Lower bound of a quadratic form defined on a direct sum of Sobolev spaces of divided regions

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1 Introduction

We consider first the eigenvalue problem of the Schrödinger equation for the space dimension 1. The Schrödinger equation with the semiclassical parameter h is written as $(-h^2\Delta + V)u = Eu$. Here $V \in C^3(\mathbb{R})$ is a real-valued function, $E \in \mathbb{R}$ is the eigenvalue and $u \in L^2(\mathbb{R})$ is the eigenfunction. Let us assume

$$V'(x)^2 + |V''(x)| = O(|x|^{-\rho_0}),\ |x| \to \infty,$$

for some $\rho_0 > 1$, $V(x) = E_0$ has two solutions $x_- < x_+$, $V(x) < E_0$ for $x \in (x_-, x_+)$, $\pm V'(x_\pm) > 0$ and $\liminf_{|x|\to\infty} V(x) > E_0$. Choose $x_1 \in (x_-, x_+)$ and set $\rho_1 := \min\{\rho_0 - 1, 1\} > 0$. Then there exists a solution $u_+(x)$ (resp., $u_-(x)$) on (x_1, ∞) (resp., $(-\infty, x_1)$) such that

$$\begin{aligned} u_\pm(x) =& Ch^{1/6}(V(x) - E)^{-1/4} \exp\left(\mp h^{-1} \int_{x_\pm}^{x} \sqrt{V(y) - E}dy\right) \\ &\times \left(1 + O\left(\left|\int_{x_\pm}^{x} \sqrt{V(y) - E}dy\right|^{-\rho_1}\right)\right), \end{aligned}$$

as $x \to \pm\infty$ (cf. [6]). We define $\mathcal{A}(E) := \int_{x_-(E)}^{x_+(E)} \sqrt{E - V(x)}dx$. Considering the condition that $u_+(x)$ and $u_-(x)$ are connected at x_1, i.e. that $(u_+(x_1), u'_+(x_1)) = (u_-(x_1), u'_-(x_1))$, we can see that eigenvalue E in a neighborhood of E_0 satisfies

$$\mathcal{A}(E) = \pi(n + 1/2)h + O(h^2).$$

The corresponding eigenfunction is $u_+(x)$ (resp., $u_-(x)$) on (x_1, ∞) (resp., $(-\infty, x_1)$).

Connection of local solutions gives exceptionally detailed information in one-dimensional cases. When the space dimension is greater than 1, the exact connection of local functions can not be achieved. In addition, local solutions themselves can not be constructed exactly. However, local behaviors of eigenfunctions are strongly affected by the local behavior of the potential. Therefore, in numerical analysis by discretization (finite-dimensional approximation) we need to choose basis functions that have local behaviors close to the true eigenfunctions.

The augmented plane wave (APW) method is a method for periodic lattices based on such an idea. It was proposed by Slater [4]. The APW method is preferred, because the method converges rapidly and it is independent of the degree of localization of electrons (cf. [2]).

2 APW method

We consider Schrödinger equation in $\mathbb{R}^n,\ n \geq 2$:

$$(-\Delta + V)u = Eu.$$

We assume that the potential V is periodic in the sense that $V(x+T) = V(x)$ for any $T \in \mathbb{R}^n$ such that

$$T = l_1 a_1 + \cdots + l_n a_n,$$

where $a_1, \dots, a_n \in \mathbb{R}^n$ are primitive translation vectors and $l_1, \dots, l_n \in \mathbb{Z}$. For fixed $k \in \mathbb{R}^n$ we seek generalized eigenfunction that satisfies

$$u(x+T) = e^{ik\cdot T} u(x),$$

for any lattice vector T (u is called Bloch function). The eigenvalues of the Bloch functions and their dependence on k play important roles in the theory of metal, insulator and semiconductor. Let $D := \{x = \sum_{i=1}^n c_i a_i : \forall i,\ 0 < c_i < 1\}$ be the unit cell. We devide the unit cell D into regions as $D = \Omega_1 \cup \left(\bigcup_{\alpha=2}^N \overline{\Omega}_\alpha \right)$,

$$\begin{aligned} \Omega_\alpha &:= \{x : |x - \bar{x}_\alpha| < R_\alpha\},\ \alpha = 2, \dots, N, \\ \Omega_1 &:= D \setminus \left(\bigcup_{\alpha=2}^N \overline{\Omega}_\alpha \right), \end{aligned}$$

where $\bar{x}_\alpha,\ \alpha = 2, \dots, N$ are atomic sites and $R_\alpha > 0$ (see Figure 1).

We assume

$$V(x) = \begin{cases} V(|x - \bar{x}_\alpha|), & x \in \Omega_\alpha,\ \alpha = 2, \dots, N \\ 0 & x \in \Omega_1 \end{cases},$$

which is called Muffin-Tin potential. If e.g. $V(|x - \bar{x}_\alpha|) = \frac{1}{|x - \bar{x}_\alpha|},\ x \in \Omega_\alpha$, the Bloch function u in $\mathbb{R}^n$ restricted to the unit cell D is an eigenfunction of the selfadjoint operator $-\Delta + V$ in $L^2(D)$ with the domain

$$\begin{aligned} &\{u \in H^2(D) : \forall j,\ u(x + a_j) = e^{ik\cdot a_j} u(x), \\ &\quad (G_j \cdot \nabla) u(x + a_j) = e^{ik\cdot a_j} (G_j \cdot \nabla) u(x),\ \text{for } x = \sum_{l \neq j} c_l a_l,\ 0 < c_l < 1\}, \end{aligned}$$

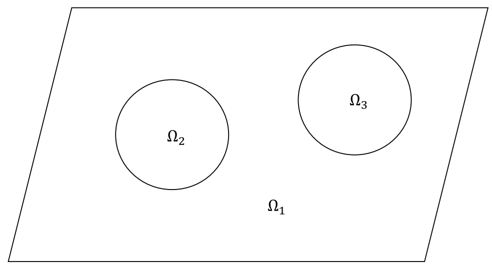

Figure 1: Regions in the unit cell

where $a_1, \dots, a_n$ are primitive translation vectors and G_i is the reciprocal lattice vector such that $G_i \cdot a_j = 2\pi\delta_{ij}$.

In Ω_1 the eigenfunction u is given by the linear combination of the plane waves

$$v_G(x) = e^{i(k+G)\cdot x},$$

where G is a reciprocal lattice vector, i.e. G is a vector such that $(G \cdot T)/(2\pi) \in \mathbb{Z}$ for any lattice vector T.

In $\Omega_\alpha,\ \alpha \geq 2$, we consider the linear combination

$$v_G(x) = e^{i(k+G)\cdot \bar{x}_\alpha} \sum_{l,m} A_{lm}^{\alpha,k+G} \chi_l^\alpha(r_\alpha, E) Y_{lm}(\theta_\alpha, \varphi_\alpha),$$

where $l = 0, 1, 2, \dots,\quad m = -l, \dots, l$, $(r_\alpha, \theta_\alpha, \varphi_\alpha)$ is the polar coordinates of $x - \bar{x}_\alpha$, $Y_{lm}(\theta, \varphi)$ is the spherical harmonics and $\chi_l^\alpha(r, E)$ is the radial function depending on the parameter E (chosen later to be an eigenvalue). The coefficients $A_{lm}^{\alpha,k+G} \in \mathbb{C}$ are determined so that two expressions of $v_G(x)$ will coincide on the boundary $\partial\Omega_\alpha$.

In order to determine $A_{lm}^{\alpha,k+G}$, we use a well-known expansion of the plane wave $e^{i(k+G)\cdot x}$ with respect to the center $\bar{x}_\alpha$:

$$e^{i(k+G)\cdot x} = 4\pi e^{i(k+G)\cdot \bar{x}_\alpha} \sum_{lm} i^l j_l(r' r_\alpha) Y_{lm}^*(\theta', \varphi') Y_{lm}(\theta_\alpha, \varphi_\alpha),$$

where $(r_\alpha, \theta_\alpha, \varphi_\alpha)$ and (r', θ', φ') are polar coordinates of $x - \bar{x}_\alpha$ and $k + G$ respectively, and j_l is the spherical Bessel function. From the condition that this expression coincides with the expression of $v_G(x)$ inside Ω_α on the boundary $\partial\Omega_\alpha$ it follows that

$$A_{lm}^{\alpha,k+G} = 4\pi i^l \frac{j_l(r' R_\alpha) Y_{lm}^*(\theta', \varphi')}{\chi_l^\alpha(R_\alpha, E)}, \quad l = 0, 1, 2, \dots, \quad m = -l, \dots, l.$$

The eigenfunction u is obtained as a linear combination of $u^i = v_{G_i}(x)$ considering the secular equation for u^i, where G_i ranges through reciprocal lattice vectors. Since $v_G(x)$ itself depends on the eigenvalue E, the problem to determine the linear combination is not a usual eigenvalue problem of a matrix. We denote $v_G(x)$ by $v_G(x, E)$ to clarify the dependence on E.

3 Secular equation and the Rayleigh-Ritz method

Let X be a Hilbert space, A be a semibounded selfadjoint operator, $\{u^1, \dots, u^M\} \in \mathcal{D}(A)$ (or form domain of A) be linearly independent. We define $h_{ij} := \langle u^i, Au^j \rangle$, actually, $\langle \nabla u^i, \nabla u^j \rangle + \langle u^i, Vu^j \rangle$ for $A = -\Delta + V$ and $s_{ij} := \langle u^i, u^j \rangle$. Set $H = (h_{ij}),\ S = (s_{ij})$.

The secular equation is the following

$$\det(H - ES) = 0, \quad E \in \mathbb{R}.$$

Let $\tilde{E}_1, \dots, \tilde{E}_M \in \mathbb{R}$ be solutions to the secular equation. In particular, if $\langle u^i, u^j \rangle = \delta_{ij}$, then $S = I$ and $\tilde{E}_1, \dots, \tilde{E}_M$ are eigenvalues of H. Let $E_1, \dots, E_M \in \mathbb{R}$ be the M lowest eigenvalues of A. Then we have

$$\tilde{E}_m \geq E_m,\ m = 1, \dots, M.$$

This method is called the Rayleigh-Ritz method.

Since the energy E obtained by the APW method satisfies the secular equation for $v_{G_i}(x, E)$, if $v_{G_i}(x, E)$ were in $H^1(D)$, E would be an upper bound of the true eigenvalue. However, since there exist infinitely many coefficients $A_{lm}^{\alpha, k+G}, \quad l = 0, 1, 2, \dots, \quad m = -l, \dots, l$ of $v_G(x, E)$ to be determined, in practical calculation the expansion is cut off at some finite l. Hence $v_G(x, E)$ has discontinuity on $\partial\Omega_\alpha$, and thus $v_G(x, E) \notin H^1(D)$. Therefore, $\tilde{E}_m$ can be smaller than E_m. Recall that decrease of the value $\tilde{E}_m$ obtained from the secular equation in the usual Rayleigh-Ritz method means that the value has been improved, because it is an upper bound.

4 Purpose of the present result and the main result

It would be very useful if there exists a method to use different basis sets in different divided regions and to estimate the error due to the discontinuity of functions on intersections of the boundaries of the regions. The purpose of the present research is the following.

- Estimate the effect of the discontinuity of functions on the boundary $\partial\Omega_\alpha$ to the solution $\tilde{E}_m$ of the secular equation not only in APW method but also in general eigenvalue problems.

Here note that the basis functions in the APW method work only for the special setting. They are plane waves and products of spherical harmonics and radial functions centered at atomic sites. They work for the Muffin-Tin potential, but for general potentials they are not good choices for the basis functions.

Let $\Omega \subset \mathbb{R}^n$ be a region with bounded $\partial\Omega$. We define

$$\langle \tilde{u}, \tilde{v} \rangle_\Omega := \int_\Omega \tilde{u}^*(x)\tilde{v}(x)dx, \quad \tilde{u}, \tilde{v} \in L^2(\Omega),$$

$$\langle u, v \rangle := \int_{\mathbb{R}^n} u^*(x)v(x)dx, \quad u, v \in L^2(\mathbb{R}^n).$$

Let $T_{l-1} : H^l(\Omega) \to \bigoplus_{m=0}^{l-1} H^{l-m-1/2}(\partial\Omega)$ be the trace operator in Ω satisfying

$$T_{l-1}\tilde{u} = \left(\tilde{u}|_{\partial\Omega}, \left.\frac{\partial \tilde{u}}{\partial n}\right|_{\partial\Omega}, \dots, \left.\frac{\partial^{l-1}\tilde{u}}{\partial n^{l-1}}\right|_{\partial\Omega} \right),$$

for $\tilde{u} \in C^l(\overline{\Omega})$. Note that if $\tilde{u} \in H^l(\Omega)$, $l \geq 1$, we have $T_0\tilde{u} \in H^{l-1/2}(\partial\Omega)$ because it is the first component of $T_{l-1}\tilde{u}$. We denote $T_0\tilde{u}$ also by $\tilde{u}|_{\partial\Omega}$.

We assume

(A) $\Omega_\alpha \cap \Omega_\beta = \emptyset$, $\alpha \neq \beta$, $\bigcup_{\alpha=1}^N \overline{\Omega}_\alpha = \mathbb{R}^n$, $\partial\Omega_\alpha$ is of class C^3 and bounded, and each $\partial\Omega_\alpha \cap \partial\Omega_\beta$, $\alpha \neq \beta$ is a connected component of $\partial\Omega_\alpha$ or the empty set (cf. Figure 2).

(B) There exist $0 \leq a < 1$ and $b \geq 0$ such that for any $\tilde{u}_\alpha \in H^1(\Omega_\alpha)$

$$\langle \tilde{u}_\alpha, |V|\tilde{u}_\alpha \rangle_{\Omega_\alpha} \leq a\|\nabla\tilde{u}_\alpha\|^2_{L^2(\Omega_\alpha)} + b\|\tilde{u}_\alpha\|^2_{L^2(\Omega_\alpha)}, \quad \alpha = 1, \dots N,$$

and for any $u \in H^2(\mathbb{R}^n)$

$$\|Vu\|_{L^2(\mathbb{R}^n)} \leq a\|\Delta u\|_{L^2(\mathbb{R}^n)} + b\|u\|_{L^2(\mathbb{R}^n)}.$$

(C) There exist $M \in \mathbb{N}$ isolated eigenvalues $E_1, \dots, E_M$ of the selfadjoint operator $-\Delta + V$ in $L^2(\mathbb{R}^n)$ with the domain $H^2(\mathbb{R}^n)$ in ascending order at the bottom of the spectrum, and there exists $d \geq 0$ such that $E_m \leq d$, $m = 1, \dots, M$.

We denote $\sum_{\alpha=1}^N \langle \tilde{u}_\alpha, \tilde{v}_\alpha \rangle_{\Omega_\alpha}$ also by $\langle u, v \rangle$ for $u = (\tilde{u}_1, \dots, \tilde{u}_N), v = (\tilde{v}_1, \dots, \tilde{v}_N) \in \bigoplus_{\alpha=1}^N L^2(\Omega_\alpha)$. Let $u^i = (\tilde{u}_1^i, \dots, \tilde{u}_N^i) \in \bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)$, $i = 1, \dots, M$, $\langle u^i, u^j \rangle = \delta_{ij}$. $h_{ij} := \langle \nabla u^i, \nabla u^j \rangle + \langle u^i, Vu^j \rangle$, where $\nabla u^i := (\nabla\tilde{u}_1^i, \dots, \nabla\tilde{u}_N^i)$, $\langle \nabla u^i, \nabla u^j \rangle := \sum_{\alpha=1}^N \langle \nabla\tilde{u}_\alpha^i, \nabla\tilde{u}_\alpha^j \rangle_{\Omega_\alpha}$ and $\langle \nabla\tilde{u}_\alpha, \nabla\tilde{v}_\alpha \rangle_{\Omega_\alpha} := \sum_{l=1}^n \langle \partial_{x_l}\tilde{u}_\alpha, \partial_{x_l}\tilde{v}_\alpha \rangle_{\Omega_\alpha}$. We denote by $\tilde{E}_m = \tilde{E}_m(u^1, \dots, u^M)$ the mth eigenvalue of $H = (h_{ij})$ in ascending order.

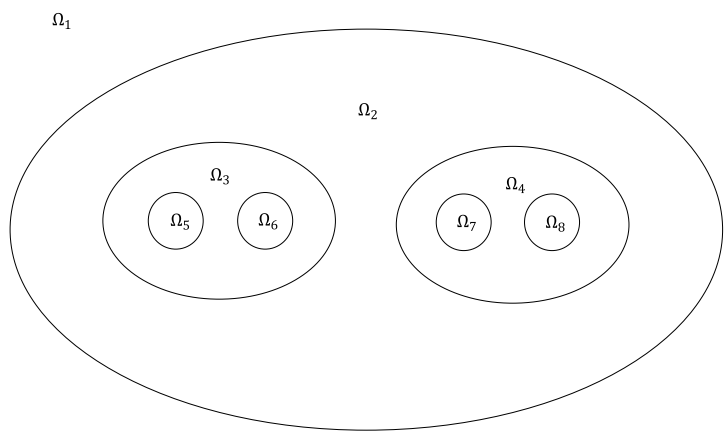

Figure 2: Example of the arrangement of regions

5 Main results

The following is our main theorem.

Theorem 5.1. *Under the assumptions (A), (B) and (C) there exist constants $C, \delta > 0$ depending only on $\{\Omega_\alpha\}$, a, b and d such that if*

$$M \sum_{i=1}^{M} \sum_{\alpha \neq \beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)} < \delta,$$

we have

$$\tilde{E}_m \geq E_m - CM^2 \sum_{i=1}^{M} \sum_{\alpha \neq \beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)},$$

for any $1 \leq m \leq M$.

From $u \in H^2(\mathbb{R}^n)$ we can construct $(\tilde{u}_1, \ldots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)$ by $\tilde{u}_\alpha(x) = u(x),\ x \in \Omega_\alpha$. Conversely, for $(\tilde{u}_1, \ldots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)$ we define $u \in L^2(\mathbb{R}^n)$ by $u(x) = \tilde{u}_\alpha(x),\ x \in \Omega_\alpha$. In this sense we have

$$H^2(\mathbb{R}^n) \subsetneq \bigoplus_{\alpha=1}^{N} H^2(\Omega_\alpha) \subsetneq L^2(\mathbb{R}^n).$$

Theorem 5.1 means that the effect of discontinuity of u on the boundaries $\partial\Omega_\alpha \cap \partial\Omega_\beta$ to $\tilde{E}_m$ is estimated by the difference of the boundary values $\|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)}$. Combining the result with the min-max principle for

$-\Delta + V$ on $L^2(\mathbb{R}^n)$ we have

$$E_m \geq \inf_{\substack{u^1,\dots,u^M \in \bigoplus_{\alpha=1}^N H^2(\Omega_\alpha) \\ \langle u^i, u^j \rangle = \delta_{ij} \\ \sum_{i,\alpha\neq\beta} \|\tilde{u}^i_\alpha|_{\partial\Omega_\alpha} - \tilde{u}^i_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}} \leq \epsilon}} \tilde{E}_m(u^1,\dots,u^M) \geq E_m - CM^2\epsilon,$$

for sufficiently small $\epsilon \geq 0$, which coincides with the principle of the Rayleigh-Ritz method when $\epsilon = 0$.

The lower bound deteriorates as M increases. However, after solving the secular equation, we obtain corresponding linear combinations φ^m of the basis functions such that $\langle \nabla\varphi^m, \nabla\varphi^m\rangle + \langle \varphi^m, V\varphi^m\rangle = \tilde{E}_m$. Thus to estimate $\tilde{E}_{m_0}$ for a fixed m_0 a posteriori, we have only to consider $\varphi^1, \dots, \varphi^{m_0}$, and therefore, the lower bound with M and u^i replaced by m_0 and φ^i holds. In particular, for the a posteriori estimate of $\tilde{E}_1$, M is always 1.

Even when $\{u^i\}$ is not orthonormalized, considering the orthonormalization we can see that the same form of estimate holds for the eigenvalues obtained by solving the secular equation. However, for the constant δ not to be very small and C not to be very large the discontinuity should not become large by the orthonormalization.

Next let us consider the case of APW method. Let $\{a_1, \dots, a_n\}$ be a base of $\mathbb{R}^n$ and set $D := \{x = \sum_{i=1}^n c_i a_i : \forall i,\ 0 < c_i < 1\}$. We assume

(A') $\Omega_\alpha \cap \Omega_\beta = \emptyset,\ \alpha \neq \beta$, $\bigcup_{\alpha=1}^N \overline{\Omega}_\alpha = \overline{D}$, $\partial\Omega_\alpha \cap D$ is of class C^3, and each $\partial\Omega_\alpha \cap \partial\Omega_\beta,\ \alpha \neq \beta$ is a connected component of $\partial\Omega_\alpha$ or the empty set.

(B') There exist $0 \leq a < 1$ and $b \geq 0$ such that for any $\tilde{u}_\alpha \in H^1(\Omega_\alpha)$

$$\langle \tilde{u}_\alpha, |V|\tilde{u}_\alpha\rangle_{\Omega_\alpha} \leq a\|\nabla\tilde{u}_\alpha\|^2_{L^2(\Omega_\alpha)} + b\|\tilde{u}_\alpha\|^2_{L^2(\Omega_\alpha)}, \quad \alpha = 1, \dots N,$$

and for any $u \in \mathcal{D}_k$

$$\|Vu\|_{L^2(D)} \leq a\|\Delta u\|_{L^2(D)} + b\|u\|_{L^2(D)},$$

where $\mathcal{D}_k$ is defined by

$$\begin{aligned}\mathcal{D}_k := \{&u \in H^2(D) : \forall j,\ u(x + a_j) = e^{ik\cdot a_j}u(x), \\ &(G_j\cdot\nabla)u(x + a_j) = e^{ik\cdot a_j}(G_j\cdot\nabla)u(x),\ \text{for } x = \sum_{l\neq j} c_l a_l,\ 0 < c_l < 1\},\end{aligned}$$

Under (B') it can be proved that the operator $-\Delta + V$ in $L^2(D)$ with the domain $\mathcal{D}_k$ is a semibounded selfadjoint operator, and its spectrum is discrete with the eigenvalues $E_m = E_m(k),\ m = 1, 2, \dots$ such that $E_m \to \infty$ as $m \to \infty$. Moreover, each $E_m(k)$ (labeled in ascending order) depends analytically on k except at points in a real-analytic subset of $\mathbb{R}^n$ on which $E_m(k)$ is degenerated.

(C') There exist $M \in \mathbb{N}$ isolated eigenvalues $E_1, \ldots, E_M$ of the selfadjoint operator $-\Delta + V$ in $L^2(D)$ with the domain $\mathcal{D}_k$ in ascending order at the bottom of the spectrum, and there exists $d \geq 0$ such that $E_m \leq d,\ m = 1, \ldots, M$.

We may assume $\partial\Omega_1 \cap \partial D \neq \emptyset$, that is, Ω_1 is the interstitial region. We set

$$Q_k := \{u = (\tilde{u}_1, \ldots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^{N} H^1(\Omega_\alpha) : \forall j,\ \tilde{u}_1(x + a_j) = e^{ik\cdot a_j}\tilde{u}_1(x), \quad \text{for } x = \sum_{l \neq j} c_l a_l,\ 0 < c_l < 1\},$$

$u^i = (\tilde{u}^i_1, \ldots, \tilde{u}^i_N) \in Q_k \cap (\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)),\ i = 1, \ldots, M,\ \langle u^i, u^j\rangle = \delta_{ij}\ h_{ij} := \langle \nabla u^i, \nabla u^j\rangle + \langle u^i, V u^j\rangle$. We denote by $\tilde{E}_m$ the mth eigenvalue of (h_{ij}) in ascending order. Our another main theorem is the following.

Theorem 5.2. *Under the assumptions (A'), (B') and (C') there exist constants $C, \delta > 0$ depending only on $\{\Omega_\alpha\}$, a, b and d such that if*

$$M \sum_{i=1}^{M} \sum_{\alpha \neq \beta} \|\tilde{u}^i_\alpha|_{\partial\Omega_\alpha} - \tilde{u}^i_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)} < \delta,$$

we have

$$\tilde{E}_m \geq E_m - CM^2 \sum_{i=1}^{M} \sum_{\alpha \neq \beta} \|\tilde{u}^i_\alpha|_{\partial\Omega_\alpha} - \tilde{u}^i_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)},$$

for any $1 \leq m \leq M$.

The essence of the proof of Theorems 5.1 and 5.2 is the equivalence of two semi-norms in the Sobolev space concerned with discontinuity of the functions. For the proof of the equivalence we need to prove several results about the Sobolev space.

6 Outline of the proof

Let $\Omega_\alpha \subset \mathbb{R}^n,\ \alpha = 1, \ldots, N$ be regions with boundaries of class C^l, $l \geq 1$ such that $\Omega_\alpha \cap \Omega_\beta = \emptyset,\ \alpha \neq \beta$. We denote by D the region such that $\bigcup_{\alpha=1}^N \overline{\Omega}_\alpha = \overline{D}$. We denote by T^α_{l-1} the trace operator in Ω_α (cf. [5]). The following can be proved by the divergence theorem using a partition of unity and C^l mappings that map the boundaries to hyperplanes.

Proposition 6.1. *Assume that* $\tilde{u}_\alpha \in H^l(\Omega_\alpha)$, $\alpha = 1, \dots, N$, *and define* $u \in L^2(D)$ *by* $u(x) = \tilde{u}_\alpha(x)$ *for* $x \in \Omega_\alpha$. *Then* $u \in H^l(D)$ *if and only if*

$$(T^\alpha_{l-1}\tilde{u}_\alpha)(x) = (JT^\beta_{l-1}\tilde{u}_\beta)(x),\ x \in \partial\Omega_\alpha \cap \partial\Omega_\beta,$$

for any $\alpha \neq \beta$ *such that* $\partial\Omega_\alpha \cap \partial\Omega_\beta \neq \emptyset$, *where* $J : \bigoplus_{m=0}^{l-1} H^{l-m-1/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta) \to \bigoplus_{m=0}^{l-1} H^{l-m-1/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)$ *is defined by*

$$J\boldsymbol{g} := (g_0, \dots, (-1)^m g_m, \dots, (-1)^{l-1} g_{l-1}),$$

for $\boldsymbol{g} = (g_0, \dots, g_{l-1}) \in \bigoplus_{m=0}^{l-1} H^{l-m-1/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)$.

Let $(H^1_0(\Omega))^\perp$ be the orthogonal complement of $H^1_0(\Omega)$ in $H^1(\Omega)$.

Lemma 6.2. *Let* Ω *be a region with a bounded boundary of class* C^3. *Then there exists a constant* $C > 0$ *such that*

$$\|u\|_{H^2(\Omega)} \leq C\|u|_{\partial\Omega}\|_{H^{3/2}(\partial\Omega)},$$

for any $u \in (H^1_0(\Omega))^\perp \cap H^2(\Omega)$.

We have a decomposition $H^2(\Omega_\alpha) = (H^1_0(\Omega_\alpha) \cap H^2(\Omega_\alpha)) \bigoplus ((H^1_0(\Omega_\alpha))^\perp \cap H^2(\Omega_\alpha))$. Obviously we have $\sum_{\alpha\neq\beta}\|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)} = 0$ for $(\tilde{u}_1, \dots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N (H^1_0(\Omega_\alpha) \cap H^2(\Omega_\alpha))$. Therefore, one would expect that the norm of $(\tilde{u}_1, \dots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N ((H^1_0(\Omega_\alpha))^\perp \cap H^2(\Omega_\alpha))$ could be estimated using $\sum_{\alpha\neq\beta}\|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)}$. However, this is not the case, because on $\partial\Omega_\alpha \cap \partial\Omega_\beta$ the values of $\tilde{u}_\alpha|_{\partial\Omega_\alpha}$ and $\tilde{u}_\beta|_{\partial\Omega_\beta}$ can cancel out. In order to avoid this, we decompose an element in $\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)$ into a sum of tuples that have nonzero difference $\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}$ only on different $\partial\Omega_\alpha \cap \partial\Omega_\beta$ on which the difference is given by $\tilde{u}_\alpha|_{\partial\Omega_\alpha}$ because $\tilde{u}_\beta|_{\partial\Omega_\beta} = 0$.

We suppose that Ω_α, $\alpha = 1, \dots, N$ are regions satisfying (A) or (A'). Then for any $1 \leq \alpha \leq N$ there exists a region $\hat{\Omega}^\alpha \subset \mathbb{R}^n$ satisfying the following condition. In the case of (A) (resp., (A')) if Ω_α is bounded (resp., $\partial\Omega_\alpha \cap \partial D = \emptyset$), then $\Omega_\alpha \subset \hat{\Omega}^\alpha$, $\partial\hat{\Omega}^\alpha \subset \partial\Omega_\alpha$ and $\partial\hat{\Omega}_\alpha$ has only one connected component. If Ω_α is unbounded (resp., $\partial\Omega_\alpha \cap \partial D \neq \emptyset$), then $\hat{\Omega}^\alpha = \mathbb{R}^n$ (resp., $\hat{\Omega}^\alpha = D$) in the case of (A) (resp., (A')). Intuitively, $\hat{\Omega}^\alpha$ is the region obtained by filling up the holes in Ω_α.

We denote connected components of $\partial\Omega_\alpha$ that enclose bounded regions not including points in Ω_α by $(\partial\Omega_\alpha)_1, \dots, (\partial\Omega_\alpha)_{P_\alpha}$ (if such connected components exist), and denote the bounded region in $\mathbb{R}^n$ whose boundary is $(\partial\Omega_\alpha)_p$ by $\hat{\Omega}_{\alpha,p}$. (Intuitively, $\hat{\Omega}_{\alpha,p}$, $p = 1, \dots, P_\alpha$ are holes in Ω_α.) Then there exists some $1 \leq \beta \leq N$ such that $\hat{\Omega}^\beta = \hat{\Omega}_{\alpha,p}$.

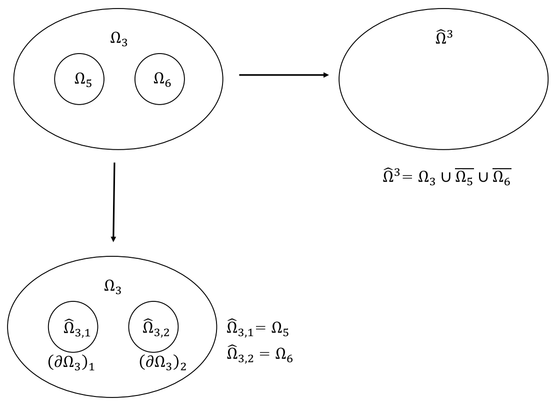

Figure 3: Definitions of the regions

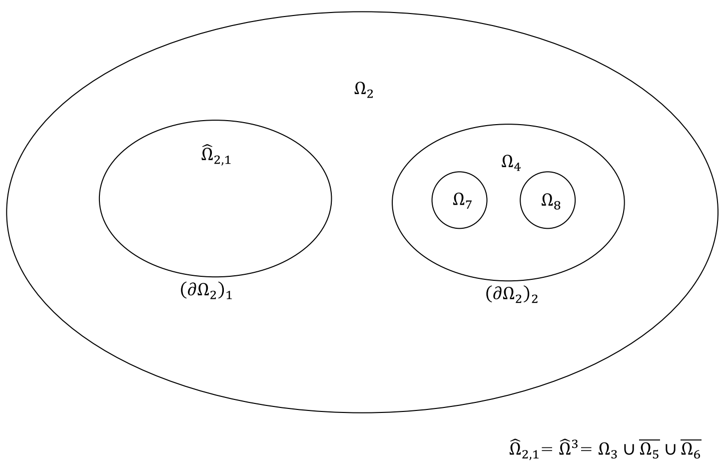

Figure 4: Definitions of the regions

For example $\hat{\Omega}^2 = \Omega_2 \cup \overline{\Omega_3} \cup \overline{\Omega_5} \cup \overline{\Omega_6} \cup \overline{\Omega_4} \cup \overline{\Omega_7} \cup \overline{\Omega_8}$.

We shall consider the case of (A). Let $u_\alpha \in H^2(\hat{\Omega}^\alpha)$. If we set $\tilde{u}_\beta \in H^2(\Omega_\beta)$ by $\tilde{u}_\beta(x) = u_\alpha(x),\ x \in \Omega_\beta$ for $\Omega_\beta \subset \hat{\Omega}^\alpha$ and $\tilde{u}_\beta = 0$ for $\Omega_\beta \not\subset \hat{\Omega}^\alpha$, we can identify $u_\alpha \in H^2(\hat{\Omega}^\alpha)$ with $(\tilde{u}_1, \ldots, \tilde{u}_N) \in \bigoplus_{\beta=1}^N H^2(\Omega_\beta)$. In this sense we have

$$H^2(\hat{\Omega}^\alpha) \subset \bigoplus_{\beta=1}^N H^2(\Omega_\beta),$$

and therefore, we have

$$\sum_{\alpha=1}^{N} H^2(\hat{\Omega}^\alpha) \subset \bigoplus_{\beta=1}^{N} H^2(\Omega_\beta).$$

In fact, the opposite inclusion holds.

Lemma 6.3.

$$\sum_{\alpha=1}^{N} H^2(\hat{\Omega}^\alpha) = \bigoplus_{\beta=1}^{N} H^2(\Omega_\beta).$$

Let X be a Hilbert space and Y a closed subspace of X. We define $\mathrm{dist}\,(u,Y) := \inf_{w\in Y}\|u-w\|_X$, for $u \in X$, where $\|\cdot\|_X$ is the norm in X.

Theorem 6.4. *Assume (A) and let* $X = \bigoplus_{\alpha=1}^{N} H^2(\Omega_\alpha)$ *and* $Y = H^1(\mathbb{R}^n) \cap (\bigoplus_{\alpha=1}^{N} H^2(\Omega_\alpha))$. *Then there exists a constant* $C > 0$ *depending only on* $\{\Omega_\alpha\}$ *such that for any* $u \in X$ *we have*

$$C^{-1}\mathrm{dist}\,(u,Y) \le \sum_{\alpha\neq\beta} \|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)} \le C\mathrm{dist}\,(u,Y).$$

We also have the corresponding result for the case of (A').

Theorem 6.4 means that the semi-norms $\mathrm{dist}\,(u,Y)$ and $\sum_{\alpha\neq\beta}\|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)}$ are equivalent. ($\mathrm{dist}\,(u,Y) \ge 0$ and $\mathrm{dist}\,(au,Y) = |a|$ $\mathrm{dist}\,(u,Y)$ are obvious. To see $\mathrm{dist}\,(u+v,Y) \le \mathrm{dist}\,(u,Y) + \mathrm{dist}\,(v,Y)$, for any $\epsilon > 0$ choose $w_1, w_2 \in Y$ such that $\|u-w_1\|_X \le \mathrm{dist}\,(u,Y)+\epsilon$, $\|v-w_2\|_X \le \mathrm{dist}\,(v,Y)+\epsilon$, and note $\|u+v-(w_1+w_2)\|_X \le \mathrm{dist}\,(u,Y)+\mathrm{dist}\,(v,Y)+2\epsilon$.)

Since the true eigenfunctions are in Y, it follows from the right inequality that in order to approximate a true eigenfunction by $u \in \bigoplus_{\alpha=1}^{N} H^2(\Omega_\alpha)$ we must make the semi-norm $\sum_{\alpha\neq\beta}\|\tilde{u}_\alpha|_{\partial\Omega_\alpha} - \tilde{u}_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)}$ small. From this fact we can see that Theorems 5.1 and 5.2 are plausible. However, it is the left inequality that is used for the proof of the theorems, and it is much more difficult to prove than the right inequality.

Finally we need a lemma about orthonormalization of a basis in a Hilbert space. We set the norms $\|x\|_1 := \sum_{i=1}^{M}|x_i|$, $\|x\|_2 := (\sum_{i=1}^{M}|x_i|^2)^{1/2}$, $\|x\|_\infty := \max_{1\le i\le M}|x_i|$, $\|A\| := \sup_{x\neq 0}\frac{\|Ax\|}{\|x\|}$, $\|A\|_1 = \max_{1\le j\le M}\sum_{i=1}^{M}|a_{ij}|$ and $\|A\|_\infty = \max_{1\le i\le M}\sum_{j=1}^{M}|a_{ij}|$ (cf. [1]).

Lemma 6.5. *Let* $\Psi^i, \ldots, \Psi^M$ *be linearly independent vectors in a Hilbert space* $\mathcal{H}$ *such that if we define a matrix* $\mathcal{E} = (\epsilon_{ij})$ *by*

$$\langle \Psi^i, \Psi^j \rangle = \delta_{ij} + \epsilon_{ij},$$

we have $2\|\mathcal{E}\|_1 + \epsilon_{\max} < 1$, *where* $\epsilon_{\max} := \max_{1\le i\le M}|\epsilon_{ii}|$. *Then there exists an* $M \times M$ *matrix* B *such that* $(\hat{\Psi}^1, \ldots, \hat{\Psi}^M)^T := B(\Psi^1, \ldots, \Psi^M)^T$ *satisfies* $\langle \hat{\Psi}^i, \hat{\Psi}^j \rangle = \delta_{ij}$ *and* $\|B - I_M\|_\infty < (2\|\mathcal{E}\|_1 + \epsilon_{\max})(1 - 2\|\mathcal{E}\|_1 - \epsilon_{\max})^{-1}$.

$H = (h_{ij}),\ h_{ij} := \langle \nabla u^i, \nabla u^j \rangle + \langle u^i, Vu^j \rangle$ is diagonalized by an $M \times M$ unitary matrix $Y = (y_{ij})$ as $\bar{Y} H Y^T = \mathrm{diag}\,[\tilde{E}_1, \ldots, \tilde{E}_M]$.

Denoting $Y(u^1, \ldots, u^M)^T$ again by $(u^1, \ldots, u^M)^T$ we may assume that H is a diagonal matrix from the beginning. Here note that if we denote the old functions by $(u^1_{\mathrm{Old}}, \ldots, u^1_{\mathrm{Old}})^T$ and the new ones by $(u^1_{\mathrm{New}}, \ldots, u^1_{\mathrm{New}})^T = Y(u^1_{\mathrm{Old}}, \ldots, u^1_{\mathrm{Old}})^T$, the discontinuity of the new functions is estimated as

$$\begin{aligned} &\|(\tilde{u}^i_{\mathrm{New}})_\alpha|_{\partial\Omega_\alpha} - (\tilde{u}^i_{\mathrm{New}})_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)} \\ &\quad \le \sum_{j=1}^{M} \|(\tilde{u}^j_{\mathrm{Old}})_\alpha|_{\partial\Omega_\alpha} - (\tilde{u}^j_{\mathrm{Old}})_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)}. \end{aligned}$$

If there exists $M' < M$ such that $\tilde{E}_{M'+1}, \ldots, \tilde{E}_M > d$, from the assumption $E_i \le d$ the inequality for these eigenvalues are obvious and we have only to consider $(u^1, \ldots, u^{M'})$ and $M' \times M'$ matrix with entries $h_{ij},\ 1 \le i, j \le M'$. Thus we may assume that $\tilde{E}_1, \ldots, \tilde{E}_M \le d$ from the beginning.

From

$$\langle \nabla u^i, \nabla u^i \rangle + \langle u^i, Vu^i \rangle = \tilde{E}_i \le d,$$

we obtain

$$\|\nabla u^i\| \le \left(\frac{d+b}{1-a} \right)^{1/2} = C,$$

where $\|w\| := \langle w, w \rangle$. By Theorem 6.4 we can decompose u^i as $u^i = \Psi^i + \Phi^i$, where $\Psi^i \in H^1(\mathbb{R}^n) \cap (\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha))$ and

$$\|\Phi^i\|_{\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)} \le C \sum_{\alpha \ne \beta} \|\tilde{u}^i_\alpha|_{\partial\Omega_\alpha} - \tilde{u}^i_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)}.$$

Since $u^i = \Psi^i + \Phi^i$, we have

$$\|\nabla \Psi^i\| \le C + \|\nabla \Phi^i\|.$$

Moreover, from $\|u^i\| = 1$ it follows that

$$\|\Psi^i\| \le 1 + \|\Phi^i\|.$$

We define an $M \times M$ matrix $\check{H} = (\check{h}_{ij})$ by

$$\check{h}_{ij} := \langle \nabla \Psi^i, \nabla \Psi^j \rangle + \langle \Psi^i, V\Psi^j \rangle.$$

Then we have $\|H - \check{H}\|_\infty \le C((1+\epsilon')\epsilon'' + \epsilon' M)$, where $\epsilon' := \max_{1 \le i \le M}(\|\Phi^i\| + \|\nabla \Phi^i\|)$ and $\epsilon'' := \sum_{j=1}^M (\|\Phi^j\| + \|\nabla \Phi^j\|)$. By Lemma 6.5 if

$$3((1+\epsilon')\epsilon'' + \epsilon' \sqrt{M}) < 1/2, \tag{6.1}$$

there exists an $M \times M$ matrix B such that $(\hat{\Psi}^1, \ldots, \hat{\Psi}^M) := B(\Psi^1, \ldots, \Psi^M)^T$ satisfies $\langle \hat{\Psi}^i, \hat{\Psi}^j \rangle = \delta_{ij}$ and $\|B - I_M\|_\infty \le C(\epsilon'' + \epsilon' \sqrt{M})$. We define $\hat{H} = (\hat{h}_{ij})$ by

$$\hat{h}_{ij} := \langle \nabla \hat{\Psi}^i, \nabla \hat{\Psi}^j \rangle + \langle \hat{\Psi}^i, V\hat{\Psi}^j \rangle.$$

Then $\hat{H} = \bar{B}\check{H}B^T$ and $\|\hat{H} - \check{H}\|_\infty \le CM(\epsilon'' + \epsilon'\sqrt{M})(1 + \epsilon'' + \epsilon'\sqrt{M})$ which yields $\|\hat{H} - \check{H}\|_\infty \le CM(\epsilon'' + \epsilon'\sqrt{M})$ under (6.1).

Combining the estimate above we obtain $\|H - \hat{H}\|_\infty \le C\tilde{\epsilon}$ with $\tilde{\epsilon} := \epsilon'' + \epsilon' M + M(\epsilon'' + \epsilon'\sqrt{M})$. Since $\hat{\Psi}^i \in H^1(\mathbb{R}^n)$, by the Rayleigh-Ritz method the eigenvalues $\hat{E}_i$ of $\hat{H}$ are estimated as $\hat{E}_i \ge E_i,\ i = 1, \ldots, M$. By the perturbation theorem of matrices and $\|A\|_2 \le (\|A\|_\infty \|A\|_1)^{1/2} = \|A\|_\infty$ for an Hermitian matrix A, we can also see that $|E_i - \hat{E}_i| \le \|H - \hat{H}\|_\infty$. Thus we obtain

$$\tilde{E}_i \ge \hat{E}_i - C\tilde{\epsilon} \ge E_i - C\tilde{\epsilon}.$$

The result immediately follows from this, $\epsilon' := \max_{1\le i\le M}(\|\Phi^i\| + \|\nabla\Phi^i\|)$, $\epsilon'' := \sum_{j=1}^M (\|\Phi^j\| + \|\nabla\Phi^j\|)$,

$$\|\Phi^i\|_{\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha)} \le C \sum_{\alpha\ne\beta} \|\tilde{u}^i_\alpha|_{\partial\Omega_\alpha} - \tilde{u}^i_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)},$$

and

$$\begin{aligned}&\|(\tilde{u}^i_{\text{New}})_\alpha|_{\partial\Omega_\alpha} - (\tilde{u}^i_{\text{New}})_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)} \\ &\quad\le \sum_{j=1}^M \|(\tilde{u}^j_{\text{Old}})_\alpha|_{\partial\Omega_\alpha} - (\tilde{u}^j_{\text{Old}})_\beta|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha\cap\partial\Omega_\beta)}.\end{aligned}$$

The proof of Theorem 5.2 is almost the same as that of Theorem 5.1. We have only to modify Lemma 6.3 so that $\tilde{u}^i_1$ and ψ^i_1 satisfy the boundary condition: $u(x+a_j) = e^{ik\cdot a_j}u(x)$, for $x = \sum_{l\ne j} c_l a_l,\ 0 < c_l < 1$. For the estimate $\hat{E}_i \ge E_i$ we use that $-\Delta + V$ with the domain

$$\begin{aligned}\mathcal{D}_k := \{u \in H^2(D) : \forall j,\ & u(x+a_j) = e^{ik\cdot a_j}u(x), \\ (G_j\cdot\nabla)u(x+a_j) &= e^{ik\cdot a_j}(G_j\cdot\nabla)u(x),\ \text{for } x = \sum_{l\ne j} c_l a_l,\ 0 < c_l < 1\}\end{aligned}$$

is the selfadjoint operator associated with the quadratic form $\langle\nabla u, \nabla u\rangle_D + \langle u, Vu\rangle_D$ with the form domain

$$\begin{aligned}Q_k := \{u \in H^1(D) :& \forall j,\ u(x+a_j) = e^{ik\cdot a_j}u(x), \\ &\text{for } x = \sum_{l\ne j} c_l a_l,\ 0 < c_l < 1\}.\end{aligned}$$

where $D := \{x = \sum_{i=1}^n c_i a_i : \forall i,\ 0 < c_i < 1\}$.

7 An example (Three-dimensional square well)

We consider the eigenvalue problem $(-\Delta + V)u = Eu$ in $\mathbb{R}^3$

$$V(x) := \begin{cases} -V_0 & |x| < a \\ 0 & |x| \ge a \end{cases},$$

where $V_0 > 0$ is a constant. If the function space is restricted to that with angular momentum 0, the solution is

$$u(x) = (4\pi)^{-1/2} r^{-1} \chi(r),$$

where $r := |x|$, $\chi(r) = A \sin \alpha r,\ r < a$ and $\chi(r) = Ce^{-\beta r},\ r \geq a$ (cf. [3, Section 15]). Here $A, C \in \mathbb{R}$ are constants and $\alpha := (V_0 - |E|)^{1/2}$, $\beta := |E|^{1/2}$. The condition that the radial function is linearly dependent at $|x| = a$ is given by $\alpha \sin \alpha a - \beta \cos \alpha a = (V_0 - |E|)^{1/2} \sin(V_0 - |E|)^{1/2} a - |E|^{1/2} \cos(V_0 - |E|)^{1/2} a = 0$.

The eigenvalue is determined by this condition. If $\frac{\pi^2}{4} < V_0 a^2 \leq \frac{9\pi^2}{4}$, there exists only one eigenvalue. When $V_0 = 1$ and $a = \pi$, by solving the equation above numerically, we obtain the eigenvalue $E_1 = -0.457591$.

The coefficients for the normalized eigenfunctions are

$$A = 0.657960,\ C = 4.05791.$$

We change A and C (increase A and decrease C) under $\|u\| = 1$ and evaluate

$$\tilde{E}_1 = \langle \nabla u, \nabla u \rangle + \langle u, Vu \rangle.$$

Thus u is no longer continuous on the boundary $\partial\Omega_2 = \{x : |x| = a\}$, where $\Omega_1 := \{x : |x| > a\}$ and $\Omega_2 := \{x : |x| < a\}$. We obtain the estimate

$$\begin{aligned} \tilde{E}_1 \geq & -0.457591 - 0.271962 \|u|_{\partial\Omega_1} - u|_{\partial\Omega_2}\|_{L^2(\partial\Omega_2)} \\ & - O(\|u|_{\partial\Omega_1} - u|_{\partial\Omega_2}\|^2_{L^2(\partial\Omega_2)}). \end{aligned}$$

Since in this case the boundary value is constant and $H^{3/2}$ norm is equivalent to L^2 norm on the boundary, we can see that the order with respect to $\|u|_{\partial\Omega_1} - u|_{\partial\Omega_2}\|_{L^2(\partial\Omega_2)}$ in the main theorem can not be improved.

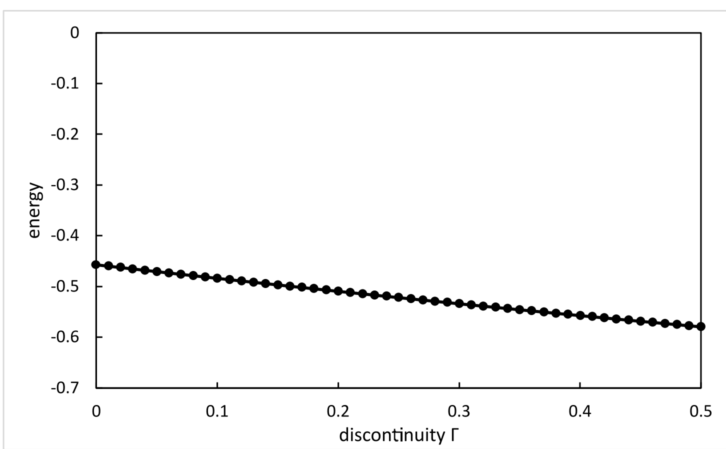

Figure 5: Energy dependence on discontinuity

For $\Gamma := \|u|_{\partial\Omega_1} - u|_{\partial\Omega_2}\|_{L^2(\partial\Omega_2)} = 0.1$ we have

$$\tilde{E}_1 = -0.484263 < E_1 = -0.457591.$$

For $\Gamma = \|u|_{\partial\Omega_1} - u|_{\partial\Omega_2}\|_{L^2(\partial\Omega_2)} = 0.5$ we have $\tilde{E}_1 = -0.579822$.

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References

[1] F. Chatelin. *Eigenvalues of matrices.* John Wiley & Sons, Chichester, 1993.

[2] G. Grosso and G. P. Parravicini. *Solid state physics.* Academic Press, Orland, 2000.

[3] L. I. Schiff. *Quantum mechanics.* McGraw-Hill, New York, 1968.

[4] J. C. Slater. Wave functions in a periodic potential. *Phys. Rev.*, 51:846–851, 1937.

[5] J. Wloka. *Partial differential equations.* Cambridge University Press, Cambridge, 1987.

[6] D. R. Yafaev. The semiclassical limit of eigenfunctions of the schrödinger equation and Bohr-Sommerfeld quantization condition, revisited. *Algebra i Analiz.*, 22:270–291, 2010. (Translation in St. Petersburg Math. J. 22 (2011), 1051-1067.).