Last week: Wave mechanics

1. Particles, fields, interactions
2. Electromagnetic waves and energy scales
3. Particle-wave duality and de Broglie's relation
4. Wavefunction as a descriptor of an electron
5. Schrödinger equation (time dependent)
6. Plane wave solves it for the free electron, provided the dispersion relation $E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ is satisfied

Time-dependent Schrödinger's equation

(Newton's 2nd law for quantum objects)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+\mathrm{V}(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

1925-onwards: E. Schrödinger (wave equation), W. Heisenberg (matrix formulation), P.A.M. Dirac (relativistic)

Stationary Schrödinger's Equation (I)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+\mathrm{V}(\vec{r},*)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

Stationary Schrödinger's Equation (II)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \mathrm{V}(\vec{r})\right]\varphi(\vec{r}) = \mathrm{E}\varphi(\vec{r})$$

From one equation to two simpler ones

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + \mathrm{V}(\vec{r},t)\Psi(\vec{r},t) = i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

Separation of variables

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \mathrm{V}(\vec{r})\right]\varphi(\vec{r}) = \mathrm{E}\varphi(\vec{r})$$

$$i\hbar\frac{d}{dt}f(t) = E\,f(t)$$

Stationary Schrödinger's Equation (III)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

1. It's not proven – it's postulated, and it is confirmed experimentally
2. It's an "eigenvalue" equation: it has a solution only for certain values (discrete, or continuum intervals) of E
3. For those eigenvalues, the solution ("eigenstate", or "eigenfunction") is the complete descriptor of the electron in its equilibrium ground state, in a potenitial V(r).
4. As with all differential equations, boundary conditions must be specified
5. Square modulus of the wavefunction = probability of finding an electron

Time dependence

$$i\hbar\frac{d}{dt}f(t) = Ef(t)$$ ⇒

Free particle: $\Psi(x,t)=\varphi(x)f(t)$

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(x)=E\varphi(x)$$

$$i\hbar\frac{d}{dt}f(t)=Ef(t)$$

A simple differential equation

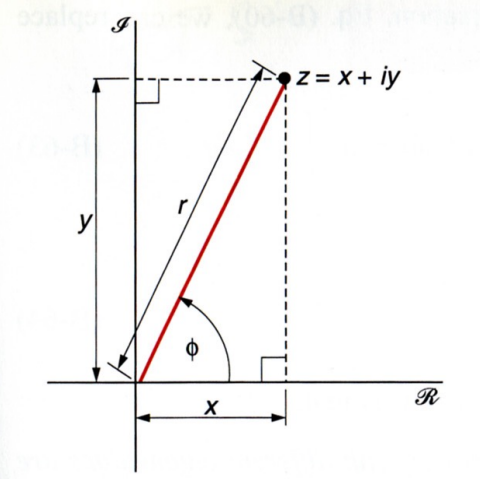


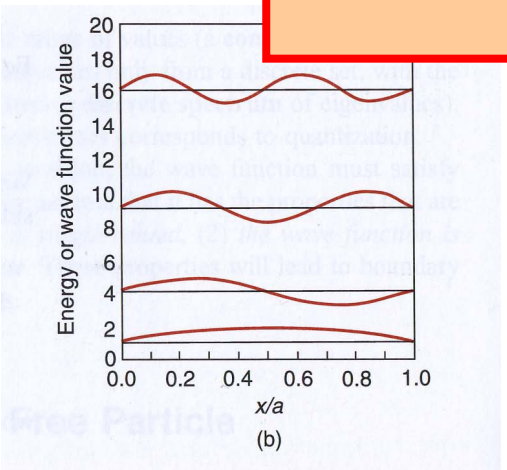
Figure B.6. The Argand Plane. A point in this diagram represents a complex number either in the form $x + iy$ or $re^{i\phi}$.

Infinite Square Well (I)
(particle in a 1-dim box)

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$

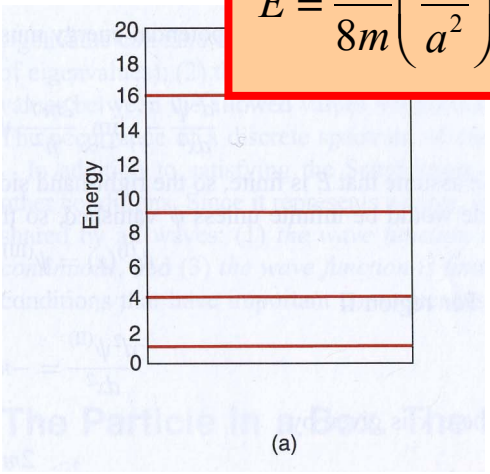
Infinite Square Well (II)

$$\varphi(x) = C\sin\left(\frac{l\pi x}{a}\right)$$



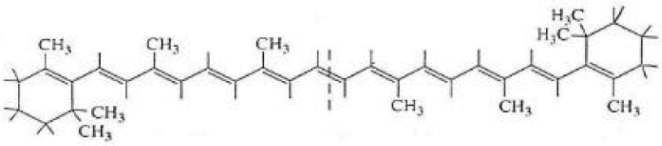
Infinite Square Well (III)

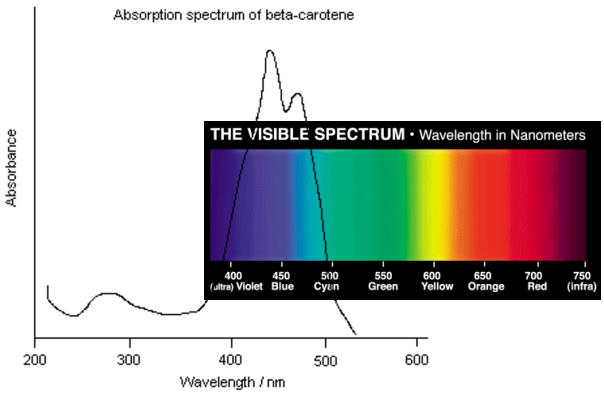
$$E = \frac{h^2}{8m}\left(\frac{l^2}{a^2}\right)$$



The power of carrots

- β-carotene





Particle in a 2-dim box

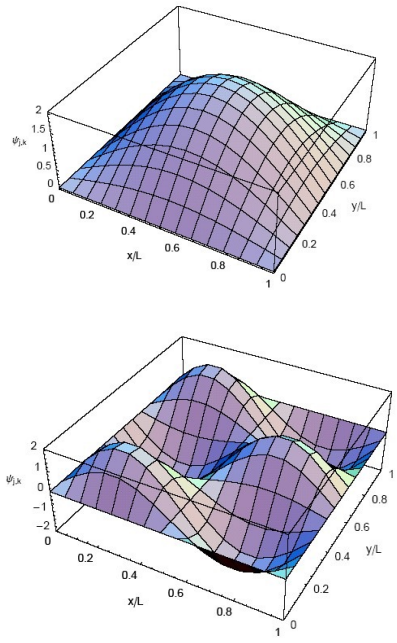
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)=E\,\varphi(x,y)$$

Particle in a 2-dim box

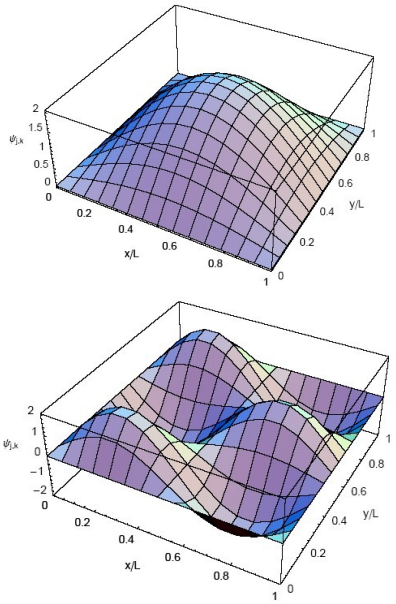
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)=E\,\varphi(x,y)$$

$$\varphi(x,y)=C\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)$$

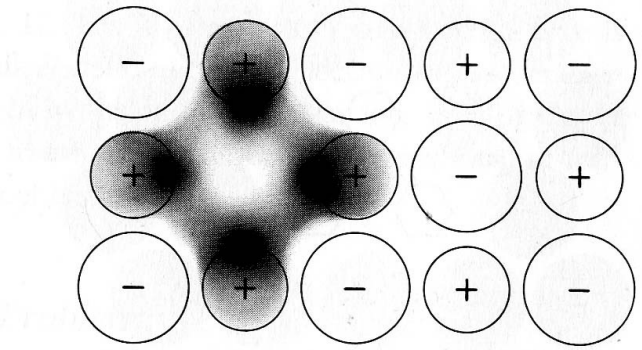
$$E=\frac{h^2}{8m}\left(\frac{l^2}{a^2}+\frac{m^2}{b^2}\right)$$



Particle in a 3-dim box: *Farbe* defect in halides (e^- bound to a negative ion vacancy)



$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\phi(x,y,z)=E\,\phi(x,y,z)$$



From Carl Zeiss to MIT

PHYSICAL REVIEW VOLUME 120, NUMBER 6 DECEMBER 15, 1960

Color Centers in Cesium Halide Single Crystals*

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(Received August 12, 1960)

Color centers have been investigated in the CsCl-type alkali halides. Cesium chloride, bromide, and iodide single crystals were grown from the melt and CsCl crystals also from solution. Coloration was produced by 130-kv x rays, 3.0-Mev electrons, and by electrolysis. In CsI coloration resulted from electrolysis only. The absorption of uncolored and colored crystals has been measured from 0.175 to 3.5 μ at 25°, −78°, and −190°C. After coloration all three crystals show one strong band in the visible (near infrared for CsI) and several weaker bands at shorter and longer wavelengths, which shift with temperature change. The spectral positions in mμ for a number of the bands at −190°C are:

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8	λ_9	λ_{10}
CsCl	227		270	370	430	579	715	780	855	980
CsBr	241	~270	~315	390	480	646	(780)	840	(~930)	1055
CsI	270	330		425	535	750			1050	1185

The strongest band (λ_6) behaves similarly to the F band in the NaCl-type alkali halides. The half-width of the band (0.20 to 0.23 ev at −190°C) and its increase with temperature, the shifting of the band maximum toward longer wavelengths upon warming to room temperature (by ~0.08 ev), and the conversion by bleaching with light into other bands support the assignment of this band as the F band. The spectral position of the band maximum approximately follows the Mollwo relation ($\lambda_{max}=\text{const}\ d^n$, where d=interionic distance and $n=2.5$).

Bleaching experiments suggest the assignment of the band λ_{10} as the M band and the bands between the F and M bands as R bands. The origin of the ultraviolet bands is still uncertain.

Molecular Limits to the Quantum Confinement Model in Diamond Clusters

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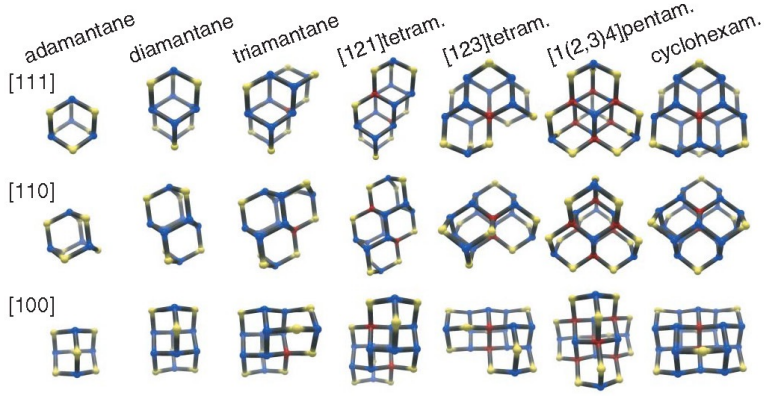
(Received 13 May 2005; published 7 September 2005)

The electronic structure of monodispersed, hydrogen-passivated diamond clusters (diamondoids) in the gas phase has been studied with x-ray absorption spectroscopy. The data show that the bulk-related unoccupied states do not exhibit any quantum confinement. Additionally, density of states below the bulk absorption edge appears, consisting of features correlated to CH and CH_2 hydrogen surface termination, resulting in an effective redshift of the lowest unoccupied states. The results contradict the commonly used and very successful quantum confinement model for semiconductors, which predicts increasing band edge blueshifts with decreasing particle size. Our findings indicate that in the ultimate size limit for nanocrystals a more molecular description is necessary.



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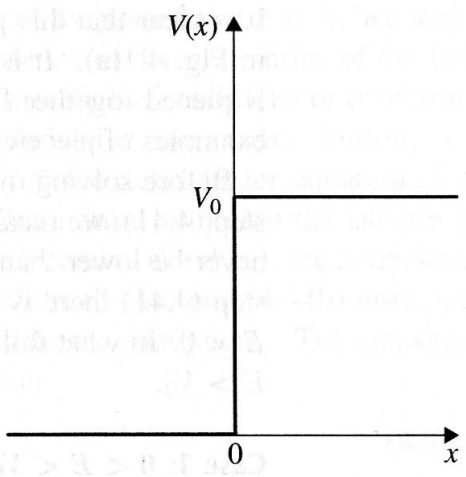
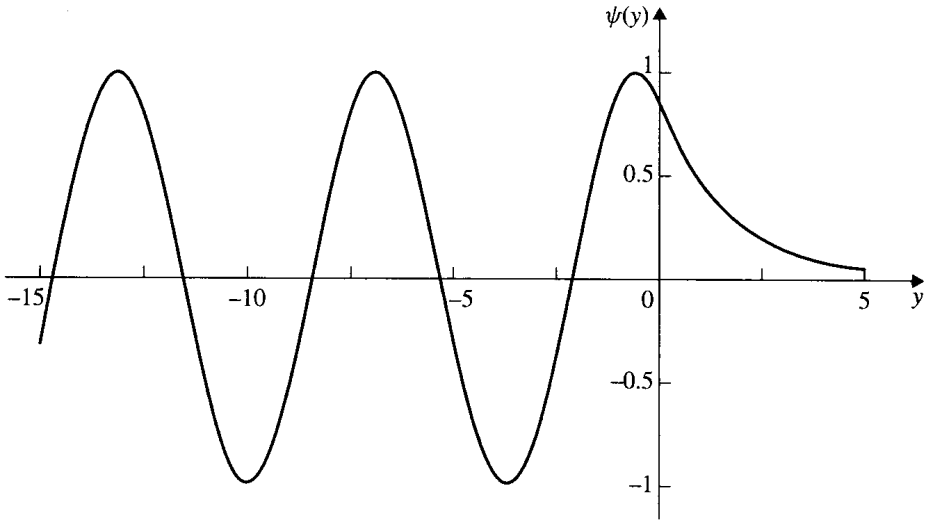
Metal Surfaces (I)

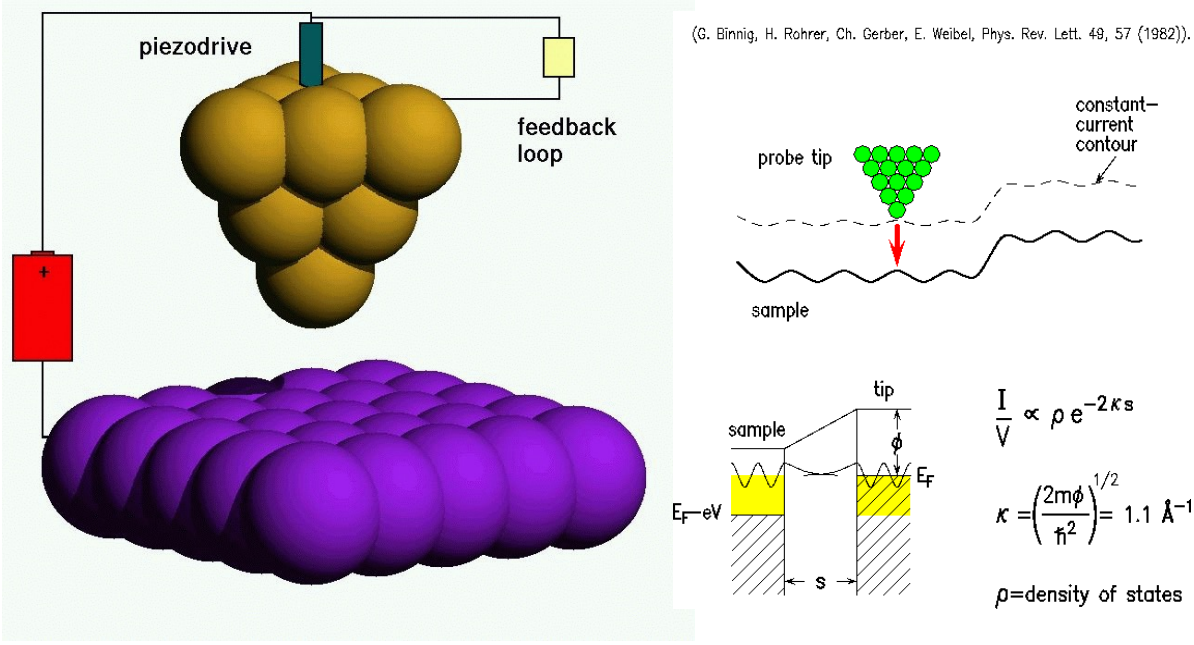
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$



Metal Surfaces (II)



Scanning Tunnelling Microscopy

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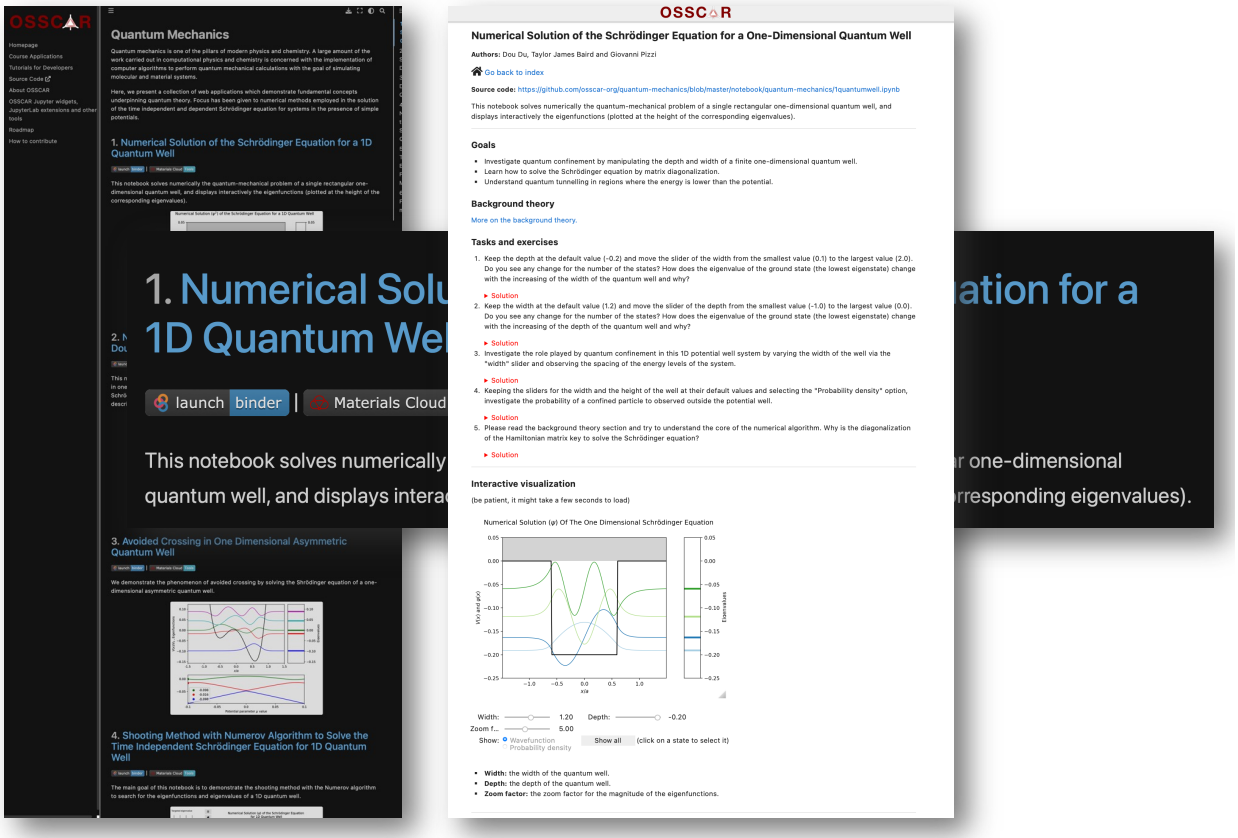
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Authors: Dou Du, Taylor James Baird and Giovanni Pizzi
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Goals
Background theory
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Numerical Solution (φ) Of The One Dimensional Schrödinger Equation

Energy from Wavefunctions

Schrödinger equation: operator, eigenvalues

E can be obtained as an “expectation value”

Dirac Notation

Dirac’s <bra|kets> (elements of vector space)

Scalar product (induces a metric → Hilbert space)

Physical Observables from Wavefunctions

Eigenvalue equation:

Expectation values for the operator (energy)

4 concepts

- Operators
- Eigenvalues
- Eigenfunctions
- Expectation values

Operators: Linear, Hermitian

Examples: (d/dx) and i(d/dx)

Product of operators, and commutators

Hermitian Operators

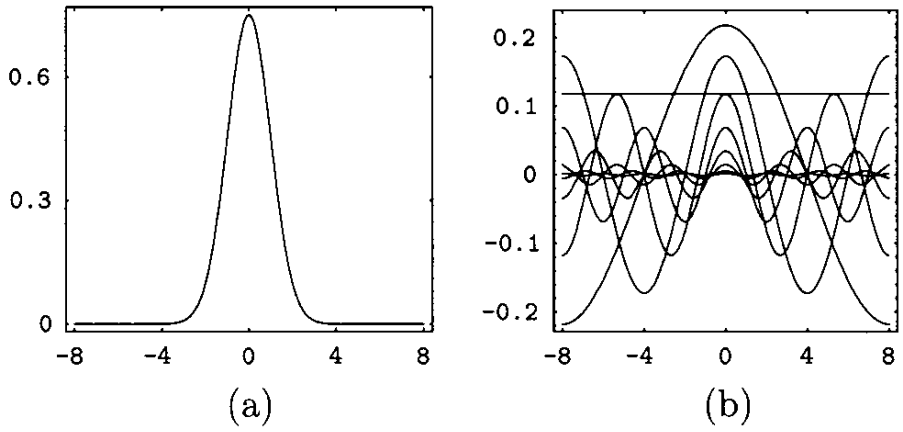
1. The eigenvalues of a Hermitian operator are real

2. Two eigenfunctions corresponding to different eigenvalues are orthogonal

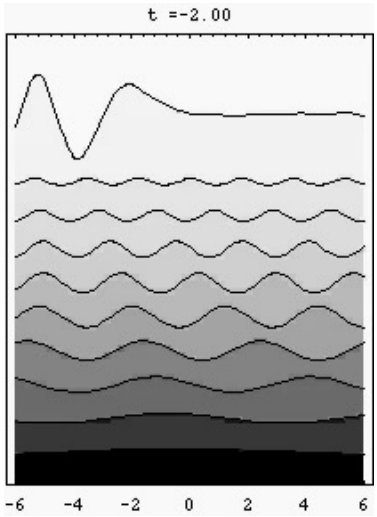
3. The set of eigenfunctions of a Hermitian operator is complete

4. Commuting Hermitian operators have a set of common eigenfunctions

The set of eigenfunctions of a Hermitian operator is complete



The set of eigenfunctions of a Hermitian operator is complete



Commuting Hermitian operators have a set of common eigenfunctions