LOWER BOUND OF A QUADRATIC FORM DEFINED ON A DIRECT SUM OF SOBOLEV SPACES OF DIVIDED REGIONS

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1. Introduction

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

$$(-\Delta + V)u = Eu, \tag{1.1}$$

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. 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 $u_\alpha^i,\ i = 1, 2, \dots$ in different regions $\Omega_\alpha,\ \alpha = 1, \dots, N$. However, these linear combinations can not 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.

The problem of this method 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.

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 and an example in which the problem as above arises. 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 $a_1, \dots, a_n$. 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

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

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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 $E_m \to \infty$ $(m \to \infty)$. We divide D into regions as $D = \Omega_1 \cup \left(\bigcup_{\alpha=2}^{N} \overline{\Omega}_\alpha\right)$,

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

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

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

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 $\Omega_\alpha,\ \alpha \geq 2$, 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.

2. Main result

Set $Q_k := \{u = (\tilde{u}_1, \ldots, \tilde{u}_N) \in \bigoplus_{\alpha=1}^{N} H^1(\Omega_\alpha); \forall j,\ \tilde{u}_1(x + a_j) = e^{ik\cdot a_j}\tilde{u}_1(x),\ x = \sum_{l\neq j} c_l a_l,\ 0 < c_l < 1\}$. We assume relative boundedness of V and that there exist $0 \leq a < 1,\ b \geq 0$ such that

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

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

Theorem 2.1. *There exist constants $C, \delta > 0$ depending only on $\{\Omega_\alpha\}$, a, b and d such that if*

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

we have for any $1 \leq m \leq M$,

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

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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