34 Linear Operators

A linear partial differential operator is understood as a linear map from a function space into another function space. The most important case for physicists may be the linear map on a Hilbert space. We will discuss the meaning of self-adjointness of an operator in conjunction to quantum mechanics in Part A. Part B discusses spectral decomposition of an operator. Part C is a short summary of spectrum theory.

Key words: linear operator (symmetric, self-adjoint), operator extension, observable, spectral decomposition, decomposition of unity, spectral measure, semibound operator, spectrum (essential, point, discrete, absolute continuous), compact operator, Hilbert-Schmidt theorem.

Summary:
(1) In quantum mechanics, self-adjoint linear operators are regarded as observables. The reason why self-adjointness is required can be glimpsed in **34A.2-5**. [Notice that the explanation is probably very different from the one given in physics courses, because in the ordinary quantum mechanics courses self-adjointness is never explained correctly.]
(2) Spectral decomposition is a generalization of diagonalization of matrices, and is the theoretical underpinning of separation of variables (**34B.3**, **34B.6**).
(3) Whether we may apply the spectral decomposition to a partial differential operator can be checked very formally (**34B.5**).
(4) Spectrum of an operator is often directly related to physical observables as electronic and phonon spectra. A clear definition of spectrum must be recognized (**34C.2**). Physicists call absolutely continuous spectrum band spectrum, and point spectrum discrete spectrum (**34C.8**). Cantor-set like spectrum has also become relevant to physics, which is the singular continuous spectrum.

34.A Self-Adjointness

34A.1 Linear operator.[416] As discussed in **20.9** the superposition principle requires that the quantum mechanical state is described by a vector in a vector space (→**20.1**) (Hilbert space →**20.3**) V. A linear operator A is a linear map from a subspace $D(A)$ of V into V. $D(A)$ is called the *domain* of A, and $AD(A) \equiv \{Az : z \in D(A)\}$ is called the *range* of A. In quantum mechanics it is assumed that a linear operator (with appropriate properties) A corresponds to a dynamical variable (*observable*), and that for a state $|x\rangle$, the expectation value of the observable A is given by $\langle x|A|x\rangle$.[417]

Example. The domain of d/dx in $L_2([a,b])$ (→**20.5(2)**) is not the whole space, because d/dx cannot be operated on non-differentiable functions.[418] However, since $C^1([a,b])$ is dense in $L_2([a,b])$, the domain of d/dx is dense in $L_2([a,b])$.

34A.2 When can a linear operator be an observable?

(1) Let A be a linear operator on a Hilbert space V (→**20.3**). If $D(A)$ is dense in V and Hermitian (i.e., $\langle x|Ay\rangle = \langle Ax|y\rangle$[419]), we say A is *symmetric.* Since this is a necessary and sufficient condition for $\langle x|A|x\rangle$ to be real, physical observables must at least be symmetric.

(2) However, this is not enough, because the extension of A may not be symmetric. An operator $\tilde{A}$ such that $D(\tilde{A}) \supset D(A)$ and $A = \tilde{A}$ on $D(A)$ is called an *extension* of A. Unfortunately, indeed some symmetric operators are extended to non-symmetric operators.[420] The whole Hilbert space should be physically meaningful, so that symmetry is not enough to characterize a respectable observable.

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[416]The most authoritative (and accessible) reference is T. Kato, *Perturbation Theory for Linear Operators* (Springer, 1966).

[417]Dirac explicitly assumes these, while Landau and Lifshitz use spectral decomposition to justify the assumption. However, all the assumptions have come from the observations based on finite dimensional linear algebra.

[418]More precisely, $df/dx \in L_2([a,b])$ is required.

[419]Of course, this means

$$\int \overline{x(t)}(Ay)(t)dt = \int \overline{(Ax)(t)}y(t)dt.$$

[420]An example from H. Ezawa, *Quantum Mechanics III* (Iwanami, 1972) p26. follows. Let $V = L_2(\boldsymbol{R})$. The operator Z is defined by

$$Z\psi(x) = -i\left(x^3\frac{d}{dx} + \frac{d}{dx}x^3\right)\psi(x) \tag{34.1}$$

(3) It is important that a symmetric operator A which corresponds to a 'physical observable' should not be extended further. A condition is the self-adjointness. To understand this statement, we need the following entries.

34A.3 Adjoint operator. Let A be an operator on a Hilbert space V whose domain is dense. Let $D(A^*)$ be the totality of $x \in V$ such that

$$\langle x|Ay\rangle = \langle z|y\rangle \tag{34.3}$$

for all $y \in D(A)$ for some $z \in V$. For $x \in D(A^*)$ z is unique: if there were two z_1 and z_2, then $\langle z_1 - z_2|y\rangle = 0$ for $\forall y \in D(A)$. Since $D(A)$ is dense, this implies $z_1 = z_2$. Thus there is a unique map $x \to z$. We will write this as $z = A^*x$, defining a linear map A^*. This is called the *adjoint* of A.

For example, $-id/dx$ defined on C_0^1 [421] is self-adjoint:

$$\int d\tau \overline{f(x)} \left(-i\frac{d}{dx}\right) g(x) = \int d\tau \left\{\overline{-i\left(\frac{d}{dx}f(x)\right)}\right\} g(x), \tag{34.4}$$

so that indeed $(-id/dx)^* = -id/dx$.

34A.4 Self-adjoint operator. If A is a linear operator with a dense domain and $A = A^*$ (i.e., $D(A) = D(A^*)$ and symmetric), then A is called a *self-adjoint operator.*

34A.5 Observable should be at least self-adjoint. We know that an observable must be a symmetric operator. However, A^* is obviously its extension, so it is natural to interpret that A^* is 'the' observable. However, we know that this may not be symmetric. This strongly suggests that observables must be self-adjoint, so that we will never encounter imaginary eigenvalues. Later, we will learn that for a self-adjoint operator, we can unambiguously determine (define) the probability of observing a particular value (or a particular range of the values) for any state in the state space thanks to the spectral decomposition theorem (→**34B.3**). This justifies the identification.

with the dense domain spanned by $\{H_n e^{-x^2/2}\}$ (→**21B.6**). It is easy to check that Z is symmetric. However, if this is applied to

$$\varphi(x) = x^{-3/2}e^{-1/4x^2}, \text{ for } x > 0; \quad \text{otherwise } \varphi(x) = 0, \tag{34.2}$$

we know $Z\varphi(x) = -i\varphi(x)$ (except at $x = 0$; this exception may be ignored, because we are in a L_2-space), so that $\langle\varphi|Z|\varphi\rangle = -i$, the expectation value is purely imaginary!

[421] C^1 functions with compact supports, i.e., they vanish outside sufficieintly large sphere centeres at the origin.

34.B Spectral Decomposition

34B.1 Spectral decomposition in finite dimensional space. Consider a normal linear operator[422] A on a <u>finite</u> dimensional vector space. Let $\{\lambda\}$ be its eigenvalues, and $|\lambda\rangle$ be the corresponding normalized eigenkets. Then, we have the following *spectral decomposition* formula

$$A = \sum_\lambda |\lambda\rangle\lambda\langle\lambda| = \sum_\lambda \lambda P(\lambda), \tag{34.5}$$

where $P(\lambda)$ is the orthogonal projection (→**20.18**) to the eigenspace belonging to λ.

$$1 = \sum_\lambda |\lambda\rangle\langle\lambda| = \sum_\lambda P(\lambda) \tag{34.6}$$

is called a *decomposition of unity* (→**20.15**). If we can have this decomposition, we can spectral decompose the operator. How can we generalize this to the operators on a Hilbert space (→**20.3**)?

34B.2 Decomposition of unity in Hilbert space. This is, for physicists, just (→**20.23**)

$$1 \equiv \int_{-\infty}^{\infty} |\nu\rangle w(\nu) d\nu \langle\nu|, \tag{34.7}$$

where $|\nu\rangle$ is an eigenket or *improper eigenket* (because it may not be normalizable), and w is a weight function (let us call $w(\nu)$ a *spectral weight*). To find improper eigenkets is called the *generalized eigenvalue problem* (**35.5** solves the problem.).

34B.3 Theorem. Let A be a self-adjoint operator (→**34A.4**) on a Hilbert space V. Then, there is a unique decomposition of unity

$$1 = \int |\nu\rangle w(\nu) \langle\nu| \tag{34.8}$$

such that

$$A = \int_{-\infty}^{\infty} \nu\, |\nu\rangle w(\nu) d\nu \langle\nu|. \tag{34.9}$$

34B.4 Why do we pay attention to spectral decomposition?

[422] If a linear operator A satisfies $A^*A = AA^*$, then we say A is a *normal* operator. Its matrix representation is a *normal matrix* and is diagonalizable with a unitary transformation. Actually, a necessary and sufficient condition for a matrix A to be diagonalizable with a unitary transformation is that A is normal.

It is a fundamental tool to understand operators, and is a very useful tool for quantum mechanics. In our current partial differential equation context, the spectral decomposition is of superb importance with respect to, as the reader should have already guessed, the separation of variables (→**18**, **23**). However, to understand the justification of the method in general, we need almost all the machineries of elementary functional analysis. First of all, most partial differential operators are not self-adjoint. For example, the Laplacian with a homogeneous Dirichlet condition is only symmetric. Hence, to use the operator theory, we must consider the self-adjoint extension (→**34A.2**) of the differential operator. Rather heavy tools are required to obtain it, but the result boils down to:

34B.5 Practical conclusion. The following is a practical conclusion about differential operators:
(1) If $P(x,D)$ is formally self-adjoint, i.e.,

$$\int_\Omega f(x)P(x,D)g(x)dx = \int \left(P^T(x,D)f(x)\right)g(x)dx, \tag{34.10}$$

where

$$P^T(x,D)f(x) = \sum_{|\alpha|\le m}(-D)^\alpha(a_\alpha(x)f(x)), \tag{34.11}$$

for

$$P(x,D)f(x) = \sum_{|\alpha|\le m} a_\alpha(x)D^\alpha, \tag{34.12}$$

(This guarantees that the operator is symmetric (→**34A.2**)) and
(2) if $P(x,D)$ is *semibounded*, i.e., for any sufficiently differentiable $f \in L_2(\Omega)$, there is a positive α such that

$$\pm\int_\Omega f(x)P(x,D)f(x)dx \le \alpha\|f\|^2 \tag{34.13}$$

for $+$ or $-$, then (thanks to Friedrichs-Freudenthal's theorem[423]), then P can be extended to a self-adjoint operator and,
(A) The totality of normalized eigenfunctions $\{u_n\}$ of the operator:

$$P(x,D)u_n(x) = \lambda_n u_n(x), \tag{34.14}$$

makes an orthonormal basis for $L_2(\Omega)$,
and
(B) we may justify the separation of variables:

[423] See K. Yosida, *Functional Analysis* (Springer, 1980 Sixth edition), Chapter XI, Section 7, Theorem 2.

34B.6 Justification of separation of variables. Let Ω be a region and P be a partial differential operator (with appropriate boundary conditions) on $L_2(\Omega)$ satisfying the consitions (1) and (2) in **34B.5**. Then there is an appropriate weight w ($\rightarrow$**34B.3**) such that the solution to

$$L_t u = P(x, D)u, \tag{34.15}$$

where L_t is a differential operator with respect to time, is given by φ such that

$$L_t\langle\lambda|\varphi\rangle = \int \mu\langle\lambda|\mu\rangle w(\mu) d\mu\langle\mu|\varphi\rangle \;\; [= \lambda\langle\lambda|\varphi\rangle]. \tag{34.16}$$

The formula inside [ ] holds if the spectrum is discrete (if not, the formula is not simple as we will see in **36.5**).

Discussion.
(A) The extension may be understood formally as follows. Let L^* be the formal adjoint of L. Then the operator $\hat{L}$ introduced as follows is the extension of L (that is, $\hat{L}^* = \hat{L} \supset L$).

$$\langle u|\hat{L}v\rangle = \langle L^* u|v\rangle. \tag{34.17}$$

(B) We have encountered the following equation in **23.9** (2)

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2}\right] R = -\lambda^2 R \tag{34.18}$$

with the boundary conditions $R(a) = R(b) = 0$ ($a < b$). The eigenfunctions are written in terms of the following 'esoteric' functions $I_{im}(x)$ and $K_{im}(x)$. We wish to demonstrate that the eigenfunctions of this problem makes a complete system. We wish to use the 'high-tech' functional analytic weapon. That is:
(1) Demonstrate that the operator is formally self-adjoint.
(2) Demonstrate that the operator is semibounded ($\rightarrow$**25B.14**).
(C) With the aid of the same argument as above demonstrate that the totality of spherical harmonics makes a complete set of functions. That is, demonstrate that

$$L^2 \equiv \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{34.19}$$

is formally self-adjoint and semibounded.[424]

[424]Do not forget an appropriate weight when you perform integration. This also applies to (B).

34.C Spectrum

34C.1 Introduction to spectrum. Physicists usually write for a linear operator

$$L|\lambda\rangle = \lambda|\lambda\rangle \tag{34.20}$$

and say that λ is an eigenvalue. However, if L is a linear operator acting on a subset of a Hilbert space, then the equation makes sense, strictly speaking, only when $|\lambda\rangle$ is in the Hilbert space (That is, $|\lambda\rangle$ is normalizable →**20.3**). We know this is not always the case. If we rewrite (34.20) as

$$(L - \lambda)|\lambda\rangle = 0, \tag{34.21}$$

we realize that what we wish to mean by (34.20) is that $(L-\lambda)^{-1}$ is not a bounded operator: a linear operator A is a *bounded operator*, if its operator norm (→**12.2**) is bounded: $\|A\| \equiv \sup_{a\in D(A)} \|Aa\|/\|a\| < +\infty$.

34C.2 Resolvent, resolvent set. Let L be a linear operator on a Hilbert space V with a dense domain (→**34A.1**). The operator

$$R(\lambda) \equiv (L - \lambda I)^{-1} \tag{34.22}$$

is called the *resolvent* of L. If the domain of $R(\lambda)$ is dense, and $R(\lambda)$ is bounded on its domain, then λ is called a *regular point*. The totality of the regular points of L is called the *resolvent set* of L and is denoted by $\rho(L)$.

Notice that if $\lambda, \mu \in \rho(L)$, then

$$R(\lambda) - R(\mu) = (\lambda - \mu)R(\lambda)R(\mu). \tag{34.23}$$

This is called the *resolvent equation*.

Exercise.
(1) Demonstrate the resolvent equation.
(2) Construct the resolvent kernel (i.e., $R(x, y; \lambda) \equiv \langle x|(L-\lambda)^{-1}|y\rangle$) for $L = -d^2/dx^2$ with the boundary condition $u'(0) = u'(1) = 0$. Cf. **20.28**, **20.29**.

34C.3 Spectrum. Let L be a linear operator whose domain is dense in a Hilbert space V. Then $\sigma(L) \equiv \boldsymbol{C} \setminus \rho(L)$ is called the *spectrum* of L. In other words, λ is a point in the spectrum of L, if $(L-\lambda)^{-1}$ is not defined, or even if it is defined, its domain is not dense in V, or even if dense, it is not a bounded operator.

34C.4 Classification of spectrum. Let T be a linear operator whose domain is dense in a Hilbert space V.
(1) If $T - \lambda$ is not one to one, that is, there is a nonzero ket $|u\rangle$[425] such

[425] Of course, the ket must be in the Hilbert space. That is, it must be normalizable.

that $A|u\rangle = \lambda|u\rangle$, we say λ is an eigenvalue. The totality of such λ is called the *point spectrum* of T.
(2) If $T - \lambda$ is one to one, but if $R(\lambda)$ is not a bounded linear operator, and
(21) if the domain of $R(\lambda)$ is dense, then we say λ belongs to the *continuous spectrum.*
[(22) if the domain of $R(\lambda)$ is not dense, then we say λ belongs to the residual spectrum.]

34C.5 Discrete and essential spectrum. The totality of eigenvalues is called the *point spectrum* σ_p. The union of the continuous spectrum and the set of eigenvalues of infinite multiplicity is called the *essential spectrum* and is denoted by $\sigma_{ess}(L)$. $\sigma(L) \setminus \sigma_{ess}(L)$ is called the *discrete spectrum* and is denoted by $\sigma_{disc}(L)$.

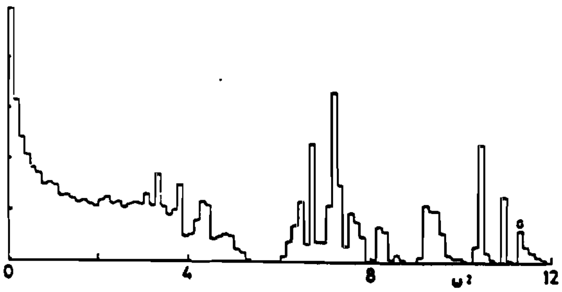
34C.6 Classification of continuous spectrum. Let L be a linear operator whose domain is in a Hilbert space V with a continuous spectrum $\sigma_c(L)$. It is classified as follows:

Let $w(\lambda)$ be the spectral weight (→**34B.2**). If for any set $A \subset \sigma_c(L)$ with measure zero (→**19.3**) $\int_A |\lambda\rangle w(\lambda) d\lambda \langle\lambda| V = \{0\}$, we say the spectrum is absolutely continuous, and the continuous spectrum is called an *absolutely continuous* spectrum. The definition applies to a subset of $\sigma_c(L)$, so we may say the operator L has an absolutely continuous spectrum in $[a,b]$, if $\int_a^b |\lambda\rangle w(\lambda) d\lambda \langle\lambda| VV$ is a nontrivial subspace of the Hilbert space V, but for any measure zero subset Q of $[a,b]$ $\int_Q |\lambda\rangle w(\lambda) d\lambda \langle\lambda| V = \{0\}$. Otherwise, we say L has a *singular continuous spectrum* (like the one concentrated on a Cantor set).

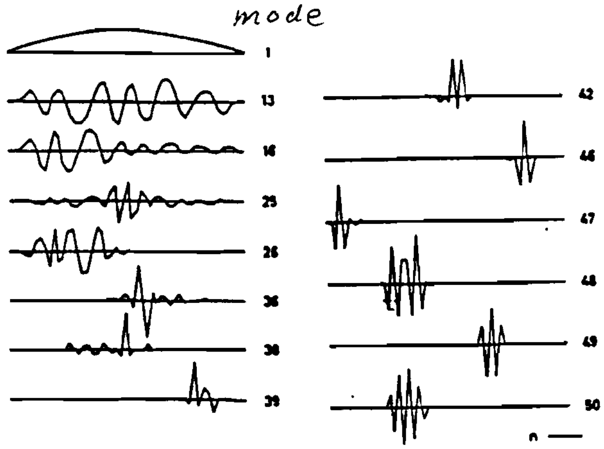
34C.7 Pure point spectrum. Let L be a linear operator whose domain is dense in a Hilbert space V. If the linear hull of the eigenspaces for all $\lambda \in \sigma_p(L)$ is dense in V, then we say L has a *pure point spectrum.*

34C.8 Are the above classification relevant to physics?.
(1) The Hamiltonian of 1D harmonic oscillator has a pure point spectrum. $\sigma = \sigma_p = \sigma_{disc}$.
(2) The Hamiltonian of a particle in a 1D periodic potential has an absolutely continuous spectrum, which physicists call a band spectrum.
(3) Consider a random 1d harmonic lattice. For example, the value of the spring constant is k or $k'(\neq k)$ chosen randomly for each spring, or a harmonic lattice with a uniform spring constant but two kinds of mass points m and $M(\neq m)$ randomly placed on the lattice points. In this case all the harmonic modes are localized (i.e., in l_2 →**20.5(1)**) and its spectrum is pure point (→**34C.7**). The reason for the localization is not very hard to understand intuitively; if there is a cluster of lighter

atoms, then they tend to behave differently from the rest. If the reader solve a finite size lattice system, then the mode localization lengths may be larger than the system size, so she would see clear localization for higher frequency modes only as illustrated below:



H:L = 1 to 1



(4) The problem in (3) is mathematically the same as the random Frenkel model; that is, the discrete Schrödinger equation with random hopping or with random site potential energy can be cast into the harmonic lattice problem. In this case localization is called the *Anderson localization.*
(5) If the spring constant or hopping probability above is chosen to be almost periodic (that is, it behaves like sin kx with k being irrational),[426] then the spectrum becomes self-similar.

In this case the eigenfunctions are not localized in the standard sense (i.e., not in l_2), but very different from the ordinary delocalized wave functions. If the largest peak is normalized, then in many cases the slow algebraic decay is observed. Experimentally, now we can fabricate almost periodic layered structures on which we can perform optical experiments. Numerically, the behavior above can be observed most easily with the most irrational $k = 1/(1 + 1/(1 + /(1 + 1/(\cdots$.

Wave function → for an almost periodic system (after Kohmoto)

[426]Physicists say a function $f(x)$ is almost periodic if $f(x)$ is a sum of periodic functions with incommensurate (not rationally related) periods.

(6) If the system exhibits only a point spectrum, then there cannot be any transport of phonons or electrons, because all the eigenfunctions are spatially localized.

Discussion.

If the system exhibits only a point spectrum, then there cannot be any transport of phonons or electrons, because all the eigenfunctions are spatially localized.

34C.9 Compact operator. If a linear operator A has a sequence of finite-dimensional operator[427] converging[428] to it, we say A is a *compact operator.* If A is self-adjoint, then, roughly speaking, we can write $A \sim \sum_{k=1}^{N} |k\rangle\lambda_k\langle k|$.

34C.10 Integral operator, Fredholm integral equation. Formally we can introduce a linear operator by the following integral[429]

$$(\Gamma u)(x) = \int_a^b dy\, w(y)K(x,y)u(y), \tag{34.24}$$

where we assume $u \in L_2([a,b],w)$ (→**20.19**), and K is an integrable function. Γ is often called a *Fredholm operator*, and K is called its *kernel.*

$$u = \Gamma u + f \tag{34.25}$$

for some function $f \in L_2([a,b],w)$ is called a *Fredholm integral equation.*

34C.11 Theorem [Hilbert-Schmidt]. Γ in **34C.10** is a compact operator, if

$$\int_a^b dx\, w(x) \int_a^b dy\, w(y)|K(x,y)|^2 < \infty. \tag{34.26}$$

Exercise.

The inverse operator of the regular Sturm-Liouville operator is compact. Demonstrate this statement. Cf. **15.6.**

34C.12 Spectral theorem for compact self-adjoint operator [Hilbert-Schmidt]. Let A be a compact self-adjoint operator (→**34C.4**) on a Hilbert space V. Then,

(1) V has an orthonormal basis $\{|e_n\rangle\}$ consisting of eigenvectors of A.

(2) Let $A|e_n\rangle = \lambda_n|e_n\rangle$. Then $\lambda_n \to 0$ as $n \to \infty$.

(3) If $|x\rangle = \sum c_n|e_n\rangle$, then $A|x\rangle = \sum c_n\lambda_n|e_n\rangle$. □

[427] A linear operator B is said to be finite dimensional, if its non-zero spectrum is point (→**34C.4**) and the total dimension of its eigenspaces is finite.

[428] with respect to the operator norm.

[429] Mathematicians introduce a measure $d\mu$ instead of w. Cf. **a19.**

Thus, almost everything true for a finite dimensional Hermitian matrix is true. The only caution we need is that we cannot freely change the order of the vectors in the basis (→**20.17**). □
Compactness implies $A \sim \sum_{k=1}^{N} |k\rangle\lambda_k\langle k|$, so intuitively, the theorem is plausible.

34C.13 Variational Principle for compact self-adjoint operator. Let A be a compact (→**32C.9**: do not forget that the theorem is NOT for any self-adjoint operator) self-adjoint linear operator on a Hilbert space V. The unit vector $|f\rangle$ which maximizes $\langle f|A|f\rangle$ is an eigenvector of A belonging to the eigenvalue with the largest modulus which is identical to $|\langle f|A|f\rangle|$. □

34C.14 Finding eigenvalues with the aid of variational principle. With the aid of **34C.13** we can determine the largest modulus eigenvalue λ_1 of a compact self-adjoint linear operator A, and a vector maximizing $F(x)$ to be denoted by $|\lambda_1\rangle$. Let V_1 be the perpendicular subspace to $|\lambda_1\rangle$. Since

$$\langle\lambda_1|A|y\rangle = \lambda_1\langle\lambda_1|y\rangle = 0, \qquad (34.27)$$

if $|y\rangle \in V_1$, so is $A|y\rangle \in V_1$. Hence we can apply the same argument to A restricted to V_1. In this way we can construct the nonincreasing sequence (in modulus) of eigenvalues $\lambda_1, \lambda_2, \cdots$.