Self-adjoint extension of the operators in quantum mechanics and its classical interpretation.

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Presentation Outline

- The role of the self-adjoint operators in quantum mechanics
- Self-adjoint extension of an operator
- Classical precursors of self-adjoint extension
- Simple example: electron capture by the dipole field of the polar molecules

Short CVs

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$$\left| A, D(A) \right|$$

$$\left| A^{+}, D(A^{+}) \right| : \quad (A\psi, \phi) = (\psi, A^{+}\phi), \quad \psi \in D(A), \phi \in D(A^{+})$$

$$(A\psi, \phi) = (\psi, A\,\phi), \;\; \forall\, \psi, \phi \in D(A) \;\; \Longrightarrow \quad D(A) \subseteq D(A^{+})$$

- (a) If $D(A) \subset D(A^{+})$, then A is called a Hermitian (symmetric) operator and one writes $A \subset A^{+}$.
- (b) If $D(A) = D(A^{+})$, then A is called a self-adjoint operator and one writes $A = A^{+}$

Operator has the self-adjoint extension, if there exists a symmetric extension of , such that

$$A \subset A_{s} = A_{s}^{+} \subset A^{+}; \quad D(A) \subset D(A_{s}) = D(A_{s}^{+}) \subset D(A^{+})$$

$$N_+ = \{\psi_+ \in D(A^+), \quad A^+\psi_+ = i\psi_+\}, \qquad \dim(N_+) = n_+$$

$$N_- = \{\psi_- \in D(A^+), \quad A^+\psi_- = -i\psi_-\}, \qquad \dim(N_-) = n_-$$

- Theorem. For an operator A with definciency indicies (n_+, n_-) there are three posibilities:
- (1) If $n_+ = n_- = 0,$ then A is self-adjoint.
- (2) If $n_+ = n_- = n \geq 1,$ then A has infinitely many self-adjoint extensions.
- (3) If $n_+ \neq n_-,$ then A has no self-adjoint extension.

Classical interpretation of self-adjoint extension.

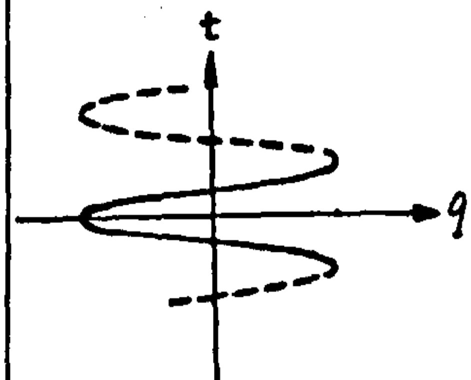
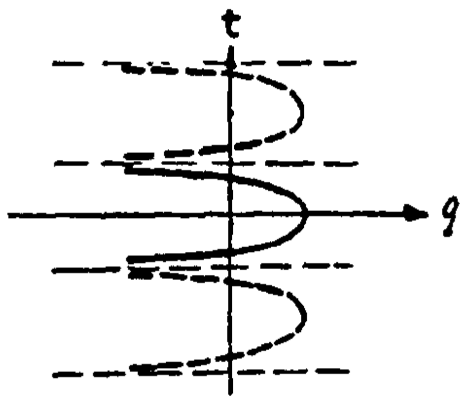
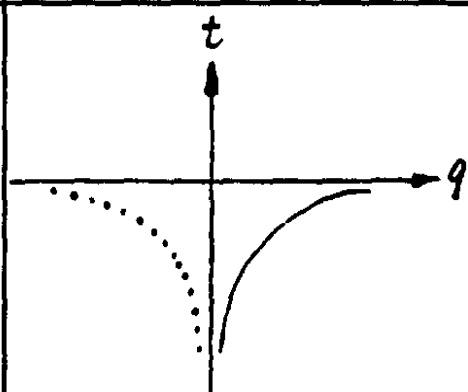
The time evolution of the wave function must be effected by a unitary transformation.

The generator of such a unitary transformation, which we identify with the Hamiltonian (up to constants), must be self-adjoint.

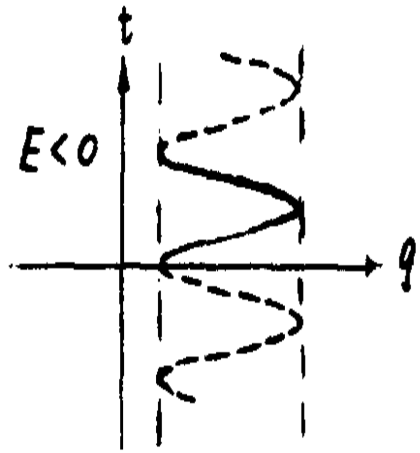
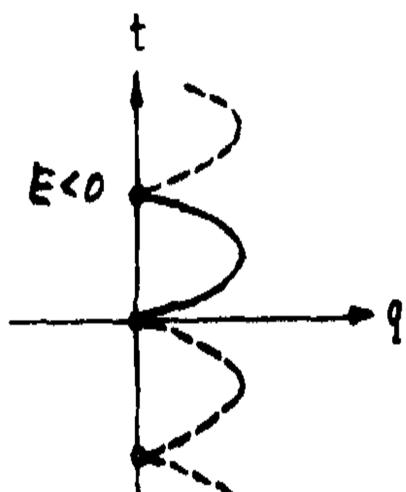
If there is no full time classical solution, then there should be no full time quantum solution, and that is exactly what happens.

$$H = \frac{p^2}{2m} + U(q);$$

$$E = \frac{m}{2}\left(\frac{dq}{dt}\right)^2 + U(q) = const \qquad t - t_0 = \pm\int \frac{dq}{\sqrt{2(E - U(q))/m}}$$

Label	Hamiltonian H	$t(q)$ of equations of motion	Classical solutions	Quantum Hamiltonian	Properties	$m = 1, 2, 3, \cdots$
a	$p^2 + q^4$		global	unique	discrete	$p^2 + q^{2m}$
b	$p^2 + q^3$		periodic	one parameter family of solution (one boundary condition)	discrete	$p^2 - q^3$ $p^2 \pm q^{2m+1}$
c	$2pq^3$		partially complex	nonexistent	none	pq^m , $m > 1$, $m =$ odd

$$H_r = \frac{p_r^2}{2m} + \frac{\vec{l}^{\,2}}{2mr^2} + V(r); \quad V(r) = -\frac{\lambda}{r^n}; \;\; (n = 1,2,\ldots); \quad \frac{dr}{dt} = 2\sqrt{E + \frac{\lambda}{r^n} - \frac{\vec{l}^{\,2}}{r^2}}$$

j	$p_r^2 - \frac{\lambda}{r} + \frac{l(l+1)}{r^2}$ $\lambda > 0$		global	unique	discrete	
k	$p_r^2 - \frac{\lambda}{r^n} + \frac{l(l+1)}{r^2}$		periodic	one parameter family of solution.	discrete	

Electron capture by the dipole field of the polar molecules.

electron capture   weakly bounded state

unstable molecular anion   enhanced scattering cross-section (anomalous scattering)

G. S. Hurst, L. B. O'Kelly and J. A. Stokdale, Nature 195, 66 (1962).

$$H_{full} = -\frac{\hbar^2}{2\mu}\nabla^2 + e\frac{Dr}{r^3}\cos\theta$$

$$H_{full}\Psi = E\Psi$$

$$\Psi(r,\theta,\phi) = \frac{1}{r}R(r)\Theta(\theta)e^{im\phi}$$

$$\left.\begin{aligned} HR(r) &\equiv \left[-\frac{d^2}{dr^2} + \frac{\lambda}{r^2}\right]R(r) = \varepsilon R(r) \\ K\Theta(\theta) &\equiv (\vec{L}^2 + d\cos\theta)\Theta(\theta) = \lambda\Theta(\theta) \end{aligned}\right\}$$

$$d = \frac{2\mu eD}{\hbar^2}$$

$$\varepsilon = \frac{2\mu E}{\hbar^2}$$

λ - dimensionless coupling constant

$$\lambda_{\min}(d_0) = -\frac{1}{4} \Rightarrow d_0 = -1.28... \Rightarrow D_0 = 1.63 \text{ Debye}$$

$\lambda < -\frac{1}{4}$ or $D > D_0$ - "fall to the center" condition , bound states with infinite negative energies.

$-\frac{1}{4} \le \lambda < 0$ or $D \le D_0$ - no ground state due to scale invariance.

Radial Hamiltonian is not self-adjoint , unless the domain of self-adjointness is specified.

Operator is Hermitian if the boundary term in the following condition is zero

$$\langle H\ \phi|\psi\rangle = \langle\phi|H\ \psi\rangle + \left(\phi^* \frac{d\psi}{dr} - \psi\frac{d\phi^*}{dr}\right)\Bigg|_0^\infty, \quad \phi\in D(H\ ), \psi\in D(H^+)$$

$$D(H\ ) = \{\phi, \phi' \in L_2(0,\infty);\ \phi(0) = \phi'(0) = 0\}$$

$$D(H^+) = \{\psi, \psi' \in L_2(0,\infty)\}$$

$$D(H) \neq D(H^+)$$

According to von Neumann’s approach

$$H^+\phi_\pm = \pm i\phi_\pm$$

$$r \to 0:$$

$$\phi_+(r) \to C_1(\nu) r^{\nu+\frac{1}{2}} + C_2(\nu) r^{-\nu+\frac{1}{2}} \qquad \phi_-(r) \to C_1^*(\nu) r^{\nu+\frac{1}{2}} + C_2^*(\nu) r^{-\nu+\frac{1}{2}}$$

$$R(r) \to D_1(\nu,q) r^{\nu+\frac{1}{2}} + D_2(\nu,q) r^{-\nu+\frac{1}{2}} \qquad \nu = \sqrt{\lambda + \frac{1}{4}} \qquad q^2 = \varepsilon,$$

$$q = i\sqrt{|\varepsilon|}$$

$$\int_0^\infty |\phi_\pm|^2 dr = \begin{cases} \infty, \Rightarrow \lambda \geq \frac{3}{4}; (n_+, n_-) = (0,0) \\ < \infty, \Rightarrow -\frac{1}{4} \leq \lambda < \frac{3}{4}; (n_+, n_-) = (1,1) \end{cases}$$

Construction of the domain of self-adjointness

$$D_\omega(H\ ): D(H\ ) \subset D_\omega(H\ ); \quad \Phi = \phi_+ + e^{i\omega}\phi_- \in D_\omega(H\ ), \quad \omega \in [0, 2\pi]$$

ω - self-adjoint extension parameter, wich classifies inequivalent boundary conditions at the origin.

$$\lim_{r\to 0}\left(\Phi^*\frac{dR}{dr}-R\frac{d\Phi^*}{dr}\right)=0$$

Boundary states   scale invariance is broken due to quantization

$$E=-\frac{\hbar^2}{2\mu}\left[\cos\frac{\pi\nu}{2}+\cot\left(\frac{\omega}{2}+\frac{\pi\nu}{4}\right)\sin\frac{\pi\nu}{2}\right]^{\frac{1}{\nu}} \qquad (0<\nu<1) \quad (D<D_0)$$

$$E=-\frac{\hbar^2}{2\mu}\exp\left[\frac{\pi}{2}\cot\frac{\omega}{2}\right] \qquad (\nu=0) \quad (D=D_0)$$

$$;\ B=-\frac{\sinh\left(\frac{\pi g}{2}\right)\sin\omega}{1+\cosh\left(\frac{\pi g}{2}\right)\cos\omega}$$

$$E_n=-\frac{\hbar^2}{2\mu}\exp\left[\frac{1}{g}\left(\arctan B-2\pi n\right)\right] \qquad (D\geq D_0) \quad (n=0,1,2,\dots) \quad (g=i\nu, g>0)$$

Thank You for attention