ON THE GROUND STATE OF QUANTUM LAYERS

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1. Introduction

The problem is from mesoscopic physics: let \( p: \Sigma \rightarrow \mathbb{R}^3 \) be an embedded surface in \( \mathbb{R}^3 \), we assume that

1. \( \Sigma \) is orientable, complete, but non-compact;
2. \( \Sigma \) is not totally geodesic;
3. \( \Sigma \) is asymptotically flat in the sense that the second fundamental form goes to zero at infinity.

On can build a quantum layer \( \Omega \) over such a surface \( \Sigma \) as follows: as a differentiable manifold, \( \Omega = \Sigma \times [-a, a] \) for some positive number \( a \). Let \( \vec{N} \) be the unit normal vector of \( \Sigma \) in \( \mathbb{R}^3 \). Define

\[
\tilde{p}: \Omega \rightarrow \mathbb{R}^3
\]

by

\[
\tilde{p}(x, t) = p(x) + t\vec{N}(x).
\]

Obviously, if \( a \) is small, then \( \tilde{p} \) is an embedding. The Riemannian metric \( ds^2_\Omega \) is defined as the pull-back of the Euclidean metric via \( \tilde{p} \). The Riemannian manifold \( (\Omega, ds^2_\Omega) \) is called the quantum layer.

Let \( \Delta = \Delta_\Omega \) be the Dirichlet Laplacian. Then we make the following

**Conjecture 1.** *Using the above notations, and further assume that*

\[
(1.1) \quad \int_{\Sigma} |K|d\Sigma < +\infty.
\]

*Then the ground state of \( \Delta \) exists.*

We make the following explanation of the notations and terminology:

1. \( \Omega \) is a smooth manifold with boundary. The Dirichlet Laplacian is the self-adjoint extension of the Laplacian acting on \( C_0^\infty(\Omega) \);
2. By a theorem of Huber \[4\], if \( (1.1) \) is valid, then \( \Sigma \) is differmorphic to a compact Riemann surface with finitely many points removed. Moreover, White \[10\] proved that if

\[
\int_{\Sigma} K^-d\Sigma < +\infty,
\]

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then
\[ \int_\Sigma |K| d\Sigma < +\infty. \]

Thus (1.1) can be weakened.

(3) Since \( \Delta \) is a self-adjoint operator, the spectrum of \( \Delta \) is the disjoint union of two parts: pure point spectrum (eigenvalues of finite multiplicity) and the essential spectrum. The ground state is the smallest eigenvalue with finite multiplicity.

(4) The conjecture was proved under the condition
\[ \int_\Sigma K d\Sigma \leq 0 \]

in [2, 1] by Duclos, Exner and Krejčířík and later by Carro n, Exner, and Krejčířík. Thus the remaining case is when
\[ \int_\Sigma K d\Sigma > 0. \]

By a theorem of Hartman [3], we know that
\[ \int_\Sigma K = 2\pi\chi(\Sigma) - \sum \lambda_i \]

where \( \lambda_i \) are the isoperimetric constants at each end of \( \Sigma \). Thus we have
\[ \chi(\Sigma) > 0 \]

and \( g = 0 \). The surface must be diffeomorphic to \( \mathbb{R}^2 \). However, even through the topology of the surface is completely known, this is the most difficult case for the conjecture.

2. VARIATIONAL PRINCIPLE

It is well known that
\[ \sigma_0 = \inf_{f \in C_0^\infty(\Omega)} \frac{\int_{\Omega} |\nabla f|^2 d\Omega}{\int_{\Omega} f^2 d\Omega} \]

is the infimum of the Laplacian, and

\[ \sigma_{\text{ess}} = \sup_K \inf_{f \in C_0^\infty(\Omega \setminus K)} \frac{\int_{\Omega} |\nabla f|^2 d\Omega}{\int_{\Omega} f^2 d\Omega} \]

is the infimum of the essential spectrum, where \( K \) is running over all the compact subset of \( \Omega \). Since \( \Omega = \Sigma \times [-a, a] \), it is not hard to see that

\[ \sigma_{\text{ess}} = \sup_{K \subset \Sigma} \inf_{f \in C_0^\infty(\Omega \setminus K \times [-a, a])} \frac{\int_{\Omega} |\nabla f|^2 d\Omega}{\int_{\Omega} f^2 d\Omega}, \]

where \( K \) is running over all the compact set of \( \Sigma \).

By definition, we have \( \sigma \leq \sigma_{\text{ess}} \). Furthermore, we have

**Proposition 2.1.** If \( \sigma_0 < \sigma_{\text{ess}} \), then the ground state exists and is equal to \( \sigma_0 \).
Let \((x_1, x_2, t)\) be a local coordinate system of \(\Sigma\). Then \((x_1, x_2, t)\) defines a local coordinate system of \(\Omega\). Such a local coordinate system is called a Fermi coordinate system. Let \(x_3 = t\) and let \(ds^2 = G_{ij}dx_idx_j\). Then we have

\[
G_{ij} = \begin{cases} 
(p + t\vec{N})_{x_i}(p + t\vec{N})_{x_j} & 1 \leq i, j \leq 2; \\
0 & i = 3, \text{ or } j = 3, \text{ but } i \neq j; \\
1 & i = j = 3.
\end{cases}
\]

We make the following definition: let \(f\) be a smooth function of \(\Omega\). Then we define

\[
Q(f, f) = \int_\Omega |\nabla f|^2d\Omega - \kappa^2 \int_\Omega f^2d\Omega; \\
Q_1(f, f) = \int_\Omega |\nabla' f|^2d\Omega; \\
Q_2(f, f) = \int_\Omega \left(\frac{\partial f}{\partial t}\right)^2d\Omega - \kappa^2 \int_\Omega f^2d\Omega,
\]

where \(|\nabla' f|^2 = \sum_{i,j=1}^{2} G^{ij} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j}|^2\).

Obviously, we have

\[
Q(f, f) = Q_1(f, f) + Q_2(f, f).
\]

It follows that

\[
\int_\Omega |\nabla f|^2d\Omega = \int_\Omega |\nabla' f|^2d\Omega + \int_\Omega \left(\frac{\partial f}{\partial t}\right)^2d\Omega
\]

for a smooth function \(f \in C^\infty(\Omega)\), where

\[
|\nabla' f|^2 = \sum_{1 \leq i, j \leq 2} G^{ij} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j}
\]

is the norm of the horizontal differential. Apparently, we have

\[
\int_\Omega |\nabla f|^2d\Omega \geq \int_\Omega \left(\frac{\partial f}{\partial t}\right)^2d\Omega.
\]

Let \(ds^2 = g_{ij}dx_idx_j\) be the Riemannian metric of \(\Sigma\) under the coordinates \((x_1, x_2)\). Then we are above to compare the matrices \((G_{ij})_{1 \leq i, j \leq 2}\) and \((g_{ij})\), at least outside a big compact set of \(\Sigma\). By (2.3), we have

\[
G_{ij} = g_{ij} + tp_{x_i}\vec{N}_{x_j} + tp_{x_j}\vec{N}_{x_i} + t^2\vec{N}_{x_i}\vec{N}_{x_j}.
\]

We assume that at the point \(x\), \(g_{ij} = \delta_{ij}\). Then we have

\[
|G_{ij} - \delta_{ij}| \leq 2a|B| + a^2|B|^2,
\]

where \(B\) is the second fundamental form of the surface \(\Sigma\). Thus we have the following conclusion:
Proposition 2.2. For any \( \varepsilon > 0 \), there is a compact set \( K \) of \( \Sigma \) such that on \( \Sigma \setminus K \) we have
\[
(1 - \varepsilon) \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \leq \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \leq (1 + \varepsilon) \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}.
\]
In particular, we have
\[
(1 - \varepsilon)^2 d\Sigma dt \leq d\Omega \leq (1 + \varepsilon)^2 d\Sigma dt.
\]
\(\square\)

Let \( \kappa = \frac{\pi}{2a} \). Then we proved the following:

Lemma 2.1. Using the above notations, we have
\[
\sigma_{\text{ess}} \geq \frac{\pi^2}{4a^2}.
\]

Proof. Let \( K \) be any compact set of \( \Sigma \). If \( f \in C_0^\infty(\Omega \setminus K) \), then by Proposition 2.2, we have
\[
\int_{\Omega} \left( \frac{\partial f}{\partial t} \right)^2 d\Omega \geq (1 - \varepsilon)^2 \int_{\Sigma} \int_{-a}^{a} \left( \frac{\partial f}{\partial t} \right)^2 dt d\Sigma \geq (1 - \varepsilon)^2 \int_{\Sigma} f^2 dtd\Sigma,
\]
where the last inequality is from the 1-dimensional Poincaré inequality. Thus by using Proposition 2.2 again, we have
\[
\int_{\Omega} |\nabla f|^2 d\Omega \geq \frac{(1 - \varepsilon)^2}{(1 + \varepsilon)^2} \kappa^2 \int_{\Sigma} f^2 dtd\Sigma,
\]
for any \( \varepsilon \). Thus we have
\[
\sigma_{\text{ess}} \geq \frac{(1 - \varepsilon)^2}{(1 + \varepsilon)^2} \kappa^2
\]
and the lemma is proved. \(\square\)

Remark 2.1. Although not needed in this paper, we can actually prove that \( \sigma_{\text{ess}} = \kappa^2 \). To see this, we first observe that since the second fundamental form of \( \Sigma \) is bounded, there is a lower bound for the injectivity radius. As a result, the volume of the surface \( \Sigma \) is infinite. By the assumption, the Gauss curvature is integrable. Thus \( \Sigma \) is parabolic (cf. [5]). From the above, we conclude that for any \( \varepsilon, C > 0 \) and any compact sets \( K \subset K' \) of \( \Sigma \), there is a smooth function \( \varphi \in C_0^\infty(\Sigma \setminus K') \) such that
\[
\varphi \equiv 1 \text{ on } K, \quad \int_{\Sigma} \varphi^2 d\Sigma > C, \quad \text{and} \quad \int_{\Sigma} |\nabla \varphi|^2 d\Sigma < \varepsilon.
\]

Let \( \tilde{\varphi} = \varphi \chi \), where \( \chi = \cos \kappa t \). Then \( \tilde{\varphi} \) is a function on \( \Omega \) with compact support. Since the second fundamental form goes to zero at infinity, by Proposition 2.2 for \( K' \) large enough, we have
\[
\int_{\Omega} |\nabla \tilde{\varphi}|^2 d\Omega < 4a\varepsilon.
\]
Thus from (2.4) and Proposition 2.2 again, we have
\[ Q(\tilde{\phi}, \tilde{\phi}) < 4a\varepsilon + (1 + \varepsilon)^2 \int_{\Sigma} \varphi^2 d\Sigma \int_{-a}^{a} \left( \frac{\partial \chi}{\partial t} \right)^2 dt \]
\[ - (1 - \varepsilon)^2 \kappa^2 \int_{\Sigma} \varphi^2 d\Sigma \int_{-a}^{a} \chi^2 dt. \]
A straightforward computation gives
\[ \int_{-a}^{a} \left( \frac{\partial \chi}{\partial t} \right)^2 dt = \kappa^2 \int_{-a}^{a} \chi^2 dt. \]
Thus
\[ Q(\tilde{\phi}, \tilde{\phi}) \leq 4a\varepsilon + 4a\varepsilon \int_{\Sigma} \varphi^2 d\Sigma. \]
By the definition of \( \sigma_{\text{ess}} \), we have
\[ \sigma_{\text{ess}} - \kappa^2 \leq \frac{Q(\tilde{\phi}, \tilde{\phi})}{\int_{\Omega} \varphi^2 d\Omega} \leq \frac{4\varepsilon(1 + \int_{\Sigma} \varphi^2 d\Sigma)}{(1 - \varepsilon)^2 \int_{\Sigma} \varphi^2 d\Sigma}. \]
We let \( \varepsilon \to 0 \) and \( C \to \infty \), then we have \( \sigma_{\text{ess}} \leq \kappa^2 \), as needed.

3. The upper bound of \( \sigma_0 \)

It is usually more difficult to estimate \( \sigma_0 \) from above. In [7, Theorem 1.1], we proved the following

**Theorem 3.1.** Let \( \Sigma \) be a convex surface in \( \mathbb{R}^3 \) which can be represented by the graph of a convex function \( z = f(x, y) \). Suppose \( 0 \) is the minimum point of the function and suppose that at \( 0 \), \( f \) is strictly convex. Furthermore suppose that the second fundamental form goes to zero at infinity. Let \( C \) be the supremum of the second fundamental form of \( \Sigma \). Let \( Ca < 1 \). Then the ground state of the quantum layer \( \Omega \) exists.

In this section, we generalize the above result into the following:

**Theorem 3.2.** Let \( \Sigma \) be a complete surface in \( \mathbb{R}^3 \) with nonnegative Gauss curvature but not totally geodesic. Furthermore suppose that the second fundamental form of \( \Sigma \) goes to zero at infinity. Let \( C \) be the supremum of the second fundamental form of \( \Sigma \). Let \( Ca < 1 \). Then the ground state of the quantum layer \( \Omega \) built over \( \Sigma \) with width \( a \) exists.

**Remark 3.1.** Since for all convex function \( f \) in Theorem 3.1, the Gauss curvature is nonnegative, the above theorem is indeed a generalization of Theorem 3.1. On the other hand, by a theorem of Sacksteder [9], any complete surface of nonnegative curvature is either a developable surface or the graph of some convex function. At a first glance, it seems that there is not much difference between the surfaces in both theorems. However, we have to use a complete different method to prove this slight generalization.
Proof of Theorem 3.2. If the Gauss curvature is identically zero, then by \cite[Theorem 2]{8}, the ground state exists.

If the Gauss curvature is positive at one point, then by using the theorem of Sacksteder \cite{9}, \( \Sigma \) can be represented by the graph of some convex function. If we fix an orientation, we can assume that \( H \), the mean curvature, is always nonnegative.

By a result of White \cite{10}, we know that there is an \( \varepsilon_0 > 0 \) such that for \( R > R_0 > R_1 \),

\[
\int_{\partial B(R)} ||B|| > \varepsilon_0,
\]

where \( B \) is the second fundamental form of \( \Sigma \). Since \( \Sigma \) is convex, we have

\[
H \geq \frac{1}{2} ||B||.
\]

Thus we have

\begin{equation}
(3.1) \quad \int_{B(R_2) \setminus B(R_1)} H \, d\Sigma \geq \frac{1}{2} \varepsilon_0 (R_2 - R_1)
\end{equation}

provided that \( R_2 > R_1 \) are large enough.

We will create suitable test functions using the techniques similar to \cite{2, 11, 1, 6, 8}. Let \( \varphi \in C^\infty_0 (\Sigma \setminus B(\frac{R}{2})) \) be a smooth function such that

\[
\varphi \equiv 1 \quad \text{on} \quad B(2R) \setminus B(R), \quad \int_\Sigma |\nabla \varphi|^2 d\Sigma < \varepsilon_1,
\]

where \( \varepsilon_1 \to 0 \) as \( R \to \infty \). The existence of such a function \( \varphi \) is guaranteed by the parabolicity of \( \Sigma \). Then we have, as in Remark 2.1, that

\[
Q(\varphi \chi, \varphi \chi) < 4a\varepsilon_1 + 2a\pi^2 \int_{\Sigma \setminus B(R/2)} K \varphi^2 d\Sigma.
\]

Since \( K \) is integrable, for any \( \varepsilon_2 > 0 \), there is an \( R_0 > 0 \) such that if \( R > R_0 \), we have

\[
Q(\varphi \chi, \varphi \chi) < \varepsilon_2.
\]

Now let’s consider a function \( j \in C^\infty_0 (B(\frac{4}{3}R) \setminus B(\frac{2}{3}R)) \). Consider the function \( j \chi(t)t \), where \( j \) is a smooth function on \( \Sigma \) such that \( j \equiv 1 \) on \( B(\frac{19}{12}R) \setminus B(\frac{17}{12}R); \ 0 \leq j \leq 1; \ \text{and} \ |\nabla j| < 2 \). Then there is an absolute constant \( C_1 \), such that

\[
Q(j \chi(t)t, j \chi(t)t) \leq C_1 R^2.
\]

Finally, let’s consider \( Q(\varphi \chi(t), j \chi(t)t) \). Since \( \text{supp} j \subset \{ \varphi \equiv 1 \} \), by \cite{23, 5}, \( Q_1(\varphi \chi(t), j \chi(t)t) = 0 \). Let

\[
\sigma = - \int_{-a}^a \chi'(t) \chi(t) t \, dt > 0.
\]

Then

\[
Q(\varphi \chi(t), j \chi(t)t) = -\sigma \int_{\Sigma} j d\Sigma.
\]
Let $\varepsilon > 0$. Then we have
\[
Q(\varphi(t) + \varepsilon j\chi(t)t, \varphi(t) + \varepsilon j\chi(t)t) < \varepsilon - 2\varepsilon \sigma \int \Sigma jd\Sigma + \varepsilon^2 C_1 R^2.
\]
By (3.1), we have
\[
Q(\varphi(t) + \varepsilon j\chi(t)t, \varphi(t) + \varepsilon j\chi(t)t) < \varepsilon - \frac{1}{3}\varepsilon \sigma R + \varepsilon^2 C_1 R^2.
\]
If
\[
\varepsilon < \frac{\sigma^2}{36C_1},
\]
then there is a suitable $\varepsilon > 0$ such that
\[
Q(\varphi(t) + \varepsilon j\chi(t)t, \varphi(t) + \varepsilon j\chi(t)t) < 0.
\]
Thus $\sigma_0 < \kappa^2$. \hfill $\Box$

4. Further Discussions.

We proved the following more general

**Theorem 4.1.** We assume that $\Sigma$ satisfies

1. The isopermetric inequality holds. That is, there is a constant $\delta_1 > 0$ such that if $D$ is a domain in $\Sigma$, we have
   \[
   (\text{length}(\partial D))^2 \geq \delta_1 \text{Area}(D).
   \]

2. There is another positive constant $\delta_2 > 0$ such that for any compact set $K$ of $\Sigma$, there is a curve $C$ outside the set $K$ such that if $\gamma$ is one of its normal vector in $\Sigma$, then there is a vector $\vec{a}$ such that
   \[
   \langle \gamma, \vec{a} \rangle \geq \delta_2 > 0
   \]
   for some fixed vector $\vec{a} \in \mathbb{R}^3$.

Then the ground state exists.

**Proof.** We let $\varphi$ be a smooth function such that $\text{supp} \varphi \subset B(R) \setminus B(r)$ for $R >> R/4 >> 4r >> r > 0$ large. We also assume that on $B(R/2) \setminus B(2r)$, $\varphi \equiv 1$. Let $\varepsilon_0 > 0$ be a positive number to be determined later such that
\[
\int \Sigma |\nabla \varphi|^2 \leq \varepsilon_0, \quad \int \Sigma |\varphi|^2 \leq \varepsilon_0.
\]
Note that $\varepsilon_0$ is independent of $R$.

We let $\chi = \cos \frac{\pi}{2r}t$. Then there is a constant $C$ such that
\[
Q(\varphi \chi, \varphi \chi) < C\varepsilon_0.
\]
Let $C$ be a curve outside the compact set $B(4r)$ satisfying the condition in the theorem. We let $R$ big enough that $C \subset B(R/4)$.

In order to construct the test functions, we let $\rho$ be the cut-off function such that $\rho = 1$ if $t \leq 0$ and $\rho = 0$ if $t \geq 1$ and we assume that $\rho$ is decreasing. Near the curve $C$, any point $p$ has a coordinate $(t, s)$, where
s ∈ C from the exponential map. To be more precise, let \((x_1, x_2)\) be the the local coordinates near \(C\) such that locally \(C\) can be represented by \(x_1 = 0\). Let the Riemannian metric under this coordinate system be
\[
g_{11}(dx_1)^2 + 2g_{12}dx_1dx_2 + g_{22}(dx_2)^2.
\]
The fact that \(\vec{\gamma}\) is a normal vector implies that if
\[
\vec{\gamma} = \gamma_1 \frac{\partial}{\partial x_1} + \gamma_2 \frac{\partial}{\partial x_2},
\]
then
\[
\gamma_1 g_{12} + \gamma_2 g_{22} = 0.
\]
Let \(\sigma_t(x_2)\) be the geodesic lines starting from \(x_2 \in C\) with initial vector \(\vec{\gamma}\). Then \(\sigma_t\) is the exponential map. The Jacobian of the map at \(t = 0\) is
\[
\begin{pmatrix}
\gamma_1 & \gamma_2 \\
0 & 1
\end{pmatrix}
\]
In particular, \(\gamma_1 \neq 0\) since the map must be nonsingular. A simple computation shows that \(\nabla t = \gamma_1 g^{12} \frac{\partial}{\partial x_1}\). Thus \(\nabla t\) is proportional to \(\vec{\gamma}\).

Let \(\varphi_1\) be a cut-off function such that \(\varphi_1 \equiv 1\) on \(B(R/4) \setminus B(4r)\) and \(\text{supp}(\varphi_1) \subset B(R/2) \setminus B(2r)\). We define \(\tilde{\rho}(p) = \varphi_1 \rho(t/\varepsilon_1)\), where \(\varepsilon_1\) is a positive constant to be determined. WLOG, let \(\vec{a}\) be the z-direction in the Euclidean space.

Let \(\vec{n}\) be the normal vector of \(\Sigma\). Let \(n_z\) be the z-component of \(\vec{n}\). We compute the following term
\[
Q(\varphi \chi, \tilde{\rho} n_z \chi_1) = -\int_{\Sigma} H \varphi \tilde{\rho} n_z d\Sigma \int_{-a}^a (\chi' \chi_1 t - \kappa^2 \chi \chi_1 t) dt.
\]
A straight computation shows that
\[
C_1 = \int_{-a}^a (\chi' \chi_1 t - \kappa^2 \chi \chi_1 t) dt = -1/2 \neq 0.
\]
Furthermore, we have \(H n_z = \Delta z\). As a result, we have
\[
-\int_{\Sigma} H \varphi \tilde{\rho} n_z d\Sigma = \int_{\Sigma} \nabla z \nabla \tilde{\rho} = \int_{\{t \leq \varepsilon_1\}} \nabla z \nabla \tilde{\rho}
\]
(Note that \(\varphi \equiv 1\) on the points we are interested). We have the following Taylor expansion:
\[
\nabla z \nabla \tilde{\rho}(t, x_2) = \nabla z \nabla \tilde{\rho}(0, x_2) + O(t)
\]
Since \(\int_{\{t \leq \varepsilon_1\}} O(t)/\varepsilon_1 = O(\varepsilon_1) \text{Length}(C)\), we have
\[
\int_{\Sigma} \nabla z \nabla \tilde{\rho} \geq (\delta_2 - O(\varepsilon_1)) \text{Length}(C)
\]
We choose $\varepsilon_1$ small enough, then we have
\[
\int_\Sigma \nabla z \nabla \rho \geq \frac{1}{2} \delta^2 \text{Length}(C)
\]
If we let $\varepsilon \to 0$, then that above becomes
\[- \int_\Sigma H \varphi \rho_n d\Sigma = \int_\Sigma \nabla z \nabla \rho \geq \delta^2 \text{Length}(C).
\]
Finally, we have $|\rho_n z| + |\nabla (\rho_n z)| \leq 2$, thus we have
\[
Q(\rho_n z \chi_1, \rho_n z \chi_1) \leq C \text{Area}(D),
\]
where $D$ is the domain $C$ enclosed. To summary, for any $\varepsilon < 0$, we have
\[
Q(\varphi \chi + \varepsilon \rho_n z \chi_1, \varphi \chi + \varepsilon \rho_n z \chi_1) \leq C \varepsilon_0 + 2 \varepsilon C_1 \delta \frac{\delta^2}{C^2} \text{Area}(D).
\]
Using the isoperimetric inequality, we know that if $\varepsilon_0 < \delta_1 \delta^2 / C^2$ is small enough, then
\[
Q(\varphi \chi + \varepsilon \rho_n z \chi_1, \varphi \chi + \varepsilon \rho_n z \chi_1) < 0
\]
which proves the theorem.

Using the same proof, we can prove the following:

**Theorem 4.2.** Using the same notations as in Conjecture [4], we assume further that
\[
||B||(x) \leq C/\text{dist}(x, x_0),
\]
where $x_0 \in \Sigma$ is a reference point of $\Sigma$. Then Conjecture [4] is true.

\[\square\]

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