triangle_{ijkm}$ is bounded as follows:

$$\int_{\triangle_{ijkm}} |\nabla u|^2 d\boldsymbol{x} \leq \frac{1}{2}\frac{\pi^2\rho^4}{l^3}\left\{(t_i - t_m)^2 + (t_j - t_m)^2 + (t_k - t_m)^2\right\}. \tag{4.12}$$

(for the details of the construction of u and evaluation its Dirichlet integral see Appendix 5.5, Lemma 5.3).

Thus the estimates (4.7), (4.11) and (4.12) yield (4.3).

□

Now we prove Theorem 4.2 using the above lemma.

Proof of Theorem 4.2. The key observation here is that all constants in (4.5), depending on the radius R of inclusions and the parameter γ, can be expressed in terms of $\mathcal{D}$ only. First, we note that for any tetrahedron T the length of its shortest edge l is greater than $2R$: $l > 2R$. Note that the circumsphere of any T does not contain vertices of other tetrahedra, and by the definition 3.3 the diameter 2ρ of this circumsphere is bounded as follows: $2\rho \leq \mathcal{D}R$. Then we obtain $\gamma < \frac{\mathcal{D}}{4}$. Thus, every constant in (4.5) is bounded from above by some constant depending on $\mathcal{D}$ which is a multiple of the radius of the inclusion R:

$$C_1 := 2\pi R\ln(2\gamma) + 4\pi R\left(1 - \frac{1}{2\gamma}\right) \leq C^{11}R\ln\mathcal{D} + C^{12}R\left(1 - \frac{2}{\mathcal{D}}\right),$$
$$C_2 := 4R\gamma \leq C^2 R\mathcal{D},$$
$$C_3 := \frac{1}{2}\gamma^3\pi^2\rho \leq C^3 R\mathcal{D}^3.$$

All four constants C^{11}, C^{12}, C^2 and C^3 are bounded by $C_0\mathcal{D}^3$. Hence, we have (4.3). □

4.3. Error Estimate. Here we give two theorems. Theorem 4.4 is about the leading term of the asymptotics of the effective conductivity $\widehat{A}$ as $\delta \to 0$. This leading term is defined by the discrete energy $\mathcal{I}$ (3.13) which is of order $\ln\delta$ for small δ. In Theorem 4.5 we obtain the relative error of approximation of the effective conductivity by the discrete energy (3.13) provided that the discrete network approximating the continuum problem is δ-$\mathcal{D}$ connected (definition 3.3).

We assume that there exists at least one *δ-path* connecting the upper boundary Q^+ with the lower boundary Q^-, where the δ-path is a path such that the maximum relative interparticle distance between balls centered at its vertices is bounded by δ. Then the following theorem holds.

THEOREM 4.4. *If there exists at least one δ-path connecting the upper and lower boundaries of Q then the effective conductivity $\widehat{A}$ (2.6)*

$$\widehat{A} = \frac{1}{8L_1L_2}\int_Q |\nabla u|^2 d\boldsymbol{x}.$$

satisfies the following inequality:

$$|\widehat{A} - \mathcal{I}(\mathbf{t})| < C, \quad \mathcal{I}(\mathbf{t}) > K|\ln\delta|, \quad as \quad \delta \to 0, \tag{4.13}$$

where $(t_1,\dots,t_N)$ is a solution of the discrete minimization problem (3.19), g_{ij} are defined by (3.8)

$$g_{ij} = \int_{\Pi_{ij}} \frac{d\mathbf{x}}{H_{ij}^2} \sim -\pi R \ln\delta_{ij}, \quad as \quad \delta_{ij} \to 0,$$

The constant C in (4.13) depends on measure of regularity γ, the number of inclusions N, but independent of δ. The constant K in (4.13) depends on the number of inclusions N, the radius R and their locations, but not on δ.

Proof.

By Lemma 4.3 we obtain that

$$|\widehat{A} - \mathcal{I}(\mathbf{t})| \le \sum_{\Pi_{ij}} C(t_i - t_j)^2, \tag{4.14}$$

where the constant C depends on the measure of the regularity of the ball distribution γ. By the maximum principle we have $|t_i - t_j| \le 2$, for any i, j. Then from (4.14) we have

$$|\widehat{A} - \mathcal{I}(\mathbf{t})| \le 4NC(\gamma), \tag{4.15}$$

which yields the first inequality in (4.13).

In order to prove the second inequality (4.13) we assume that there is a δ-path connecting the upper and lower boundaries of the length k (the number of vertices in the path) and consider

$$\begin{aligned}\mathcal{I}(\mathbf{t}) &\ge -\pi \sum_{short\,\Pi_{ij}} R\ln\delta_{ij}(t_i - t_j)^2 \ge \pi R|\ln\delta| \sum_{short\,\Pi_{ij}} (t_i - t_j)^2 \\ &\ge \pi R|\ln\delta| \sum_{\delta-path} (t_i - t_j)^2 \ge \pi R|\ln\delta| \min_{\mathbf{t}} \sum_{\delta-path} (t_i - t_j)^2 \\ &\sim \pi R|\ln\delta|\frac{1}{k} > K|\ln\delta|.\end{aligned}$$

Hence, we obtain (4.14).
□

THEOREM 4.5. *If the discrete network $\mathcal{G}$ for the continuum problem* (2.1) *is δ-$\mathcal{D}$ connected the relative error for the effective conductivity $\widehat{A}$ is*

$$\frac{\left|\widehat{A}-\mathcal{I}(\mathbf{t})\right|}{\mathcal{I}(\mathbf{t})} \leq \frac{C\mathcal{D}^6}{\ln\delta}, \tag{4.16}$$

where $\mathcal{I}(\mathbf{t})$ is the discrete energy defined by (3.13).

Proof. The idea of the proof: we wish to "absorb" *all* the $O(1)$ terms in (4.3) as the "smaller order corrections" into $O(\ln\delta)$ the terms and derive an estimate

$$\mathcal{I}(\mathbf{t}) \leq \widehat{A} \leq \mathcal{I}(\mathbf{t}) + O(1) \leq \mathcal{I}(\mathbf{t})\left(1+\frac{C\mathcal{D}^6}{\ln\delta}\right). \tag{4.17}$$

Then 4.16 immediately follows from (4.17).

If the distributions of balls is δ-$\mathcal{D}$ connected then from Theorems 4.1 and 4.2 we obtain the following bounds on the effective conductivity:

$$\mathcal{I}(\mathbf{t}) \leq \widehat{A} \leq \frac{1}{8L_1L_2}\left(\sum_{\Pi_{ij}}(g_{ij}+C_1)(t_i-t_j)^2 + \sum_{P_{ijk}} C_2[(t_i-t_k)^2+(t_j-t_k)^2] + \sum_{\triangle_{ijkm}} C_3[(t_i-t_m)^2+(t_j-t_m)^2+(t_k-t_m)^2]\right).$$

Applying (3.22), (3.23) and then (3.9) we have:

$$\begin{aligned}\mathcal{I}(\mathbf{t}) \leq \frac{1}{8L_1L_2}\Bigg(&\sum_{\Pi_{ij}\notin\{\Lambda_\delta\}} g_{ij}(t_i-t_j)^2 + \sum_{\Pi_{ij}\in\{\Lambda_\delta\}} g_{ij}(t_i-t_j)^2 \\ &+ C_0\mathcal{D}^3R\Bigg[\sum_{\Pi_{ij}}(t_i-t_j)^2 + \sum_{P_{ijk}}[(t_i-t_k)^2+(t_j-t_k)^2] \\ &+ \sum_{\triangle_{ijkm}} C_3[(t_i-t_m)^2+(t_j-t_m)^2+(t_k-t_m)^2]\Bigg]\Bigg),\end{aligned} \tag{4.18}$$

where $\Pi_{ij} \in \{\Lambda_\delta\}$ means that we consider the hoses only in the δ-polyhedra of the δ-$\mathcal{D}$ partition of Y. Continuing (4.18) we obtain

$$\begin{aligned}\mathcal{I}(\mathbf{t}) &\leq \frac{1}{8L_1L_2}\Bigg(\sum_{\Pi_{ij}\notin\{\Lambda_\delta\}} g_{ij}(t_i-t_j)^2 + \sum_{\Pi_{ij}\in\{\Lambda_\delta\}} g_{ij}(t_i-t_j)^2 \\ &\quad + C_0\mathcal{D}^3R\frac{\mathcal{D}^3}{4}\left[\#\Pi_{\Lambda_\delta}+\#P_{\Lambda_\delta}+\#\triangle_{\Lambda_\delta}\right]\sum_{\Pi_{ij}}(t_i-t_j)^2\Bigg) \\ &\leq \frac{1}{8L_1L_2}\left(\sum_{\Pi_{ij}\notin\{\Lambda_\delta\}} g_{ij}(t_i-t_j)^2 + \sum_{\Pi_{ij}\in\{\Lambda_\delta\}} (g_{ij}+C\mathcal{D}^6R)(t_i-t_j)^2\right)\end{aligned}$$

$$\leq \frac{1}{8L_1L_2}\left[1+\frac{C\mathcal{D}^6}{\ln\delta}\right]\sum_{\Pi_{ij}} g_{ij}(t_i-t_j)^2 = \left[1+\frac{C\mathcal{D}^6}{\ln\delta}\right]\mathcal{I}(\mathbf{t}).$$

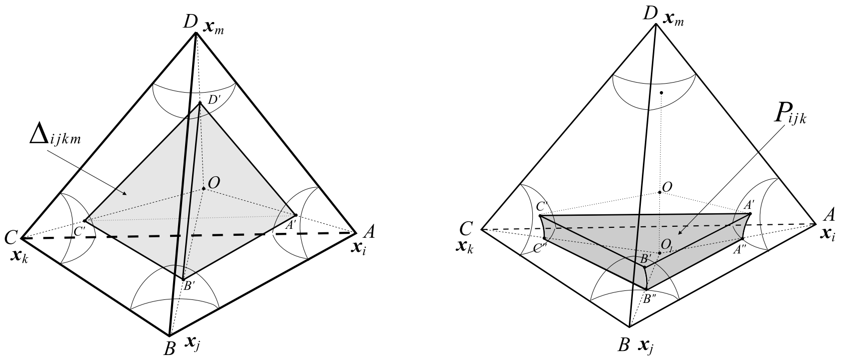
Hence, combining all the bounds we obtain (4.3):

$$\mathcal{I}(\mathbf{t}) \leq \widehat{A} \leq \left[1+\frac{C\mathcal{D}^6}{\ln\delta}\right]\mathcal{I}(\mathbf{t}).$$

□

5. Appendices.

5.1. Appendix A. Here we present an alternative construction of the hoses, prisms and tetrahedra using four pairwise neighbors $\boldsymbol{x}_i$, $\boldsymbol{x}_j$, $\boldsymbol{x}_k$ and $\boldsymbol{x}_m$, depicted in Figures 5.1, 5.2. The vertices $\boldsymbol{x}_i = A$, $\boldsymbol{x}_j = B$, $\boldsymbol{x}_k = C$ and $\boldsymbol{x}_m = D$ being connected form a tetrahedron $T = ABCD$. The point O is an intersection of the bisector planes to the edges of the tetrahedron. This point O is the Voronoi vertex $\mathcal{V}$. The projection of O on four corresponding spheres are $\pi_i(\mathcal{V}) = A'$, $\pi_j(\mathcal{V}) = B'$, $\pi_k(\mathcal{V}) = C'$ and $\pi_m(\mathcal{V}) = D'$. They form a tetrahedron $A'B'C'D'$ which is one of the tetrahedra in the central projection partition of the domain Q, denoted by Δ_{ijkm}.



(a) the tetrahedron $A'B'C'D'$ *(b) the prism $A'B'C'C''B''A''$*

FIG. 5.1. *The tetrahedron Δ_{ijkm} and the prism P_{ijk}*

Each prism contains two parts. To obtain one of them, for instance, the prism P_{ijk} between three neighbors centered at $\boldsymbol{x}_i$, $\boldsymbol{x}_j$, $\boldsymbol{x}_k$ (A, B, C) shown in Figure 5.1(b), we consider the Voronoi edge $\mathcal{E}$ that intersects $\triangle ABC$ at the point O_1. The line segment OO_1 is the part of $\mathcal{E}$, lying inside T. The arcs $A'A''$, $B'B''$ and $C'C''$ are the projections of OO_1 on the corresponding spheres ∂B_i, ∂B_j and ∂B_k. The figure $A'B'C'C''B''A''$ obtained is the part of the prism that lies inside of T.

Finally, to construct a hose, for example, Π_{ij} connecting two neighbors centered at $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ (A and B in Figure 5.2) we recall that they share a common Voronoi face $\mathcal{F}$. The part of this face lying inside the tetrahedron T being projected on these two spheres yields quadrilaterals $A'A''A'''A_B$ and $B'B''B'''B_A$ as projections. The solid between these two quadrilaterals, which is a generalized cylinder, is the part of the hose Π^{α}_{ij} connecting two neighbors B_i and B_j.

5.2. Appendix B. Here we estimate the number of the tetrahedra, prisms, hoses in the Λ_δ in terms of the parameter $\mathcal{D}$.

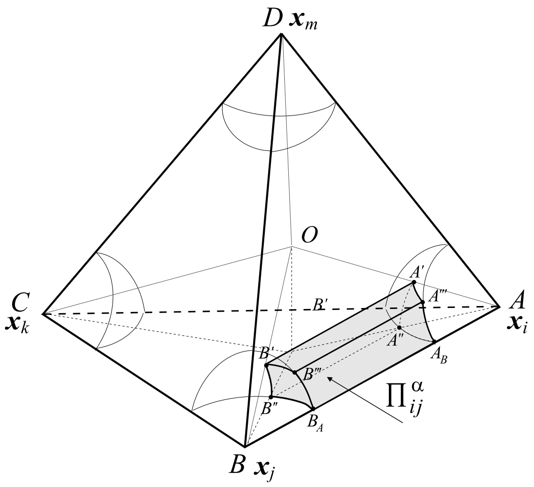


FIG. 5.2. *The part of the hose* $\Pi_{ij}^{\alpha} = A'A''A'''A_BB_AB'''B''B'$

LEMMA 5.1. *For any δ-polyhedron* Λ_δ *of δ-*$\mathcal{D}$ *partition of* Y *of the δ-subgraph* $\mathcal{G}_\delta$ *the number of tetrahedra* $\#\triangle_{\Lambda_\delta}$, *the number of prisms* $\#P_{\Lambda_\delta}$, *the number of hoses* $\#\Pi_{\Lambda_\delta}$ *in* $Int\,\Lambda_\delta$ *satisfy:*

$$\begin{aligned} (a) \quad & \#\triangle_{\Lambda_\delta} \le \frac{3}{2}\mathcal{D}^3, \\ (b) \quad & \#P_{\Lambda_\delta} \le 3\mathcal{D}^3, \\ (c) \quad & \#\Pi_{\Lambda_\delta} \le \frac{3}{2}\mathcal{D}^3. \end{aligned} \tag{5.1}$$

Proof.
By $3D$ Euler's formula:

$$\#\boldsymbol{x}_{\Lambda_\delta} - \#\Pi_{\Lambda_\delta} + \#P_{\Lambda_\delta} - \#\triangle_{\Lambda_\delta} = 1, \tag{5.2}$$

where $\#\boldsymbol{x}_{\Lambda_\delta}$ is the number of vertices $\boldsymbol{x}_i$ in Λ_δ. Since each tetrahedron has 4 faces and each face belongs to at most two tetrahedra we have the following bound:

$$\#P_{\Lambda_\delta} \ge 2\#\triangle_{\Lambda_\delta}.$$

Since each edge has 2 vertices and each vertex can belong to not more than 12 edges (due to the "kissing" number in $3D$ [6]) we obtain:

$$\#\boldsymbol{x}_{\Lambda_\delta} \ge \frac{\#\Pi_{\Lambda_\delta}}{6}.$$

From (5.2) we have

$$\#\boldsymbol{x}_{\Lambda_\delta} + \#P_{\Lambda_\delta} = \#\triangle_{\Lambda_\delta} + \#\Pi_{\Lambda_\delta} + 1 \le \frac{\#P_{\Lambda_\delta}}{2} + 6\#\boldsymbol{x}_{\Lambda_\delta} + 1.$$

which implies

$$\frac{\#P_{\Lambda_\delta}}{2} \ge 5\#\boldsymbol{x}_{\Lambda_\delta} + 1 < 6\#\boldsymbol{x}_{\Lambda_\delta}.$$

Thus, we obtain

$$\#\Pi_{\Lambda_\delta} \leq 6\#\boldsymbol{x}_{\Lambda_\delta}, \quad \#P_{\Lambda_\delta} \leq 12\#\boldsymbol{x}_{\Lambda_\delta}, \quad \#\triangle_{\Lambda_\delta} \leq 6\#\boldsymbol{x}_{\Lambda_\delta}.$$

The volume of Λ_δ is bounded from above by the volume of the ball of diameter $\mathcal{D}R$. Let M be the number of balls of radius R that can be placed into this ball. Then $\frac{4}{3}M\pi R^3 \leq \frac{\pi}{3}\mathcal{D}^3 R^3$, from which we find $\#\boldsymbol{x}_{\Lambda_\delta} \leq M \leq \frac{\mathcal{D}^3}{4}$. Then from above bounds on the number of tetrahedra, prisms and hoses we obtain (5.1). ☐

5.3. Appendix C. Here we give the estimates on the Dirichlet integral of the function u defined by (4.6).

LEMMA 5.2. *Let the function u be given by* (4.6). *Then the Dirichlet integral of this function over the hose Π_{ij} is bounded by*

$$\int_{\Pi_{ij}} |\nabla u|^2 d\boldsymbol{x} \leq \left\{ g_{ij} + \left(-2\pi R \ln\left(\frac{l}{2\rho}\right) + 4\pi R \left(1 - \frac{l}{2\rho}\right)\right)\right\}(t_i - t_j)^2. \tag{5.3}$$

Proof.

If u is given by (4.6) then its gradient is

$$\nabla u(\boldsymbol{x}) = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial u}{\partial z}\right) = (t_i - t_j)\left(-\frac{z(H_{ij})_x}{H_{ij}^2}, -\frac{z(H_{ij})_y}{H_{ij}^2}, \frac{1}{H_{ij}}\right) \tag{5.4}$$

We need to estimate the Dirichlet integral of u over the hose Π_{ij}. Let $\pi_j(\mathcal{F})$ be the lower base of the hose Π_{ij} (see Figure 4.1). Recall that the base of the hose is a convex curvilinear polygon (projection of the convex polygon on the sphere). Let S be the projection on the xy plane of the longest line segment connecting the point B_A with all the vertices of this curvilinear polygon, referred to as *half-width* of the hose (in Figure 4.1 the longest line segment connecting B_A with other vertices of $\pi_j(\mathcal{F})$ is B_AB_O, its projection on xy plane is equal to S). Then we obtain the following estimate:

$$\begin{aligned} &(t_i - t_j)^2 \int_{\Pi_{ij}} \left(\frac{\partial u}{\partial z}\right)^2 d\boldsymbol{x} = (t_i - t_j)^2 \int_{\Pi_{ij}} \frac{1}{(H_{ij})^2} d\boldsymbol{x} \\ &= (t_i - t_j)^2 \int_{\pi_j(\mathcal{F})} \frac{dx\,dy}{H_{ij}} \leq (t_i - t_j)^2 \int_{C_{ij}} \frac{dx\,dy}{H_{ij}} \end{aligned}$$

where C_{ij} is defined by

$$C_{ij} = \left\{(x, y) \in \mathbb{R}^2 : \ x^2 + y^2 \leq S^2\right\}. \tag{5.5}$$

Thus, using the formula (3.8), we obtain

$$(t_i - t_j)^2 \int_{\Pi_{ij}} \left(\frac{\partial u}{\partial z}\right)^2 d\boldsymbol{x} \leq g_{ij}(t_i - t_j)^2. \tag{5.6}$$

Next consider

$$(t_i - t_j)^2 \int_{\Pi_{ij}} \left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right] d\boldsymbol{x}$$

$$
\begin{aligned}
&= (t_i - t_j)^2 \left(\int_{\Pi_{ij}} \frac{z^2 (H_{ij})_x^2}{(H_{ij})^4} d\boldsymbol{x} + \int_{\Pi_{ij}} \frac{z^2 (H_{ij})_y^2}{(H_{ij})^4} d\boldsymbol{x} \right) \\
&\leq \frac{(t_i - t_j)^2}{4} \left(\int_{\pi_j(\mathcal{F})} \left[\frac{(H_{ij})_x^2}{H_{ij}} + \frac{(H_{ij})_y^2}{H_{ij}} \right] dx\, dy \right). \qquad (5.7)
\end{aligned}
$$

Here we used the fact that $z^2 \leq \dfrac{H_{ij}^2}{4}$ due to $z \in \left(-\dfrac{H_{ij}}{2}, \dfrac{H_{ij}}{2} \right)$.

Now look at

$$
(H_{ij})_x^2 = \frac{4x^2}{R^2 - x^2 - y^2},
$$

then

$$
\begin{aligned}
&\frac{(H_{ij})_x^2}{H_{ij}} = \frac{4x^2}{R^2 - x^2 - y^2} \frac{1}{\delta_{ij} + 2R - 2\sqrt{R^2 - x^2 - y^2}} \\
&\leq \frac{2x^2}{R^2 - x^2 - y^2} \frac{1}{R - \sqrt{R^2 - x^2 - y^2}} = \frac{2x^2}{R^2 - x^2 - y^2} \frac{R + \sqrt{R^2 - x^2 - y^2}}{x^2 + y^2}.
\end{aligned}
$$

Similarly, the estimation for $\dfrac{(H_{ij})_y^2}{H_{ij}}$ is obtained.

Thus, continuing (5.7), we have

$$
\begin{aligned}
&\frac{(t_i - t_j)^2}{4} \left(\int_{\pi_j(\mathcal{F})} \left[\frac{(H_{ij})_x^2}{H_{ij}} + \frac{(H_{ij})_y^2}{H_{ij}} \right] dx\, dy \right) \\
&\leq \frac{(t_i - t_j)^2}{4} \int_{\pi_j(\mathcal{F})} \frac{2x^2 + 2y^2}{R^2 - x^2 - y^2} \frac{R + \sqrt{R^2 - x^2 - y^2}}{x^2 + y^2} dx\, dy \\
&= \frac{(t_i - t_j)^2}{2} \int_{\pi_j(\mathcal{F})} \frac{R + \sqrt{R^2 - x^2 - y^2}}{R^2 - x^2 - y^2} dx\, dy.
\end{aligned}
$$

Similarly, we obtain that

$$
(t_i - t_j)^2 \int_{\Pi_{ij}} \left(\frac{\partial u}{\partial y} \right)^2 d\boldsymbol{x} \leq \frac{(t_i - t_j)^2}{2} \int_{\Pi_{ij}} \frac{y^2}{R^2 - x^2 - y^2} \frac{R + \sqrt{R^2 - x^2 - y^2}}{x^2 + y^2} dx\, dy.
$$

Hence

$$
\begin{aligned}
&(t_i - t_j)^2 \int_{\Pi_{ij}} \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right] d\boldsymbol{x} \leq \frac{(t_i - t_j)^2}{2} \int_{\pi_j(\mathcal{F})} \frac{R + \sqrt{R^2 - x^2 - y^2}}{R^2 - x^2 - y^2} dx\, dy \\
&\leq \frac{(t_i - t_j)^2}{2} \int_{C_{ij}} \frac{R + \sqrt{R^2 - x^2 - y^2}}{R^2 - x^2 - y^2} dx\, dy = 2\pi \int_0^S \frac{R + \sqrt{R^2 - r^2}}{R^2 - r^2} r\, dr \\
&= -\pi R \ln \left(1 - \frac{S^2}{R^2} \right) + 4\pi R \left(1 - \sqrt{1 - \frac{S^2}{R^2}} \right) \qquad (5.8)
\end{aligned}
$$

Let S be the length of the projection on the xy plane of the longest line segment connecting the point B_A with the vertices of the curvilinear quadrilateral, which is

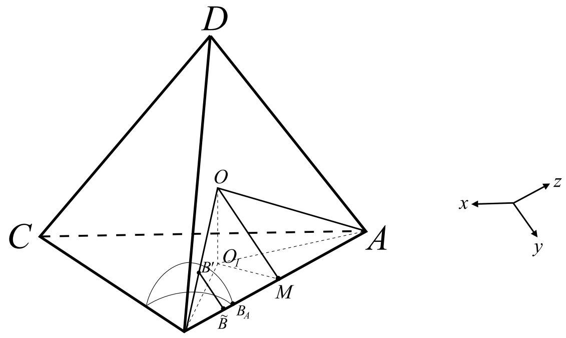


FIG. 5.3. *The construction in the triangle* $\triangle BB'\tilde{B}$

the base of the hose $\pi_j(\mathcal{F})$, see Figure 5.3 (recall that the z-axis is directed along AB). Then the projection $B'\tilde{B}$ of the line segment $B'B_A$ on the xy plane is less or equal than S. Denote the radius of the circumsphere of the tetrahedron $ABCD$ by ρ. Then in the triangle $\triangle BB'\tilde{B}$: $\rho = |BO| = \frac{|BM|}{\cos\angle OBM}$, where M is the middle-point of AB. From $\triangle BB'\tilde{B}$ we have:

$$|BB'| = R; \quad |B'\tilde{B}| \leq S; \quad \frac{S}{R} \leq \sin\angle OBM$$

then

$$\sqrt{1 - \frac{S^2}{R^2}} \geq \cos\angle OBM \geq \frac{|BM|}{\rho}.$$

Denote the length of the smallest edge of the tetrahedron $ABCD$ by l. Then $|BM| \geq \frac{l}{2}$.

Continuing (5.8), we obtain

$$-\pi R \ln\left(1 - \frac{S^2}{R^2}\right) + 4\pi R\left(1 - \sqrt{1 - \frac{S^2}{R^2}}\right) \leq -\pi R \ln\left(\frac{l^2}{4\rho^2}\right) + 4\pi R\left(1 - \frac{l}{2\rho}\right)$$

Hence

$$\int_{\Pi_{ij}} |\nabla u|^2 d\boldsymbol{x} \leq \left\{g_{ij} + 2\pi R \ln\left(\frac{2\rho}{l}\right) + 4\pi R\left(1 - \frac{l}{2\rho}\right)\right\}(t_i - t_j)^2. \qquad (5.9)$$

□

5.4. Appendix D. Here we prove the bound (4.10).

Proof. Denote by θ the smallest angle in the triangle $A'B'C'$ ($\angle C'A'B' = \theta$ in Figure 5.4). Let $\theta = \theta_1 + \theta_2 = \angle C'A'O_1 + \angle B'A'O_1$. Recall that the point O_1 is the point of the intersection of the bisectors of $\triangle A'B'C'$. Denote $\angle C'B'O_1$ by θ_3, then $\theta_1 + \theta_2 + \theta_3 = \frac{\pi}{2}$.

From $\triangle C'B'O_1$:

$$\cos\theta_3 = \sin(\theta_1 + \theta_2) = \sin\theta = \frac{|B'C'|}{2|B'O_1|}.$$

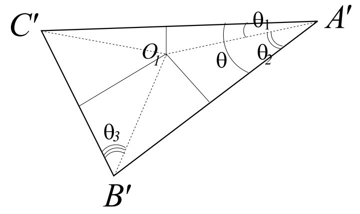


FIG. 5.4. *The triangle $A'B'C'$*

Note that $|B'O_1| \leq \rho$ then $\sin\theta \geq \dfrac{|B'C'|}{2\rho}$. Since $|B'C'| \geq l$, the formula (4.10) follows.

□

5.5. Appendix E. LEMMA 5.3. *Let four different points $\boldsymbol{A}_i$, $i = 1, \ldots, 4$ form a tetrahedron T. Let u be a linear function, taking values t_i at $\boldsymbol{A}_i$, respectively, $i = 1, \ldots, 4$. Then its Dirichlet integral over T is bounded as follows:*

$$\int_T |\nabla u|^2 d\boldsymbol{x} \leq \frac{1}{2}\frac{\pi^2\rho^4}{l^3}\left\{(t_1 - t_4)^2 + (t_2 - t_4)^2 + (t_3 - t_4)^2\right\}, \tag{5.10}$$

where ρ is the circumradius, and l is the length of the shortest edge of the tetrahedron T.

Proof. Consider the tetrahedron $T = \boldsymbol{A}_1\boldsymbol{A}_2\boldsymbol{A}_3\boldsymbol{A}_4$ (see Figure 5.5) with values of the potentials t_i at the point $\boldsymbol{A}_i$ $(i = 1, \ldots, 4)$. We choose the coordinate system so that the point $\boldsymbol{A}_4$ is the origin.

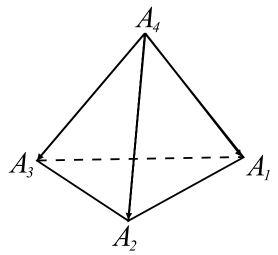


FIG. 5.5. *The tetrahedron T*

Inside the tetrahedron T the trial function $u(x, y, z)$ is linear, i.e. $u(x, y, z) = ax + by + cz + d$, where the constants a, b, c and d are to be determined. If we denote $\boldsymbol{K} = (a, b, c)$ and $\boldsymbol{X} = (x, y, z)$ then the function $u = \boldsymbol{K} \cdot \boldsymbol{X} + d$. Moreover, $u(\boldsymbol{A}_i) = t_i \Rightarrow d = t_4$, then

$$\boldsymbol{K} \cdot \boldsymbol{A}_i + t_4 = t_i, \text{ where } \boldsymbol{A}_i = (x_i, y_i, z_i),\ i = 1, 2, 3,$$

or if we denote

$$\tau_4 = 0; \quad \tau_i = t_i - t_4 \ (i = 1, 2, 3): \tag{5.11}$$

$$\boldsymbol{K} \cdot \boldsymbol{A}_i = \tau_i, \quad i = 1, 2, 3.$$

Let $\boldsymbol{B}_i = \dfrac{\boldsymbol{A}_i}{\tau_i}$ then

$$\boldsymbol{K} \cdot \boldsymbol{B}_i = 1, \quad i = 1,\, 2,\, 3. \tag{5.12}$$

which is the equation of the plane.

Then (5.12) implies that $\boldsymbol{K} \perp \boldsymbol{B}_i$, $i = 1, 2, 3$ and $\boldsymbol{K} \perp \boldsymbol{B}_1 - \boldsymbol{B}_2$, $\boldsymbol{K} \perp \boldsymbol{B}_2 - \boldsymbol{B}_3 \Rightarrow \boldsymbol{K} \| (\boldsymbol{B}_1 - \boldsymbol{B}_2) \times (\boldsymbol{B}_2 - \boldsymbol{B}_3)$ or

$$(\boldsymbol{B}_1 - \boldsymbol{B}_2) \times (\boldsymbol{B}_2 - \boldsymbol{B}_3) = \alpha \boldsymbol{K}, \tag{5.13}$$

where α is some constant to be determined. From the equation (5.13) we have

$$\boldsymbol{K} = \frac{\boldsymbol{B}_1 \times \boldsymbol{B}_2 + \boldsymbol{B}_2 \times \boldsymbol{B}_3 + \boldsymbol{B}_3 \times \boldsymbol{B}_1}{\alpha}. \tag{5.14}$$

Now substitute (5.14) into (5.12) for e.g. $i = 1$:

$$\boldsymbol{B}_1 \cdot \left(\frac{\boldsymbol{B}_1 \times \boldsymbol{B}_2 + \boldsymbol{B}_2 \times \boldsymbol{B}_3 + \boldsymbol{B}_3 \times \boldsymbol{B}_1}{\alpha} \right) = 1,$$

from what we conclude that

$$\alpha = \boldsymbol{B}_1 \cdot \boldsymbol{B}_2 \times \boldsymbol{B}_3 = \det [\boldsymbol{B}_1 \ \boldsymbol{B}_2 \ \boldsymbol{B}_3] =: \det \mathcal{B}. \tag{5.15}$$

Hence

$$\boldsymbol{K} = \frac{\boldsymbol{B}_1 \times \boldsymbol{B}_2 + \boldsymbol{B}_2 \times \boldsymbol{B}_3 + \boldsymbol{B}_3 \times \boldsymbol{B}_1}{\det \mathcal{B}} = (a,\, b,\, c). \tag{5.16}$$

Recall that our goal here is to calculate the Dirichlet integral of the function $u = \boldsymbol{K} \cdot \boldsymbol{X} + t_4$ over the tetrahedron T. Then we need to consider $\nabla u = \boldsymbol{K}^2$. Taking into account that

$$\det \mathcal{B} = \frac{1}{\tau_1 \tau_2 \tau_3} \det [\boldsymbol{A}_1 \ \boldsymbol{A}_2 \ \boldsymbol{A}_3] = \frac{1}{\tau_1 \tau_2 \tau_3} \det \mathcal{A}$$

we obtain

$$\boldsymbol{K}^2 = \frac{\left| \frac{1}{\tau_1 \tau_2} (\boldsymbol{A}_1 \times \boldsymbol{A}_2) + \frac{1}{\tau_2 \tau_3} (\boldsymbol{A}_2 \times \boldsymbol{A}_3) + \frac{1}{\tau_1 \tau_3} (\boldsymbol{A}_3 \times \boldsymbol{A}_1) \right|^2}{\frac{\det^2 \mathcal{A}}{\tau_1^2 \tau_2^2 \tau_3^2}}. \tag{5.17}$$

Using the following inequality

$$(a + b + c)^2 \leq 3a^2 + 3b^2 + 3c^2,$$

we continue the formula (5.17):

$$\begin{aligned} \boldsymbol{K}^2 &\leq \frac{\tau_1^2 \tau_2^2 \tau_3^2}{\det^2 \mathcal{A}} \left(\frac{3}{\tau_1^2 \tau_2^2} |\boldsymbol{A}_1 \times \boldsymbol{A}_2|^2 + \frac{3}{\tau_2^2 \tau_3^2} |\boldsymbol{A}_2 \times \boldsymbol{A}_3|^2 + \frac{3}{\tau_1^2 \tau_3^2} |\boldsymbol{A}_3 \times \boldsymbol{A}_1|^2 \right) \\ &= \frac{3}{\det^2 \mathcal{A}} \left(\tau_3^2 |\boldsymbol{A}_1 \times \boldsymbol{A}_2|^2 + \tau_1^2 |\boldsymbol{A}_2 \times \boldsymbol{A}_3|^2 + \tau_2^2 |\boldsymbol{A}_3 \times \boldsymbol{A}_1|^2 \right) \end{aligned} \tag{5.18}$$

Now we obtain the estimate for the Dirichlet integral of the trial function u in the tetrahedron T:

$$\int_T |\nabla u|^2 d\boldsymbol{x} \leq \frac{3}{\det^2 \mathcal{A}} |T| \left(\tau_3^2 |\boldsymbol{A}_1 \times \boldsymbol{A}_2|^2 + \tau_1^2 |\boldsymbol{A}_2 \times \boldsymbol{A}_3|^2 + \tau_2^2 |\boldsymbol{A}_3 \times \boldsymbol{A}_1|^2 \right) \tag{5.19}$$

Note that the volume of the tetrahedron $|T| = \frac{1}{6} \det \mathcal{A}$, then we continue (5.19):

$$\int_T |\nabla u|^2 d\boldsymbol{x} \leq \frac{1}{2 \det \mathcal{A}} \left(\tau_3^2 |\boldsymbol{A}_1 \times \boldsymbol{A}_2|^2 + \tau_1^2 |\boldsymbol{A}_2 \times \boldsymbol{A}_3|^2 + \tau_2^2 |\boldsymbol{A}_3 \times \boldsymbol{A}_1|^2 \right) \tag{5.20}$$

Recall that $\frac{1}{2} |\boldsymbol{A}_i \times \boldsymbol{A}_j|$ is the area of the triangle made of the vectors A_i and A_j. The area of the triangle is less than the area of the circumcircle and due to the fact that the circumradius of any triangle is less than the radius of circumsphere ρ we have $\frac{1}{2} |\boldsymbol{A}_i \times \boldsymbol{A}_j| \leq \pi \rho^2$ for any i, j.

Since $\det \mathcal{A} = \det [\boldsymbol{A}_1\, \boldsymbol{A}_2\, \boldsymbol{A}_3]$ is the volume of the parallelepiped made of the vectors $\boldsymbol{A}_1$, $\boldsymbol{A}_2$ and $\boldsymbol{A}_3$ then $\det \mathcal{A} \geq l^3$, where l, as above, is the shortest edge of the tetrahedron T.

Then from (5.20) and (5.11) we obtain (5.10).

□

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