Simple quantum mechanical examples

Mathematics GR6434, Spring 2023

What physicists call "canonical quantization" can be understood in terms of the unique non-trivial representation of the Heisenberg group and Lie algebra, which wlll be described in detail in the second lecture. For one degree of freedom the Schrödinger version of this representation is on the space of wavefunctions (functions $\psi(q)$ of a position variable q) in $L^2(\mathbf{R})$. The representation operators are given in terms of the self-adjoint operators

$$Q = q, \quad P = -i\hbar\frac{d}{dq}$$

which satisfy the Heisenberg commutation relations

$$[Q, P] = i\hbar\mathbf{1}$$

A specific quantum mechanical system will require the specification of an addtional operator, the Hamiltonian. For a single quantum particle moving in one dimension, subject to a potential $V(q)$, the Hamiltonian is

$$H = \frac{1}{2m}P^2 + V(Q) = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + V(q)$$

One would like to find the eigenfunctions and eigenvalues of this operator, i.e. find $E, \psi_E(q)$ such that

$$(-\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + V(q))\psi_E(q) = E\psi_E(q)$$

and then expand wavefunctions at an initial time $t = 0$ in terms of the energy eigenfunctions $\psi_E(q)$. The Schrödinger equation

$$i\hbar\frac{d}{dt}\psi = H\psi$$

implies that these evolve in time as

$$\psi_E(q)e^{-\frac{i}{\hbar}Et}$$

For much more detail about these examples, see any physics textbook on quantum mechanics, or [1].

1 The free particle

The case of the free particle is the case $V(q) = 0$. Using Fourier analysis, one finds that the energy eigenvalues and eigenfunctions are parametrized by $p \in \mathbf{R}$ and are given by

$$E_p = \frac{p^2}{2m}, \quad \psi_{E_p}(q) = e^{i\frac{p}{\hbar}q}$$

The spectrum of the Hamiltonian is continuous, all non-negative values in $\mathbf{R}$.

The eigenfunctions are eigenvalues of the momentum operator P with eigenvalue p. P commutes with H, so it generates a symmetry of the states (symmetry under spatial translation). If one prepares a state at time 0 with wavefunction $\psi_{E_p}(q)$ and measure its momentum at any later times, one will always get the value p (the momentum is a conserved quantity).

The eigenfunctions of the operator Q are delta-functions $\delta(q - q')$, with eigenvalue $q' \in \mathbf{R}$. Unlike the case for momentum P, one has $[Q, H] \neq 0$ and these are not energy eigenfunctions. If one prepares a state at time 0 with wavefunction $\delta(q - q')$, so localized at $q = q'$, it will immediately evolve into a linear combination of states with all possible eigenvalues of Q. Measurement of position at later times t may give all possible different values.

Note that the eigenfunctions of Q and P are not functions in $L^2(\mathbf{R})$ and in addition, the operators Q and P don't preserve $L^2(\mathbf{R})$ (multiplying or differentiating by q can take a function that is square-integrable to one that isn't). To deal with these problems simultaneously, one can define the Schwartz space $\mathcal{S}(\mathbf{R})$ of functions such that the function and its derivatives fall off faster than any power at $\pm\infty$. The dual space $\mathcal{S}'(\mathbf{R})$ of continuous linear functionals on $\mathcal{S}(\mathbf{R})$ is called the space of tempered distributions, and includes the eigenfunctions of Q and P. One has the sequence of dense inclusions

$$S(\mathbf{R}) \subset L^2(\mathbf{R}) \subset \mathcal{S}'(\mathbf{R})$$

The Fourier transform takes each term in this sequence to itself. Duality interchanges $S(\mathbf{R})$ and $S'(\mathbf{R})$, and takes $L^2(\mathbf{R})$ to itself (Riesz representation theorem).

A problem here is that elements of $\mathcal{S}'(\mathbf{R})$ like the eigenfunctions of Q and P are not in $L^2(\mathbf{Q})$. They do not have well-defined norms, so will not be vectors in a unitary representation and the Born rule can't be used for them. However, they are linear functionals on $S(\mathbf{R})$ and one can use this to replace their inner products with elements of $S(\mathbf{R})$.

To get a well-defined formalism one has two options:

- Work with states $\psi \in L^2(\mathbf{R})$, taking great care with domains and ranges of operators like P, Q and H that are applied to states. In this case, eigenfunctions of these operators are not in the state space.

- Work with the space $S'(\mathbf{R})$ and distributional states, but be careful to properly pair these only with physical states in $\mathcal{S}(\mathbf{R})$ (sometimes called "wavepackets").

2 The harmonic oscillator

The quantum harmonic oscillator is the case of a particle moving in a quadratic potential $V(q) = \frac{1}{2}m\omega^2 q^2$

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 Q^2$$

The energy eigenvalues and eigenfunctions are given by

$$E_n = \hbar\omega(n + \frac{1}{2}), \quad \psi_n(q) = H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right)e^{-\frac{m\omega}{2\hbar}q^2}$$

where $n = 0, 1, 2, \ldots$ and $H_n(q)$ are Hermite polynomials. In this case the spectrum of the operator H is discrete, energy eigenfunctions are in $L^2(\mathbf{R})$, and arbitrary $t = 0$ wavefunctions in $L^2(\mathbf{R})$ can be written as linear combinations of the $\psi_{E_n}(q)$.

The easiest way to get these results is to work not with Q and P, but with complex linear combinations of these. For smplicity, rescaling so that $m = \omega = 1$, one can choose

$$a = \frac{1}{\sqrt{2}}(Q - iP) = \frac{1}{\sqrt{2}}(q - \frac{d}{dq}), \quad a^\dagger = \frac{1}{\sqrt{2}}(Q + iP) = \frac{1}{\sqrt{2}}(q + \frac{d}{dq})$$

$a, a^\dagger$ are each others adjoints and satisfy the commutation relation

$$[a, a^\dagger] = \mathbf{1}$$

The Hamiltonian is

$$H = \frac{1}{2}(Q^2 + P^2) = \frac{1}{2}(a^\dagger a + aa^\dagger) = a^\dagger a + \frac{1}{2}$$

One can easily see that $a^\dagger$ increases the eigenvalue of H by 1, a reduces it by 1. To have a spectrum bounded below, one needs a non-zero state $\psi_0(q)$ satisfying

$$a\psi_0(q) = \frac{1}{\sqrt{2}}(q - \frac{d}{dq})\psi_0(q) = 0$$

This state will have energy $\frac{1}{2}$ and by given by

$$\psi_0(q) = e^{-\frac{1}{2}q^2}$$

The other energy eigenstates will have energy $n + \frac{1}{2}$ and can be found explicitly by applying the operator $a^\dagger$ n-times to $\psi_0(q)$, so evaluating

$$(q + \frac{d}{dq})^n e^{-\frac{1}{2}q^2}$$

Note that for the harmonic oscillator, $V(q)$ is not translation invariant, and one has $[P, H] \neq 0$ as well as $[Q, H] \neq 0$ so neither position nor momentum are conserved quantities.

For more general potentials one can have both discrete (with eigenfunctions in $L^2(\mathbf{R})$) and continuous (with eigenfunctions not in $L^2(\mathbf{R})$ components of the spectrum. The physical interpretation will involved both "bound" states which correspond to particles localized in some regions of $\mathbf{R}$ and "scattering states" which correspond to particles with possible positions extending to $+\infty$ or $-\infty$.

References

[1] Woit, P., *Quantum Theory, Groups and Representations,* Springer, 2017.