

LOWER BOUND FOR SOLUTIONS TO THE SECULAR EQUATION IN A DIRECT SUM OF THE SOBOLEV SPACES OF DIVIDED REGIONS

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1. INTRODUCTION

1.1. Connection of locally constructed solutions. We consider the Schrödinger equation

$$(1.1) \quad (-\Delta + V)u = Eu,$$

in $\mathbb{R}^n$, where Δ is the Laplacian, V is a real valued function in $\mathbb{R}^n$, u is the eigenfunction and E is the eigenvalue. When the space dimension n is 1, exceptionally detailed information of the eigenfunctions and the eigenvalues is obtained by connecting solutions constructed on intervals at the end points of the intervals (see e.g. [7, Section 34] and [9]). Since the structures of the solutions of (1.1) are strongly affected by the local behavior of the potential V (in particular, the structure of an eigenfunction of an electron in neighborhoods of nuclei is very different from that in the interstitial region), it is desirable to develop methods that construct local solutions in several regions $\Omega_1, \dots, \Omega_N$ and connect the solutions at the boundaries $\Omega_\alpha \cap \Omega_\beta$, $\alpha \neq \beta$ also in the case of $n \geq 2$.

Actually, exact local solution itself is difficult to obtain when $n \geq 2$ in general. Nevertheless, in physical situations we can speculate local basis functions that approximate the local true solutions by their linear combinations. Thus it is expected to obtain approximations of the true eigenfunctions by the linear combinations of the basis functions u_α^i , $i = 1, 2, \dots$ in different regions Ω_α , $\alpha = 1, \dots, N$. However, these linear combinations cannot be connected exactly on the boundaries $\Omega_\alpha \cap \Omega_\beta$, $\alpha \neq \beta$ as stated above. Instead, in practical calculations a feasible method would be to construct linear combinations u^i , $i = 1, \dots, M$ that have only small discontinuity on the boundaries $\Omega_\alpha \cap \Omega_\beta$ first, and then solve the secular equation by these functions u^i as in the Rayleigh-Ritz method.

Here let us recall the secular equation and the Rayleigh-Ritz method. Let X be a Hilbert space, A be a semibounded selfadjoint operator in X , q be the quadratic form associated with A , and $Q \subset X$ be the form domain of q . For linearly independent elements $\{u^1, \dots, u^M\} \in Q$ in X we set $h_{ij} := q(u^i, u^j)$ and $s_{ij} := \langle u^i, u^j \rangle$. The secular equation for $E \in \mathbb{R}$ is defined by

$$\det(H - ES) = 0,$$

where $H = (h_{ij})$, $S = (s_{ij})$. In particular, if $\{u^i\}$ is orthonormal, S is a unit matrix and E is an eigenvalue of H . Let $\tilde{E}_1 \leq \dots \leq \tilde{E}_M$ be solutions to the secular equation and $E_1 \leq \dots \leq E_M$ be the M lowest eigenvalues of A . Then by the min-max principle (cf. [6, Theorem XIII.1, 2]) we have

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

The evaluation of eigenvalues E_m based on this inequality is called the Rayleigh-Ritz method.

The problem of the method in the second paragraph is that the relation between the true eigenvalues and the approximations of the eigenvalues obtained by solving the secular equation are not clear as in the Rayleigh-Ritz method because of the discontinuity of the functions u^i on the boundaries $\Omega_\alpha \cap \Omega_\beta$, that is, the eigenvalues $\tilde{E}_i(u^1, \dots, u^M)$, $i = 1, \dots, M$ obtained by the secular equation are not upper bounds of the true eigenvalues, and $\inf_{\{u^1, \dots, u^M\}} \tilde{E}_i(u^1, \dots, u^M)$, $i = 1, \dots, M$ do not coincide with the true eigenvalues in contrast to the Rayleigh-Ritz method.

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1.2. Augmented plane wave (APW) method. The augmented plane wave (APW) method is one of the methods of band structure calculations in solid state physics (see e.g. [5]) and an example in which the problem as above arises. The APW method was proposed by Slater [8]. The purpose of the APW method is to obtain eigenvalues of the Bloch functions. The Bloch function is a generalized eigenfunction in a periodic lattice with the primitive translation vectors $a_1, \dots, a_n \in \mathbb{R}^n$. The Bloch function restricted to the unit cell $D := \{x = \sum_{i=1}^n c_i a_i : \forall i, 0 < c_i < 1\}$ is an eigenfunction of the selfadjoint operator $-\Delta + V$ in $L^2(D)$ (the selfadjointness can be proved under a mild assumption on the potential) with the domain

$$(1.2) \quad \mathcal{D}_k := \left\{ u \in H^2(D) : \forall j, u(x + a_j) = e^{ik \cdot a_j} u(x), (G_j \cdot \nabla) u(x + a_j) = e^{ik \cdot a_j} (G_j \cdot \nabla) u(x), \right. \\ \left. x = \sum_{l \neq j} c_l a_l, 0 < c_l < 1 \right\},$$

for some $k \in \mathbb{R}^n$, where $G_i \in \mathbb{R}^n$ is the reciprocal lattice vector such that $G_i \cdot a_j = 2\pi\delta_{ij}$. We can also prove that the spectrum of the operator is discrete, the eigenvalue E_m (labeled in ascending order) depend analytically on k if it is simple, and $E_m \rightarrow \infty$ ($m \rightarrow \infty$). We divide D into regions as $D = \Omega_1 \cup \left(\bigcup_{\alpha=2}^N \bar{\Omega}_\alpha \right)$,

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

where $\bar{x}_\alpha$, $\alpha = 2, \dots, N$ are atomic sites and $R_\alpha > 0$. We assume that the potential has the form

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

which is called Muffin-Tin potential. 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. $\forall i, G \cdot a_i / (2\pi) \in \mathbb{Z}$. On the other hand, in Ω_α , $\alpha \geq 2$, we consider the linear combination

$$v_G(x) = e^{i(k+G) \cdot \bar{x}_\alpha} \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{lm}^{\alpha, k+G} \chi_l^\alpha(r_\alpha, E) Y_{lm}(\theta_\alpha, \varphi_\alpha),$$

where $(r_\alpha, \theta_\alpha, \varphi_\alpha)$ is the polar coordinates of $x - \bar{x}_\alpha$, $\chi_l^\alpha(r_\alpha, E)$ is a radial function depending on the energy E , and coefficients $A_{lm}^{\alpha, k+G}$ are determined so that the right-hand side coincides with $e^{i(k+G) \cdot x}$ on the boundaries $\partial\Omega_\alpha$. We consider the secular equation of such waves $u^i = v_{G_i}$ for different G_i and the eigenvalue E is determined from the condition that the equation has a solution. However, in practice the infinitely many coefficients $A_{lm}^{\alpha, k+G}$ can not be calculated and we need to cut off the expansion at some finite number of coefficients. Thus u^i are discontinuous on the boundaries $\partial\Omega_\alpha$ and the problem stated above arises. As for the mathematical convergence analysis of the APW method Chen and Schneider [3] proved existence of a convergent subsequence of approximate solutions as the basis set increases and an error estimate for the subsequence.

In the theory of finite element method there is a method to use functions discontinuous on boundaries of the elements. Such a method is called nonconforming finite element method (cf. [2, section 10.3]). There are also other methods such as discontinuous Galerkin (DG) method (cf. [4]). In some cases error estimates were obtained for nonconforming method and DG method. In these analysis specific forms of basis functions play crucial roles.

2. MAIN RESULT

Set $Q_k := \{u = (\tilde{u}_1, \dots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^N H^1(\Omega_\alpha); \forall j, \tilde{u}_1(x+a_j) = e^{ik \cdot a_j} \tilde{u}_1(x), x = \sum_{l \neq j} c_l a_l, 0 < c_l < 1\}$. We assume that for any $u \in \mathcal{D}_k$

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

that there exist $0 \leq a < 1$, $b \geq 0$ such that

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

and that there exists $d \geq 0$ such that $E_m \leq d$, $m = 1, \dots, M$, where $\mathcal{D}_k$ is defined by (1.2). Let $u^i = (\tilde{u}_1^i, \dots, \tilde{u}_N^i) \in Q_k \cap (\bigoplus_{\alpha=1}^N H^2(\Omega_\alpha))$, $i = 1, \dots, M$, $\langle u^i, u^j \rangle = \delta_{ij}$ and set $h_{ij} := \langle \nabla u^i, \nabla u^j \rangle + \langle u^i, Vu^j \rangle$, where $\langle u, v \rangle := \sum_{\alpha=1}^N \langle \tilde{u}_\alpha, \tilde{v}_\alpha \rangle_{\Omega_\alpha}$ and $\nabla u^i := (\nabla \tilde{u}_1^i, \dots, \nabla \tilde{u}_N^i)$. We denote by $\tilde{E}_m$ the m th eigenvalue of the matrix (h_{ij}) . The following is the main result.

Theorem 2.1 ([1]). *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 for any $1 \leq m \leq M$,

$$\tilde{E}_m \geq E_m - CM^{5/2} \sum_{i=1}^M \sum_{\alpha \neq \beta} \|\tilde{u}_\alpha^i|_{\partial\Omega_\alpha} - \tilde{u}_\beta^i|_{\partial\Omega_\beta}\|_{H^{3/2}(\partial\Omega_\alpha \cap \partial\Omega_\beta)}.$$

Thus the difference between E_m and the infimum of $\tilde{E}_m$ with respect to $\{u^i\}$ is estimated by the discontinuity of u^i on the boundaries. We also have a similar result for nonperiodic case in $\mathbb{R}^n$.

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