Quantum Mechanics

The Schrödinger Equation: The Linear Harmonic Oscillator and the Heisenberg Algebra

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Pink Floyd: "Another Brick in the Wall (Pt. II)"

Quantum Mechanics

Exact Solutions (So Far)

- Solve in each region, patch with matching conditions:
  - If $W(x)$ crosses E discontinuously, $\Delta\psi(x_*)=0=\Delta\psi'(x_*)$;
    - If $W(x)=\lambda\,\delta(x-x_*)$, $\Delta\psi(x_*)=0$, $\Delta\psi'(x_*)=2\lambda M\,\psi(x_*)/\hbar$;
    - If $W(x)=\infty$ for $x\in[a,b]$, then $\psi(x)=0$ there, $\Delta\psi'(a)$ & $\Delta\psi'(b)$ free
  - Where $W(x)=const.$, $\psi(x)=N\sin(kx+\delta)$,
    - with $k^2=2M[E-W(x)]/\hbar^2$ if $E>W(x)$, and $k=-i\varkappa$ otherwise;
  - Where $W(x)=ax+b$, $\psi(ax+b)=A\,\mathrm{Ai}(ax+b)+B\,\mathrm{Bi}(ax+b)$,
    - with $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$ the two Airy functions;
    - use momentum representation (1st order PDE) I'LL BE BACK
  - Where $W(x)=ax^2+bx+c$, both representations: 2nd order PDE
    - Bounded from below, only bound states
    - Can be solved as PDE: $\psi(x)=N\,e^{-\alpha x^2}H_n(x)$; "_straightforward & tedious_"
    - Complete the square so $W(x)=a\,x^2$, by shifting $x\to x+x_0$ & $E\to E+E_0$;
    - Use that $\xi^2+\eta^2=\zeta_+\zeta_-$, with $\zeta_\pm=(\xi\pm i\eta)$.

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Algebraic Solution: Number Representation

- The linear harmonic oscillator (LHO) Hamiltonian

$$H = \tfrac{1}{2M}P^2 + \tfrac{1}{2}M\omega^2 Q^2 \qquad [Q,P] = i\hbar$$

representation independent

- Change variables: $a = \alpha Q + \beta P$ and $a^\dagger = (a)^\dagger$, so $[a, a^\dagger] = 1$:

$$a := \sqrt{\tfrac{M\omega}{2\hbar}}\,Q + \tfrac{i}{\sqrt{2M\hbar\omega}}\,P \qquad a^\dagger = \sqrt{\tfrac{M\omega}{2\hbar}}\,Q - \tfrac{i}{\sqrt{2M\hbar\omega}}\,P$$

$$Q = \sqrt{\tfrac{\hbar}{2M\omega}}\,(a^\dagger + a) \qquad P = i\sqrt{\tfrac{M\hbar\omega}{2}}\,(a^\dagger - a)$$

- With these new variables, the Hamiltonian is

$$H = \tfrac{1}{2}\hbar\omega(a\,a^\dagger + a^\dagger a) = \hbar\omega(a^\dagger a + \tfrac{1}{2}) = \hbar\omega\, a^\dagger a + \underbrace{\tfrac{1}{2}\hbar\omega}_{E_0}$$

- Since $H > 0$, we know that $E > 0 = W(0)$, and so $a^\dagger a > -½$.

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Algebraic Solution

- Since $H = \hbar\omega(a^\dagger a + ½)$, define $N := a^\dagger a$; then, $H = \hbar\omega(N + ½)$

$$H\,|E\rangle = E\,|E\rangle = \hbar\omega(N + \tfrac{1}{2})\,|E\rangle \qquad N\,|E\rangle = \underbrace{(E/\hbar\omega - \tfrac{1}{2})}_{:=\nu}\,|E\rangle$$

$$E = E_\nu = \hbar\omega(\nu + \tfrac{1}{2})$$

- re-label: $N\,|\nu\rangle = \nu\,|\nu\rangle \quad H\,|\nu\rangle = \hbar\omega(\nu + \tfrac{1}{2})\,|\nu\rangle$
- determine what we can about eigenvalues & eigenvectors.
- To that end, use $[a, a^\dagger] = 1$ (*Heisenberg algebra*) and calculate:

$$[N, a] = [a^\dagger a, a] = a^\dagger[a, a] + [a^\dagger, a]a = (-1)a \qquad [N, a] = -a$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger[a, a^\dagger] + [a^\dagger, a^\dagger]a = (+1)a^\dagger \qquad [N, a^\dagger] = +a^\dagger$$

- So, both a and $a^\dagger$ are eigen-operators of N.
- In addition, we continue to use $[a, a^\dagger] = 1 \;\Rightarrow\; a\,a^\dagger = 1 - a^\dagger a$
- Next, we need to find out the effect of a and $a^\dagger$ on the eigenstates of N and H.

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$$[N, a^\dagger] = +a^\dagger$$
$$[N, a] = -a$$

Algebraic Solution

- So, consider the effect of a & $a^\dagger$ on the eigenstates:

$$N(a\,|\nu\rangle) = a^\dagger a a\,|\nu\rangle = (a a^\dagger - 1)a\,|\nu\rangle = a a^\dagger a\,|\nu\rangle - a\,|\nu\rangle$$
$$= aN\,|\nu\rangle - a\,|\nu\rangle = a\nu\,|\nu\rangle - a\,|\nu\rangle = a(\nu-1)\,|\nu\rangle$$
$$N(a\,|\nu\rangle) = (\nu-1)(a\,|\nu\rangle) \qquad a\,|\nu\rangle = C_\nu\,|\nu-1\rangle$$

- To determine C_ν, use that the eigenstates are normalized:

$$\|a\,|\nu\rangle\|^2 = \|C_\nu\,|\nu-1\rangle\|^2 = \langle\nu-1|\,C_\nu^* C_\nu\,|\nu-1\rangle = |C_\nu|^2\langle\nu-1|\nu-1\rangle$$
$$= \langle\nu|\,a^\dagger a\,|\nu\rangle = \langle\nu|\,N\,|\nu\rangle = \langle\nu|\,\nu\,|\nu\rangle = \nu \qquad C_\nu = \sqrt{\nu}$$

- In perfect analogy:

$$N(a^\dagger\,|\nu\rangle) = (\nu+1)(a^\dagger\,|\nu\rangle) \qquad a^\dagger\,|\nu\rangle = D_\nu\,|\nu+1\rangle \qquad D_\nu = \sqrt{\nu+1}$$

- So,

$$N\,|\nu\rangle = \nu\,|\nu\rangle \qquad a\,|\nu\rangle = \sqrt{\nu}\,|\nu-1\rangle \qquad a^\dagger\,|\nu\rangle = \sqrt{\nu+1}\,|\nu+1\rangle$$

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$$N\,|\nu\rangle = \nu\,|\nu\rangle$$
$$a\,|\nu\rangle = \sqrt{\nu}\,|\nu-1\rangle$$
$$a^\dagger\,|\nu\rangle = \sqrt{\nu+1}\,|\nu+1\rangle$$

Algebraic Solution

- So, a & $a^\dagger$ "move" between the eigenstates, with $\Delta\nu=\pm1$
- The eigenvalue ν can only change in unit increments.
- Iterate: $(a)^k\,|\nu\rangle = \sqrt{\nu(\nu-1)\cdots(\nu-k+1)}\,|\nu-k\rangle$
  - If ν were non-integral, $\sqrt{\nu(\nu-1)\cdots(\nu-k+1)} \neq 0$
  - and $\lim_{k\to\infty} E_{\nu-k} = -\infty$ Impossible, since $H>0$
- Therefore, force ν to be integers; write n from now on.
- Then, $a\,|0\rangle = C_0\,|-1\rangle = \sqrt{0}\,|-1\rangle = 0$ $\quad a\,|0\rangle = 0,\ E_0 = \frac{1}{2}\hbar\omega$

$$a^\dagger\,|0\rangle = \sqrt{1}\,|1\rangle,\ \ a^\dagger\,|1\rangle = \sqrt{2}\,|2\rangle\ \ \ldots \qquad |n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle$$

- ...and, this is the whole Hilbert space.
  - ...because all observables are constructible from Q and P, *i.e.*, from a and $a^\dagger$, and no other state can be constructed.

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Algebraic Solution: the Number Representation

- To summarize, changing variables $Q, P \to a, a^\dagger$ allowed
  - constructing the whole Hilbert space

$$\mathscr{H} = \Big\{ |n\rangle = \tfrac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle \,:\; \langle n|n'\rangle = \delta_{n,n'},\; \sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{1} \Big\}$$

  - wherein $a\,|\nu\rangle = \sqrt{\nu}\,|\nu{-}1\rangle \qquad a^\dagger\,|\nu\rangle = \sqrt{\nu{+}1}\,|\nu{+}1\rangle$
  - and $H\,|n\rangle = E_n\,|n\rangle \qquad E_n = \hbar\omega(n{+}\tfrac{1}{2})$
- In fact, we know (much!) more!
  - Every observable $R = R(Q,P) = R(a,a^\dagger) = \sum_{p,q=0}^{\infty} c_{p,q}(a^\dagger)^p(a)^q$

$$\langle m|R(a,a^\dagger)|n\rangle = \sum_{p,q=0}^{\infty} c_{p,q}\langle m|(a^\dagger)^p(a)^q|n\rangle$$

$$= \sum_{p,q=0}^{\infty} c_{p,q}\sqrt{n(n{-}1)\cdots(n{-}q{+}1)}$$

$$\times\sqrt{(n{-}q{+}1)(n{-}q{+}2)\cdots(n{-}q{+}p)}\;\delta_{m,n-q+p}$$

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Algebraic Solution: the Number Representation

- We constructed the complete Hilbert space

$$\mathscr{H} = \Big\{ |n\rangle = \tfrac{1}{\sqrt{n!}}(\mathsf{a}^\dagger)^n\,|0\rangle : \;\; \langle n|n'\rangle = \delta_{n,n'}, \;\; \sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{1} \Big\}$$

  - and calculated all matrix elements of all observables

$$\langle m|R(\mathsf{a},\mathsf{a}^\dagger)|n\rangle = \sum_{p,q=0}^{\infty} c_{p,q}\sqrt{n(n-1)\cdots(n-q+1)} \times\sqrt{(n-q+1)(n-q+2)\cdots(n-q+p)}\,\delta_{m,n-q+p}$$

  - including state operators.

- In turn, operator eigenstates can also be expanded

$$M\,|\mu\rangle = \mu\,|\mu\rangle \qquad |\mu\rangle = \sum_{n=0}^{\infty} \mu_n\,|n\rangle \qquad \mu_n = \langle n|\mu\rangle$$

$$\mathrm{Prob}(M \mapsto \mu|\boldsymbol{\rho}) = \mathrm{Tr}\Big[\,|\mu\rangle\langle\mu|\,\boldsymbol{\rho}\Big] = \sum_{n,n',p,q} \mu_n\mu^*_{n'}\,r_{p,q}\,\langle n'|(\mathsf{a}^\dagger)^p(\mathsf{a})^q|n\rangle$$

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Algebraic Solution: the Number Representation

- In fact, we can do even more:

$$a\,|0\rangle = 0 \quad \Rightarrow \quad \left[\sqrt{\frac{M\omega}{2\hbar}}\,x + \frac{i}{\sqrt{2M\hbar\omega}}\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right]\psi_0(x) = 0$$

$$\psi_0(x) = N\,e^{-\frac{1}{2}\alpha x^2} \qquad \alpha = \frac{M\omega}{\hbar} \qquad N = \sqrt[4]{\frac{\alpha}{\pi}}$$

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left[\sqrt{\frac{M\omega}{2\hbar}}\,x - \frac{i}{\sqrt{2M\hbar\omega}}\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\right]^n \psi_0(x)$$

Just as easy for the momentum representation

- This then provides for coordinate/momentum probability distribution, such as $|\psi_n(x)|^2$, for example
- Notice: $\psi_n(x) = N_n e^{-½\alpha x^2} H_n(x)$

quadratic-exponential suppression for $x \to \pm\infty$

polynomial: oscillatory within a localized region

Quantum Mechanics I

Now, go forth and calculate!!

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