

On the completeness of the compressed modes in the eigenspace

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November 2, 2013

Abstract

This note provides a completeness result on the compressed modes introduced in [7, 8]. We prove the fact that for an unbounded Hermitian operator, the sub-eigenspace of spanned by the first M eigenfunctions can be approximated by first N compressed modes with improvable accuracy as N increases, for any fixed regularization parameter μ .

1 Introduction

In [7], the authors introduce a novel framework for obtaining spatially localized (“sparse”) solutions to a class of problems in mathematical physics that can be formulated as variational problems. The method is to add an L^1 regularization term in the variational problem, which penalizes the L^1 norm of the solution. This yields solutions called the “compressed modes”. Numerical evidences in [7, 8] show that compressed modes have compact support. In recent work [1], the author provides some interesting theoretical analysis of compressed modes. It is shown that as the L^1 regularization term in the variational problem vanishes, the compressive modes converge in the L^2 norm to a unitary transformation of eigenfunctions of the original Hamiltonian. The idea of obtaining sparse solutions by ℓ^1 minimization can also be found in other work such as [5, 3, 2, 4, 9]. The regularization parameter for the L^1 term is used to balance between the consistency with the original problem and the sparsity of the solution.

In [7] the authors consider the time-independent Schrödinger’s equation for the independent particles, where the Hamiltonian is defined as

$$\hat{H} = -\frac{1}{2}\Delta + V(x), \tag{1}$$

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which is an unbounded positive-definite Hermitian operator. The variational problem for the ground state energy of N particles is proposed as

$$E_0 = \min_{\Phi_N} \sum_{j=1}^N \langle \phi_j, \hat{H} \phi_j \rangle \quad \text{s.t.} \quad \langle \phi_j, \phi_k \rangle = \delta_{jk}. \quad (2)$$

The solutions $\Phi_N = \{\phi_i\}_{i=1}^N$ are a set of orthonormal eigenfunctions corresponding to eigenvalues $\{\lambda_i\}_{i=1}^N$, where the eigenvalues are arranged in non-decreasing order. Any unitary transformation of $\{\phi_i\}_{i=1}^N$ also gives a set of solutions to this variational problem. In history, in order to obtain localized solutions to this problem, people choose the solutions to be some unitary transformation of the eigenfunctions, such that the solutions are “maximally localized”, which are called the localized Wannier functions [10, 6].

Different from this approach, the compressed modes are constructed by solving a new variational problem

$$E = \min_{\Psi_N} \sum_{j=1}^N \left(\frac{1}{\mu} |\psi_j|_1 + \langle \psi_j, \hat{H} \psi_j \rangle \right) \quad \text{s.t.} \quad \langle \psi_j, \psi_k \rangle = \delta_{jk}, \quad (3)$$

where the minimizers $\Psi_N = \{\psi_j\}_{j=1}^N$ are called the compressed modes for the variational problem (2), and $|\psi_j|_1 = \int_{\Omega} |\psi_j(x)| dx$. The compressed modes $\{\psi_i\}_{i=1}^N$ are shown to be more localized than the Wannier functions. But unlike Wannier functions, they cannot be obtained by a unitary transformation of the eigenfunctions of \hat{H} . We note that in [1] it was shown that for fixed N , a unitary transformation of the compressed modes and their associated eigenvalues converge as μ approaches infinity to their limiting values, which are eigenfunctions and eigenvalues of \hat{H} . In this paper we answer a different and important question, namely for fixed μ , under some unitary transformation, these compressed modes can approximate the eigenfunctions in a systematically improved manner as N increases. This result characterizes the closeness between the space spanned by the compressed modes and the true eigen space.

The rest of the paper is organized as follows. In Section 2, we formally describe the main result. In Section 3, we state the key lemmas that would be used in the proof of the main result, which is given in Section 4. The proofs to the lemmas are put in the appendix. In the end, we make some concluding remarks.

2 Main result

In general, let \hat{H} be an unbounded positive-definite Hermitian operator. It is well known that \hat{H} has discrete eigenvalues approaching infinity, and the corresponding eigen-functions can form a set of orthonormal basis in $L^2(\Omega)$, where Ω is the domain in consideration. We assume that Ω is bounded. Denote λ_i the eigenvalues for \hat{H} arranged in ascending order,

and ϕ_i be the corresponding orthonormal eigenfunctions. The first N compressed modes associated with \hat{H} refer to the solution to the variational problem (3). We claim the following result:

Theorem 1. *Given any fixed parameter μ , the first N compressed modes up to an unitary transformation, denoted by $\{\xi_1, \dots, \xi_N\}$, satisfies*

$$\|\phi_i - \xi_i\|_2^2 \leq \frac{2NC_\Omega}{\mu(\lambda_{N+1} - \lambda_i)}, \quad (4)$$

for $i = 1, \dots, N$, where C_Ω is a constant depending only on Ω .

If the eigenvalues $\{\lambda_i\}$ satisfies

$$\lim_{i \rightarrow \infty} \frac{i}{\lambda_i} = 0, \quad (5)$$

then for fixed integer $M < N$ and $i = 1, \dots, M$,

$$\|\phi_i - \xi_i\|_2 \leq \frac{2NC_\Omega}{\mu(\lambda_{N+1} - \lambda_M)}. \quad (6)$$

As a result,

$$\lim_{N \rightarrow \infty} \|\phi_i - \xi_i\|_2 = 0 \quad (7)$$

uniformly for $i = 1, \dots, M$.

Remark 1. *As an example, let $\hat{H} = -\frac{1}{2}\Delta$ and Ω be a finite interval, then the eigenvalues satisfy (5), in which the above theorem holds.*

3 Some useful lemmas

For the positive-definite unbounded Hermitian operator \hat{H} , the set of eigenfunctions $\{\phi_i\}_{i=1}^\infty$ is an orthonormal basis in $L^2(\Omega)$ up to a normalization. Let $\{\psi_1, \dots, \psi_N\}$ be a set of orthonormal functions in $L^2(\Omega)$. In particular, they can be the first N compressed modes. Then each ψ_j has an linear expansion

$$\psi_j = \sum_{i=1}^{\infty} a_{ji} \phi_i, \quad (8)$$

where a_{ji} are the coordinates of ψ_j under the basis $\{\phi_i\}$.

By the orthogonality of ψ_j 's, we have

$$\sum_{i=1}^{\infty} a_{ji}^* a_{ki} = \delta_{jk}, \quad (9)$$

where δ_{jk} is the Dirac delta function. A special case is that

$$\sum_{i=1}^{\infty} |a_{ji}|^2 = 1, \quad (10)$$

for $j = 1, \dots, N$.

Our first lemma is concerned with the summation of $|a_{ji}|^2$ in the first dimension, which is also given as Lemma 3.1 in [1].

Lemma 1. *In the previous notations,*

$$\sum_{j=1}^N |a_{ji}|^2 \leq 1, \quad (11)$$

for $i = 1, 2, \dots$

Proof. See the appendix. □

In the next lemma, we give an estimate of the error of the approximate energy in (3) to the true energy given by (2).

Lemma 2.

$$E_0 \leq E \leq E_0 + \frac{NC_{\Omega}}{\mu}, \quad (12)$$

where E and E_0 are defined in (3) and (2).

Proof. See the appendix. □

Remark 2. *In the definition of the variational problem (3), by replacing the L^1 term by any functional bounded by L^2 norm, the energy E still satisfies upper estimate*

$$E \leq E_0 + C_{\Omega}N/\mu, \quad (13)$$

for some constant C_{Ω} depending only on Ω .

A corollary of this lemma, also shown in [1], is that if $\mu \rightarrow \infty$, $E \rightarrow E_0$, which shows the consistency of the variational form (3) with (2).

The more important lemma, as follows, gives an sharper lower bound of E than that in Lemma 2.

Lemma 3. *Let the first N compressed modes be ψ_1, \dots, ψ_N . Use the notation in (8) and denote*

$$a_i = \sum_{j=1}^N |a_{ji}|^2, \quad (14)$$

for $i = 1, 2, \dots$

Then we have

$$\sum_{k=1}^N \langle \psi_k, \hat{H} \psi_k \rangle = \sum_{i=1}^N \lambda_i + \sum_{i=1}^N (1 - a_i)(\lambda_{N+1} - \lambda_i) + \sum_{i=N+1}^{\infty} a_i(\lambda_i - \lambda_{N+1}). \quad (15)$$

As a consequence, a lower bound for E is given by

$$E \geq E_0 + \sum_{i=1}^N (1 - a_i)(\lambda_{N+1} - \lambda_i). \quad (16)$$

Proof. Proof by standard calculation. Given in the appendix. \square

4 Proof of the main theorem

By (8), the compressed modes ψ_j has coordinates $\{a_{ji}\}_{i=1}^{\infty}$ under the basis $\{\phi_i\}_{i=1}^{\infty}$. Under an unitary transformation $U \in \mathbb{C}^{N \times N}$, $\{\psi_j\}_{j=1}^N$ are transformed to $\{\xi_j\}_{j=1}^N$, where each ξ_j has coordinates $\{b_{ji}\}_{i=1}^{\infty}$ under the basis $\{\phi_i\}_{i=1}^{\infty}$. More exactly,

$$U \begin{pmatrix} a_{1i} \\ a_{2i} \\ \vdots \\ a_{Ni} \end{pmatrix} = \begin{pmatrix} b_{1i} \\ b_{2i} \\ \vdots \\ b_{Ni} \end{pmatrix}, \quad (17)$$

for $i = 1, \dots$, and

$$\xi_j = \sum_{i=1}^{\infty} b_{ji} \phi_i, \quad (18)$$

for $j = 1, \dots, N$. By QR decomposition, there exists such an U that

$$\begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1N} \\ b_{21} & b_{22} & \cdots & b_{2N} \\ \vdots & \vdots & \cdots & \vdots \\ b_{N1} & b_{N2} & \cdots & b_{NN} \end{pmatrix} \quad (19)$$

is upper triangular, that is, $b_{ji} = 0$ for $i < j$, and b_{jj} are non-negative real numbers. Because unitary transformation preserves the length of the vector,

$$\sum_{j=1}^N |b_{ji}|^2 = \sum_{j=1}^N |a_{ji}|^2 = a_i. \quad (20)$$

Since $\{\xi_j\}_{j=1}^\infty$ are orthonormal,

$$\sum_{i=1}^{\infty} |b_{ji}|^2 = 1. \quad (21)$$

Because $b_{ji} = 0$ for $i < j \leq N$, for $i = 1, \dots, N$, we rewrite (20) as

$$\sum_{j=1}^i |b_{ji}|^2 = a_i, \quad (22)$$

and for $j = 1, \dots, N$, (21) becomes

$$\sum_{i=j}^{\infty} |b_{ji}|^2 = 1. \quad (23)$$

Next we show that

$$|b_{ii}|^2 \geq \sum_{j=1}^i a_j - (i-1). \quad (24)$$

for $i = 1, \dots, N$.

By (22),

$$|b_{ii}|^2 = a_i - \sum_{j=1}^{i-1} |b_{ji}|^2, \quad (25)$$

From (23) we know

$$|b_{ji}|^2 \leq 1 - \sum_{k=j}^{i-1} |b_{jk}|^2. \quad (26)$$

Therefore, for $i = 1, \dots, N$

$$\begin{aligned} |b_{ii}|^2 &\geq a_i - \sum_{j=1}^{i-1} \left(1 - \sum_{k=j}^{i-1} |b_{jk}|^2 \right) \\ &= a_i - (i-1) + \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} |b_{jk}|^2 \\ &= a_i - (i-1) + \sum_{k=1}^{i-1} \sum_{j=1}^k |b_{jk}|^2 \\ &= a_i - (i-1) + \sum_{k=1}^{i-1} a_k \\ &= \sum_{k=1}^i a_k - (i-1). \end{aligned} \quad (27)$$

By Lemma 2 and 3, we have an estimate of a_i as defined in (14) as

$$\sum_{i=1}^N (1 - a_i)(\lambda_{N+1} - \lambda_i) \leq \frac{NC_\Omega}{\mu}, \quad (28)$$

where $a_i \leq 1$ as proved in Lemma 1. Because $\{\lambda_i\}$ are non-decreasing,

$$\sum_{k=1}^i (1 - a_k) \leq \frac{NC_\Omega}{\mu(\lambda_{N+1} - \lambda_i)}, \quad (29)$$

which is combined with (27) to give

$$1 \geq a_i \geq |b_{ii}|^2 \geq 1 - \frac{NC_\Omega}{\mu(\lambda_{N+1} - \lambda_i)}, \quad (30)$$

for $i = 1, \dots, N$. By our construction, b_{ii} are non-negative real numbers, so

$$(1 - b_{jj})^2 \leq 1 - b_{jj}^2 \leq \frac{NC_\Omega}{\mu(\lambda_{N+1} - \lambda_j)}. \quad (31)$$

Now we calculate $\|\phi_i - \xi_i\|_2^2$. We note (18) and write

$$\|\phi_j - \xi_j\|^2 = \left\| (b_{jj} - 1)\phi_j + \sum_{i=1, i \neq j}^{\infty} b_{ji}\phi_i \right\|^2 \quad (32)$$

Since $\{\phi_i\}_{i=1}^{\infty}$ are orthonormal,

$$\begin{aligned} \|\phi_j - \xi_j\|^2 &= (b_{jj} - 1)^2 + \sum_{i=1, i \neq j}^{\infty} |b_{ji}|^2 \\ &= (b_{jj} - 1)^2 + 1 - b_{jj}^2 \\ &\leq 1 - b_{jj}^2 + 1 - b_{jj}^2 \\ &\leq \frac{2NC_\Omega}{\mu(\lambda_{N+1} - \lambda_j)}. \end{aligned} \quad (33)$$

From this inequality we can conclude that for a fixed $\mu > 0$ and integer M , if eigenvalues of \hat{H} satisfy (5), then for $j = 1, \dots, M$, $\|\phi_j - \xi_j\|^2$ converges uniformly to 0 as $N \rightarrow \infty$.

5 Conclusion

In this short note, we prove a completeness theorem on the compressed modes. As discussed in Remark 2, the result in Theorem 1 still holds, up to a change in the constant coefficient, if the L^1 term is replaced by any functional bounded by L^2 norm in the variational problem (3).

By changing the variational formulation (3) to

$$E = \min_{\Psi_N} \sum_{j=1}^N \langle \psi_j, \hat{H} \psi_j \rangle + \frac{1}{\mu} |\Psi_N|_1 \quad \text{s.t.} \quad \langle \psi_j, \psi_k \rangle = \delta_{jk}, \quad (34)$$

where $|\Psi_N|_1$ denotes the 1-norm of the matrix, we can improve the estimate of $\|\phi_i - \xi_i\|_2^2$ to

$$\|\phi_i - \xi_i\|_2^2 \leq \frac{2C_\Omega}{\mu(\lambda_{N+1} - \lambda_i)}, \quad (35)$$

In this case the requirement (5) on the eigenvalues can be relaxed to

$$\lim_{i \rightarrow \infty} \lambda_i = \infty, \quad (36)$$

and $\|\phi_i - \xi_i\|_2^2$ converges uniformly to 0 as N goes to infinity, for $i = 1, \dots, M$ with M fixed.

A Proof of the lemmas

A.1 Proof of Lemma 1

The proof of this lemma is also given in [1], and here we give a different one. By (9) (the orthogonality condition), for any $\epsilon > 0$ and fixed N , there exists $n > N$ such that

$$A_n = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{N1} & a_{N2} & \cdots & a_{Nn} \end{pmatrix} \quad (37)$$

satisfies

$$\left| \sum_{i=1}^n a_{ji}^* a_{ki} \right| < \epsilon/N, \quad \text{for } j \neq k. \quad (38)$$

We now consider an $N \times N$ Hermitian matrix $B = (1 + \epsilon)I - A_n A_n^*$, whose j, k -th entry is

$$B_{jk} = \begin{cases} -\sum_{i=1}^n a_{ji} a_{ki}^* & \text{if } j \neq k \\ (1 + \epsilon) - \sum_{i=1}^n |a_{ji}|^2 & \text{if } j = k \end{cases}. \quad (39)$$

We note that

$$B_{jj} \geq \epsilon \quad \text{and} \quad \sum_{k \neq j, k=1}^N |B_{jk}| < \epsilon, \quad (40)$$

so B is a diagonal dominant Hermitian matrix with positive diagonal entries, hence it is positive-definite. Also $(1 + \epsilon)I - A_n^* A_n$ is an $n \times n$ positive-definite matrix, so its diagonal entries are all positive real numbers. Therefore, the diagonal entries of $A_n^* A_n$ are all less than $1 + \epsilon$, that is,

$$\sum_{j=1}^N |a_{ji}|^2 < 1 + \epsilon \text{ for } i = 1, \dots \quad (41)$$

Since $\sum_{j=1}^N |a_{ji}|^2$ is independent of ϵ , we let $\epsilon \rightarrow 0$ and obtain

$$\sum_{j=1}^N |a_{ji}|^2 \leq 1 \text{ for } i = 1, \dots \quad (42)$$

A.2 Proof of Lemma 2

Let $\Psi_N = \{\psi_j\}_{j=1}^N$ be the minimizer of (3), then

$$E > \sum_{j=1}^N \langle \psi_j, \hat{H} \psi_j \rangle \geq \min_{\Phi_N} \sum_{j=1}^N \langle \phi_j, \hat{H} \phi_j \rangle = E_0. \quad (43)$$

For any $\psi \in L^2(\Omega)$ with $\|\psi\| = 1$,

$$\int_{\Omega} |\psi| \, dx \leq \frac{1}{2} \int_{\Omega} \sqrt{|\Omega|} |\psi|^2 + \frac{1}{\sqrt{|\Omega|}} \, dx = \sqrt{|\Omega|}. \quad (44)$$

The equality holds when $|\psi| = \frac{1}{\sqrt{|\Omega|}}$ a.e. in Ω . Then

$$E = \min_{\Psi_N} \sum_{j=1}^N \left(\frac{1}{\mu} |\psi_j|_1 + \langle \psi_j, \hat{H} \psi_j \rangle \right) \leq \min_{\Psi_N} \sum_{j=1}^N \langle \psi_j, \hat{H} \psi_j \rangle + \sum_{j=1}^N \frac{1}{\mu} \sqrt{|\Omega|} = E_0 + \frac{N \sqrt{|\Omega|}}{\mu}. \quad (45)$$

A.3 Proof of Lemma 3

We note (8) and $\hat{H}\phi_i = \lambda_i\phi_i$,

$$\begin{aligned}
& \sum_{j=1}^N \langle \psi_j, \hat{H}\psi_j \rangle \\
&= \sum_{k=1}^N \sum_{i=1}^{\infty} |a_{ki}|^2 \lambda_i \\
&= \sum_{i=1}^{\infty} \sum_{k=1}^N |a_{ki}|^2 \lambda_i \\
&= \sum_{i=1}^N a_i \lambda_i + \sum_{i=N+1}^{\infty} a_i \lambda_i \\
&= \sum_{i=1}^N \lambda_i + \sum_{i=1}^N (1 - a_i)(\lambda_N - \lambda_i) + \sum_{i=1}^N (a_i - 1)\lambda_N + \sum_{i=N+1}^{\infty} a_i(\lambda_i - \lambda_N) + \sum_{i=N+1}^{\infty} a_i \lambda_N \\
&= \sum_{i=1}^N \lambda_i + \sum_{i=1}^N (1 - a_i)(\lambda_N - \lambda_i) + \sum_{i=N+1}^{\infty} a_i(\lambda_i - \lambda_N) + \left(\sum_{i=1}^{\infty} a_i \right) \lambda_N - N\lambda_N,
\end{aligned} \tag{46}$$

where a_i is defined in (14). Also we note that

$$\sum_{i=1}^{\infty} a_i = \sum_{i=1}^{\infty} \sum_{j=1}^N |a_{ji}|^2 = \sum_{j=1}^N \sum_{i=1}^{\infty} |a_{ji}|^2 = N, \tag{47}$$

where we use the fact (10). Then following (46) we have

$$\sum_{j=1}^N \langle \psi_j, \hat{H}\psi_j \rangle = \sum_{i=1}^N \lambda_i + \sum_{i=1}^N (1 - a_i)(\lambda_N - \lambda_i) + \sum_{i=N+1}^{\infty} a_i(\lambda_i - \lambda_N). \tag{48}$$

Acknowledgement

K.Y. would like to Dr. Jing Qin for her helpful discussions and comments.

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