Eigenvectors and Approximations in Quantum Mechanics

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States as information packages

- in physics, a 'model' is a prediction instrument
- everything there is to know about a system is coded in the *state* of the system
- states are modelled as unit vectors in a complex Hilbert space
- observables (such as position, momentum, energy) correspond to self adjoint operators

Example

Two key operators in quantum mechanics are the *position operator* Q and the *momentum operator* P (here in one dimension)

$$Q(\psi)(x) = x\psi(x)$$

$$P(\psi)(x) = -i\hbar\frac{d\psi}{dx}(x)$$

where $\hbar = h/2\pi$, and h is the Planck constant.

Two approaches

Eigenvector approach

- basically assuming everything works as in a finite dimensional case
- used in beginning physics courses

Wave function approach

- working in $L_2(\mathbb{R}^n)$
- used by mathematical physicists

Eigenvector approach

- for each observable, the possible observed values are eigenvalues of the corresponding operator
- the eigenvectors of the operator span the state space

Example

E.g. there is a state $|x_0\rangle$ corresponding to the position x_0.

- linear combinations of eigenstates correspond to *superpositions* of possible states, and the coefficients give the probability of observing the corresponding eigenvalue
- observation changes the state: after observing an eigenvalue, the system will be in the corresponding eigenstate

Wave function approach

- states are *wave functions*, i.e., unit vectors in $L_2(\mathbb{R}^n)$
- no eigenvalues or eigenvectors for the operators one is interested in
- the wave function gives the probability distribution of the position of a particle
- the oscillations of the wave function encode the momentum; the Fourier transform is an isometry between the position and momentum spaces of the particle

Example

The probability that for a state $\psi(x)$ (in position space) the particle is in the interval $[x_0, x_1]$ is given by

$$\int_{x_0}^{x_1} |\psi(x)|^2 dx.$$

Time evolution

The system evolves over time and this is described by a unitary *time evolution operator*

$$K^t : H \to H$$

that describes change in time interval t (the time independent case). If

the state of the system at time 0 is $\psi_0(x)$, then the state at time t is

$$\psi_t(x) = K^t(\psi_0(x)).$$

Time evolution with eigenvectors: the propagator

The propagator

$$\langle y|K^t|x\rangle$$

gives the probability amplitude for a particle to travel from position x to position y in a given time interval t.
The notation means the inner product of $|y\rangle$ and $K^t|x\rangle$, where $|x\rangle$ and $|y\rangle$ are the eigenvectors corresponding to positions x and y respectively.

Time evolution with wave functions: the kernel

In the wave function formalism, one calculates time evolution via the integral representation of the time evolution operator.
So $K(x, y, t)$ is a function such that

$$\psi_t(y) = K^t(\psi_0)(y) = \int_{\mathbb{R}} K(x, y, t)\psi_0(x)dx.$$

Are these the same?

To describe the same physical reality, both models should give the same value.

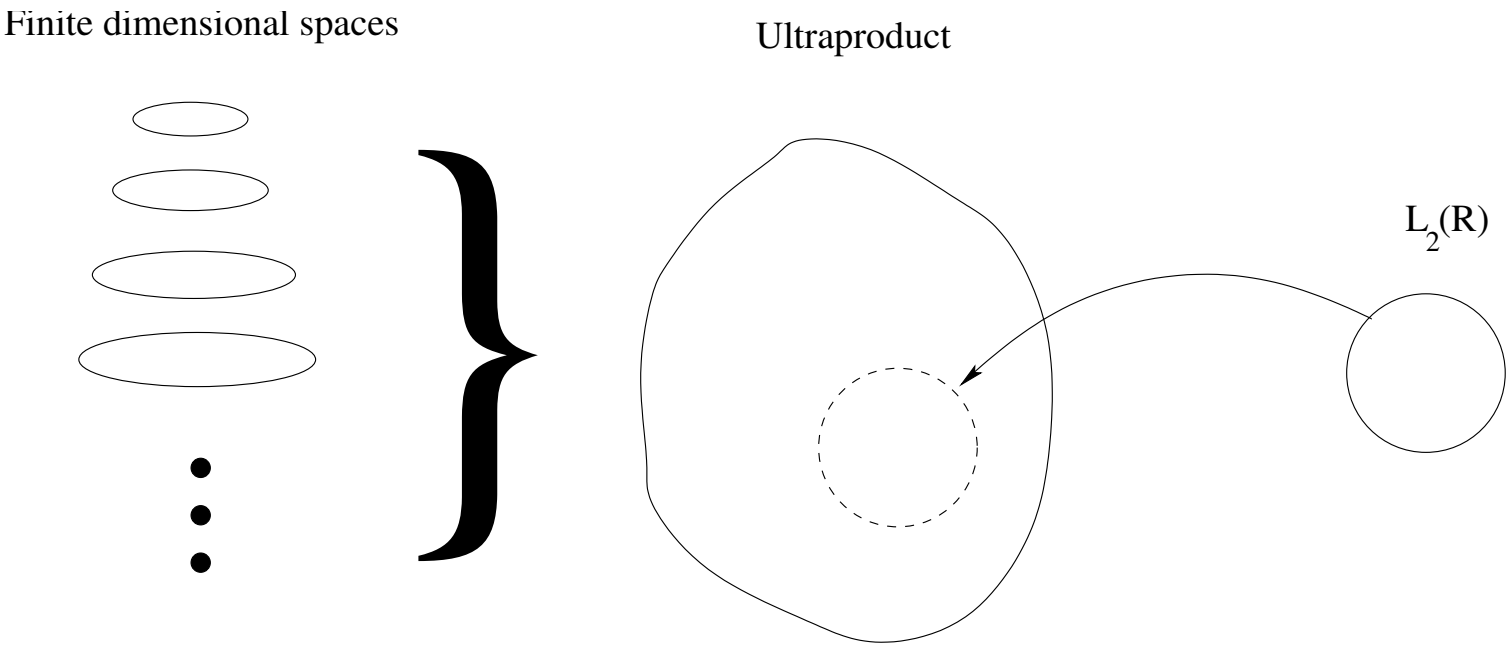
$$K(x, y, t) \stackrel{?}{=} \langle y | K^t | x \rangle$$

But how can we even compare them?

Finite dimensional approximations

- physicists seem to use the eigenvector approach as an intuitive idea, but mainly calculate by other means
- when finite dimensional models are used, it is not always clear what is meant by 'approximation'
- we give a model theoretic approach to approximations

Approximations via ultraproducts



The finite dimensional Hilbert spaces H_N

Definition

Let for each N, H_N be an N-dimensional Hilbert space with two orthogonal bases

$$\{u_n : n < N\} \quad \text{and} \quad \{v_n : n < N\}$$

such that

$$v_n = \sqrt{\frac{1}{N}} \sum_{m=0}^{N-1} e^{i2\pi nm/N} u_m$$

and thus

$$u_n = \sqrt{\frac{1}{N}} \sum_{m=0}^{N-1} e^{-i2\pi nm/N} v_m.$$

Operators in H_N

Definition

Further let

$$Q_N(u_n) = \frac{n}{\sqrt{N}} u_n \quad \text{and} \quad P_N(v_n) = \frac{hn}{\sqrt{N}} v_n,$$

and define (the unitary operators)

$$U^t = e^{itQ_N} \quad \text{and} \quad V^t = e^{itP_N}.$$

Lemma

Then the Weyl commutator relation $V^w U^t = e^{i\hbar tw} U^t V^w$ holds whenever $\sqrt{N}\hbar t$ is an integer.

Remark

In no finite dimensional space can the commutator relation $[Q, P] = i\hbar$ hold, as this requires the operators to be unbounded.

Ultraproduct of Hilbert space models

- start with indexed set of Hilbert space models H_N ($N \in \mathbb{N}$) and an ultrafilter D on $\mathbb{N}$
- define norms on elements of cartesian product $\prod_{N\in\mathbb{N}} H_N$ as ultralimits of coordinatewise norms
- cut out 'infinite part'
- mod out infinitesimals modulo D
- for operators with a uniform bound, we can define an ultraproduct operator in a straightforward fashion

But...

- the real Q and P are unbounded,
- we need P and Q for calculations, not just their exponentials.

Building unbounded operators in ultraproducts

Theorem

Let, for each $i \in I$, H_i be a complex Hilbert space and P_i a bounded operator on H_i (where the bound may vary with i). Further assume there are complete subspaces H_i^k (possibly $\{0\}$), for all $k < \omega$, such that

1. *if $k \neq l$, then H_i^k and H_i^l are orthogonal to each other,*
2. *$P_i(H_i^k) \subseteq H_i^k$,*
3. *for all $k < \omega$, there is $0 < M_k < \omega$ such that for all $i \in I$ and $x \in H_i^k$*

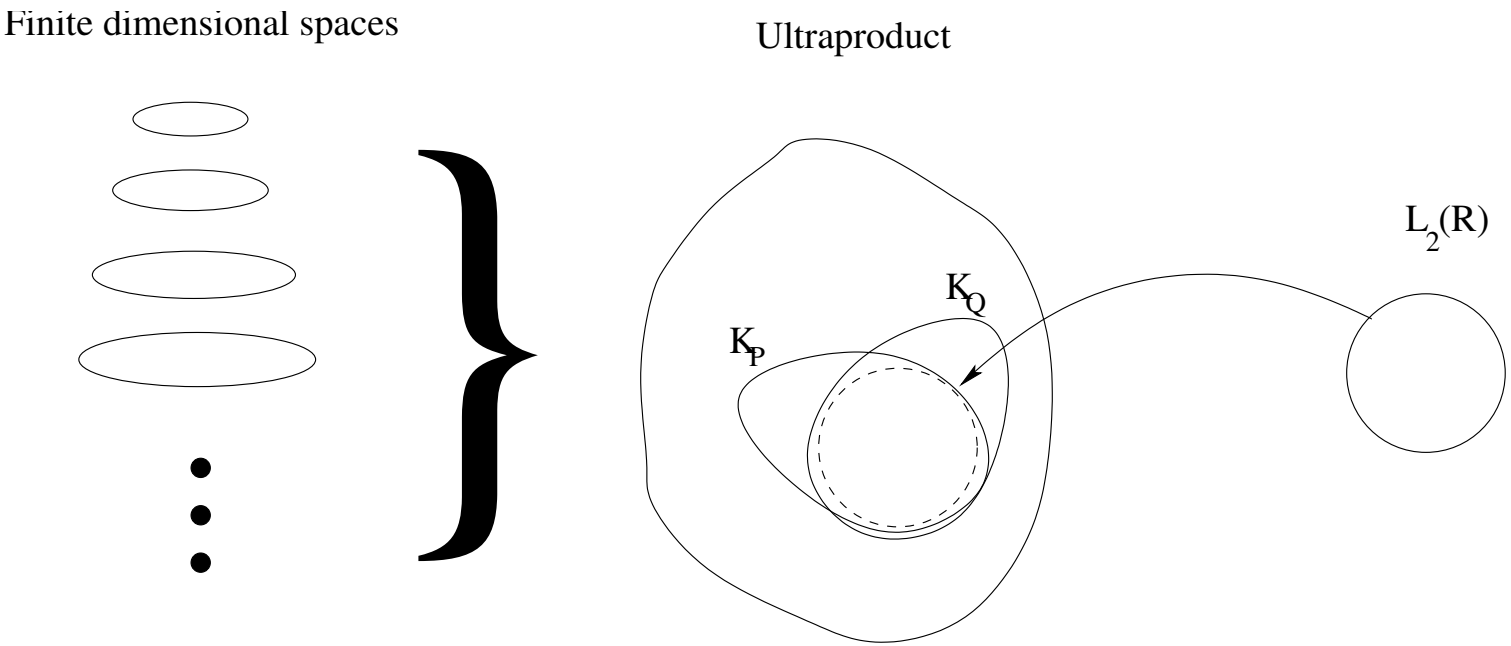
$$\frac{1}{M_k}\|x\| \leq \|P_i(x)\| \leq M_k\|x\|.$$

Theorem (continued)

Then if D is an ultrafilter on I, there is a closed subspace K of the metric D-ultraproduct of the spaces H_i where we can define the ultraproduct of the operators P_i as an unbounded operator P satisfying

1. *on a dense subset of K, $P(f/D) = (P_i(f(i)))_{i\in I}/D$ and*
2. *if for $n < \omega$, $f_n/D \in \mathrm{dom}(P)$ and both $(f_n/D)_{n<\omega}$ and $(P(f_n/D))_{n<\omega}$ are Cauchy sequences, and $(f_n/D)_{n<\omega}$ converges to f/D, then P is defined at f/D and $P(f/D) = \lim_{n\to\infty} P(f_n/D)$.*

The K-subspaces



Theorem

With the above definitions,

1. *for a dense set of t, w, the Weyl commutator relation*

$$V^w U^t = e^{i\hbar tw} U^t V^w$$

   holds,
2. *P and Q have (partially defined) unbounded ultraproducts and these operators have eigenvectors for all real positions (although they do not span the whole space),*
3. *a metric version of Łos's theorem holds when we restrict our parameters to the parts where P and Q are defined.*

Embedding the $L_2(\mathbb{R})$ model

To see that the ultraproduct model tells us something of the $L_2(\mathbb{R})$ model, we need an embedding:

Definition

In a dense set of ('nice') functions $f \in L_2$ (e.g., C_c^∞, the set of compactly supported smooth functions) let $F(f) = (F_N(f)|\ N < \omega)/D$, where for $N > 1$

$$F_N(f) = \sum_{n=0}^{(N/2)-1} N^{-1/4} f(nN^{-1/2}) u_n + \sum_{n=N/2}^{N-1} N^{-1/4} f((n-N)N^{-1/2}) u_n.$$

As F is isometric, it can be extended to all of $L_2(\mathbb{R})$.
And it maps the quantum mechanical operators Q and P correctly.

Now we can compare the propagator and the kernel

But **they differ!**

Example

When the units are chosen such that $th/2m \in \mathbb{Z}$, then for rational positions x_0, x_1 the propagator for the free particle in H_N is

$$\langle x_1 | K^t | x_0 \rangle = N^{-1/2} thm^{-1} K(x_0, x_1, t),$$

when thm^{-1} divides $\sqrt{N}(x_1 - x_0)$ and 0 otherwise, where $K(x_0, x_1, t) = (m/2\pi i\hbar t)^{1/2} e^{im(x_0 - x_1)^2/2\hbar t}$ is the value of the kernel.

What can be done?

$$\langle x_1 | K^t | x_0 \rangle = N^{-1/2} thm^{-1} K(x_0, x_1, t)$$

- the factor $N^{-1/2}$ stems from the interval corresponding to 'steps' between eigenvectors, so it can be justified
- for fixed x_0, x_1, we can argue that $\sqrt{N}(x_1 - x_0)$ is as divisible as we like, when N grows large
- we can change the embedding of $L_2(R)$ to change the operator P is mapped to, to get rid of the factor thm^{-1}
- **but** then we get the wrong probabilities (as predicted in the model)
- so the propagator is actually correct *in the model where it is calculated*

What is happening?

- calculations in N-dimensional model depend on divisibility questions – the model of dimension N only 'sees' positions that are multiples of $1\sqrt{N}$ apart; puts too much weight on these transitions, and 0 on others
- in the ultraproduct there are actually continuum many orthogonal eigenvectors for each position (corresponding to different sequences of eigenvectors in the H_Ns)
- there is no guarantee one has enough divisibility along the way in these sequences, but in a sense the average is correct
- since we cannot compute the average in the ultraproduct, we do it along the way
- this corresponds to calculating the *kernel* instead of the *propagator*

Calculating the kernel in the ultraproduct

Use

$$K(\alpha,\beta,t) = \lim_{\varepsilon\to 0} \int_{\beta-\varepsilon}^{\beta+\varepsilon} \int_{\alpha-\varepsilon}^{\alpha+\varepsilon} \phi(x)K(x,y,t)dxdy \,/\, ((2\epsilon)^2\phi(\alpha))$$

and calculate the limit in the ultraproduct,

- in the finite-dimensional models, calculate the average probability amplitude over small regions and look at the value in the ultraproduct
- in ultraproduct, look at the limit as regions shrink
- This gives the correct kernel!

Why is this interesting?

- calculations with eigenvectors are (relatively) easy
- our method gives a robust description for what approximation means

 Å. Hirvonen, T. Hyttinen. *On eigenvectors, approximations and the Feynman Propagator*, Ann. Pure Appl. Logic 170 (2019), no. 1, 109-135.