Stone-von Neumann theorem and superposition principle: superselection rule for scattering a particle on a 1D potential barrier

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based on

[1] Chuprikov N.L. On the need to revise the superposition principle for a particle with a continuous energy spectrum: superselection rule for a one-dimensional scattering. arXiv:1805.03952v3 [physics.gen-ph]

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Goal

The superposition principle is at the heart of quantum mechanics (QM), and there is a firm conviction that its modern formulation is faultless.

Our goal is to show that this is not so in the general case:

- the modern formulation of the superposition principle is justified only for a particle with a *discrete* energy spectrum;
- to a particle with a *continuous* energy spectrum it is inapplicable.

The modern formulation of the superposition principle in QM:

- a sum (“superposition") of two or more pure states of a quantum particle is another pure state of the particle;
- every pure state of a particle can be represented as a sum of two or more other pure states of the particle.

Thus, the space of pure states can not be a direct sum of nontrivial orthogonal subspaces invariant with respect to the action of the (canonical) position and momentum operators (otherwise, we would have to distinguish between pure states belonging to different subspaces).

In other words, this formulation requires that the position and momentum operators must act irreducibly in the space of pure states = the Schrödinger representation must be irreducible.

Do these (unbounded) operators obey this requirement?

There is no *rigorous* answer to this question. By F. Strocchi, “without the condition of *boundedness* the whole linear structure of the observables is in question". The present proof of the irreducibility of the Schrödinger representation is two-step:

(1) On the basis of the Stone-von Neumann theorem it is rigorously proved that the (bounded) Weyl exponentials $e^{i\hat{x}u}$ and $e^{i\hat{p}v}$ of the usual (unbounded) position and momentum operators $\hat{x}$ and $\hat{p}$ act irreducibly in the space of pure states of a particle; here $u, v \in \mathbb{R}^1$.

(2) Then, with making use of the heuristic “operational definition of observables", this result is extended onto the usual $\hat{x}$ and $\hat{p}$ operators.

“Operational definition of observables"

What is the essence of the “operational definition" (see F. Strocchi [2])? It tells us that

- due to the scale bounds of experimental apparatuses, one actually measures only *bounded* functions of x and p;
- thus, x and p are not observables in the operational sense – the unbounded $\hat{x}$ and $\hat{p}$ are rather *(physically harmless) extrapolations* of their bounded Weyl counterparts that fall under the “operational definition of observables".

[2] Strocchi F. An Introduction to the Mathematical Structure of Quantum Mechanics. A Short Course for Mathematicians. Advanced Series in Mathematical Physics. V.27. World Scientific Publishing (2005)

Intermediate conclusions

- The modern formulation of the superposition principle does not respect the unboundedness of the $\hat{x}$ and $\hat{p}$ operators $\Rightarrow$ either this formulation that imposes the tough requirement on the $\hat{x}$ and $\hat{p}$ operators, or their status, as operators representing physical observables in QM, must be revised.
- At present this controversy does not treated as a dilemma which must be resolved:
  the modern formulation is not questioned, while the *unbounded* $\hat{x}$ and $\hat{p}$ operators are treated as approximations of their *bounded* Weyl counterparts.

The superposition principle must respect the unboundedness of the position operator

It must distinguish between the discrete and continuous energy spectrum of a particle:

- Discrete energy spectrum – bound stationary states: for a given energy the probability of finding a particle at infinity is zero ⇒ the usual position operator is "effectively bounded" and, thus, can indeed be treated as an approximation of its bounded Weyl counterpart ⇒ the modern formulation of the superposition principle is true.
- Continuous energy spectrum – unbound stationary states: for a given energy the probability of finding a particle at infinity is nonzero ⇒ the unboundedness of $\hat{x}$ is essential ⇒ the modern formulation is unacceptable.

Example: Scattering a particle on a 1D potential barrier

Let $\hat{H}$ be the Hamiltonian to describe scattering a particle on a 1D potential barrier $V(x)$ which is zero outside the interval $[-a, a]$ and has no bound states; $|\psi_0\rangle$ be the initial state:

(a) $|\psi_0\rangle$ uniquelly determines the in-asymptote $|\psi_{in}\rangle = \hat{\Omega}_+|\psi_0\rangle$ and the out-asymptote $|\psi_{out}\rangle = \hat{\Omega}_-|\psi_0\rangle$, as well as the scattering state $e^{-i\hat{H}t/\hbar}|\psi_0\rangle$ that "interpolates" between these asymptotes; $\hat{\Omega}_\mp$ are the Moller operators.

(b) $|\psi_{out}\rangle = \hat{S}|\psi_{in}\rangle$ where $\hat{S} = \hat{\Omega}_-^\dagger \hat{\Omega}_+$ is the (unitary linear) scattering operator.

The subspaces of left and right asymptotes

In the distant past and future, a particle can be located both to the left and to the right of the barrier, far from it.

Thus, one has to distinguish between the *pure left* (in- and out-) asymptotes ψ_{left}^{in} and ψ_{left}^{out} and the *pure right* (in- and out-) asymptotes ψ_{right}^{in} and ψ_{right}^{out} that form the subspaces $\mathcal{H}_{left}^{in}$, $\mathcal{H}_{left}^{out}$, $\mathcal{H}_{right}^{in}$ and $\mathcal{H}_{right}^{out}$, respectively.

In the x-representation, left and right (normalized) asymptotes are infinitely differentiable functions nonzero in the disjoint spatial intervals $(-\infty, -a)$ and (a, ∞).

The spaces of in- and out-asymptotes $\mathcal{H}_{in}$ and $\mathcal{H}_{out}$ are direct sums of orthogonal subspaces of left and right asymptotes: $\mathcal{H}_{in} = \mathcal{H}_{left}^{in} \oplus \mathcal{H}_{right}^{in}, \quad \mathcal{H}_{out} = \mathcal{H}_{left}^{out} \oplus \mathcal{H}_{right}^{out} \Rightarrow$ in the distant past and furure the Schrödinger representation is reducible!

The first sign of the existence of a superselection rule

There exists an operator $\hat{T}$ such that the subspaces $\mathcal{H}_{left}^{in}$, $\mathcal{H}_{left}^{out}$, $\mathcal{H}_{right}^{in}$ and $\mathcal{H}_{right}^{out}$ are its eigenspaces of a point-like spectrum:

- $\hat{T} = \hat{P}_r - \hat{P}_l$; here $\hat{P}_r$ and $\hat{P}_l$ are projection operators defined as multiplication operators in the x-representation: $\hat{P}_r = \theta(x + a)$ and $\hat{P}_l = \theta(a - x)$; $\theta(x)$ is the Heaviside step function; $\hat{T}$ is a multiple of the identity operator.
- $\hat{T}|\psi_{right}^{in,out}\rangle = +|\psi_{right}^{in,out}\rangle$ and $\hat{T}|\psi_{left}^{in,out}\rangle = -|\psi_{left}^{in,out}\rangle$ – the subspaces $\mathcal{H}_{right}^{in}$ and $\mathcal{H}_{right}^{out}$ are its eigenspaces that correspond to the eigenvalue $+1$; while the subspaces $\mathcal{H}_{left}^{in}$ and $\mathcal{H}_{left}^{out}$ are its eigenspaces that correspond to the eigenvalue -1.

The second sign of the existence of a superselection rule

Superpositions of left and right asymptotes represent mixed vector states, rather than pure ones.

Let ψ_{out} be an arbitrary normalized out-asymptote from $\mathcal{H}_{out}$:

$$|\psi_{out}\rangle = e^{i\beta_l}\sqrt{W_{left}} \cdot |\psi^{out}_{left}\rangle + e^{i\beta_r}\sqrt{W_{right}} \cdot |\psi^{out}_{right}\rangle;$$

$0 < W_{left} < 1$, $W_{left} + W_{right} = 1$; β_l and β_r are real constants.

For any self-adjoint operator $\hat{A}$

$$\langle\psi_{out}|\hat{A}|\psi_{out}\rangle = W_{left} \cdot \langle\psi^{out}_{left}|\hat{A}|\psi^{out}_{left}\rangle + W_{right} \cdot \langle\psi^{out}_{right}|\hat{A}|\psi^{out}_{right}\rangle:$$

- This expression is typical for *mixed* states.
- It does not depend on the phases β_l and β_r – ψ_{out} is the superposition of mutually *incoherent* states.

The third sign of the existence of a superselection rule

For any self-adjoint operator $\hat{A}$

$\langle\psi^{in}_{left}|\hat{A}|\psi^{in}_{right}\rangle = \langle\psi^{out}_{left}|\hat{A}|\psi^{out}_{right}\rangle = 0$:

- transitions between the subspaces of left and right asymptotes, both in the distant past and future, are forbidden;
- the operator $\hat{A}$ and, thus, the position and momentum operators leave invariant these subspaces.

Superselection rule for scattering a particle on a 1D potential barrier

- In the spaces of in- and out-asymptotes there acts a dichotomous superselection rule that needs revising the modern formulation of the superposition principle for this scattering process:
  - a superselection operator is the operator $\hat{T}$;
  - coherent superselection sectors are the subspaces of left and right asymptotes.

Superposition principle for this 1D scattering process

- Superposition of any pure vector states from the same coherent sector is also a pure vector state from this sector.
- Superposition of any pure vector states from different coherent sectors is a mixed vector state.

Note that the Schrödinger dynamics crosses the coherent sectors (for example, for a particle impinging the barrier from the left the scattering operator transforms the left in-asymptote into the superposition of the left (reflected) and right (transmitted) out-asymptotes) $\Rightarrow$

- to calculate expectation values of observables for the whole process has no physical meaning;
- a correct quantum model of this scattering process must describe the quantum dynamics of its subprocesses – transmission and reflection – at all stages of scattering.

Conclusion

- The modern formulation of the superposition principle is inapplicable to quantum one-particle processes with a continuous energy spectrum; it is for this reason that the present models of such processes flood QM with paradoxes and unsolvable interpretational problems.
- But this formulation is quite applicable to quantum one-particle processes with a discrete energy spectrum; the present quantum models of such processes do not lead to interpretational problems.

Thank you for your attention!

Example of weight functions for left and right asymptotes

$A_{left}(k) \div A_{left}(x)$; here $A_{left}(x) = e^{-\frac{L^2 x^4}{x^2 - a^2}}$ for $x < -a$, and $A_{left}(x) \equiv 0$ for $x > -a$; L is a real constant.

$A_{right}(k) \div A_{right}(x)$; here $A_{riht}(x) = e^{-\frac{L^2 x^4}{x^2 - a^2}}$ for $x > a$, and $A_{right}(x) \equiv 0$ for $x < a$.