# Quantum Tunneling

MARIUS LUTZ

# Can we walk through walls?



[1. Marcel Aymé, „The man who could walk through walls“]

# Let‘s have a closer look…

$$SiO_2$$

[2. Wikipedia, „Quarz“]

# Structure: A story about quantum tunneling



When did we first see it?

How did we explain it?

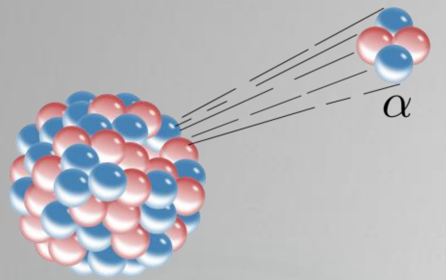
What could we explain with it?

What could we use it for?

And what does it have to do with rocks?

# First observations



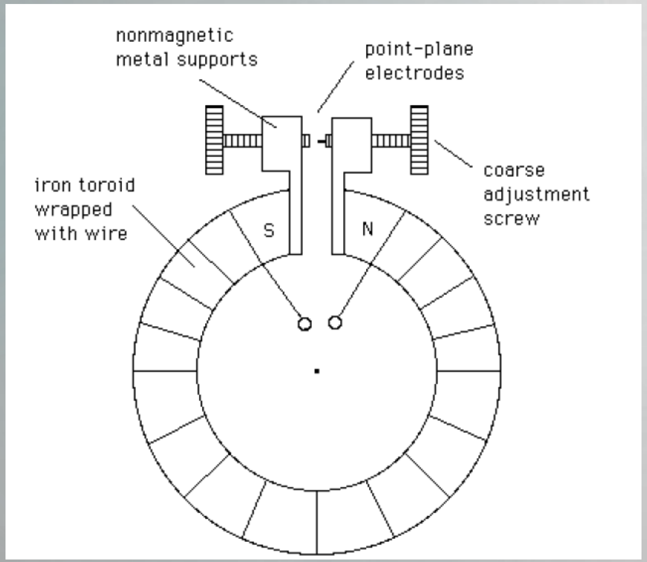



[3. Wikipedia, „Alpha decay“]

Alpha decay

In the investigation of radioactivity in the late 19th and early 20th century.

They did not know they were seeing a tunneling effect.




[4. Thomas Mark Cuff, „The STM […] The forgotten contribution of Robert Francis Earhart to the discovery of quantum tunneling.“, Hoffmann‘s Magnetic Apparatus for Bringing Electrodes Close Together]

Field Emission

Unexpected conduction regime in gases was observed and later reproduced in a vacuum.

They could not interpret their results.

# Solution: Schrödinger Equation 1926



Wave-particle duality → Wave Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H} \Psi(\mathbf{r}, t)$$

Photoelectric Effect
Zeeman/Stark Effect

Etc.

Tunneling was not known at the time

1926 № 13

ANNALEN

VIERTE FO

1. *Quantisierung a*
*von E. S*

(Dritte[1]) Mitteilung: Störungstheor
der Ba

**Einleitung.**

Wie schon am Ende de
läßt sich das praktisch zu
Eigenwerttheorie schon mit
Methoden ziemlich bedeuten

*Second Series* *December, 1926* *Vol. 28, No. 6*

THE
PHYSICAL REVIEW

AN UNDULATORY THEORY OF THE MECHANICS OF ATOMS AND MOLECULES

By E. Schrödinger

Abstract

The paper gives an account of the author's work on a new form of quantum theory. §1. The Hamiltonian analogy between mechanics and optics. §2. The analogy is to be extended to include real "physical" or "undulatory" mechanics instead of mere geometrical mechanics. §3. The significance of wave-length; macro-mechanical and micro-mechanical problems. §4. The wave-equation and its application to the hydrogen atom. §5. The intrinsic reason for the appearance of discrete characteristic frequencies. §6. Other problems; intensity of emitted light. §7. The wave-equation derived from a Hamiltonian variation-principle; generalization to an arbitrary conservative system. §8. The wave-function physically means and determines a continuous distribution of electricity in space, the fluctuations of which determine the radiation by the laws of ordinary electrodynamics. §9. Non-conservative systems. Theory of dispersion and scattering and of the "transitions" between the "stationary states." §10. The question of relativity and the action of a magnetic field. Incompleteness of that part of the theory.

Inserting this and Eq. (6) in Eq. (15) we get

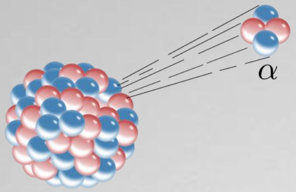
$$\Delta\psi + 8\pi^2 m(E-V)\psi/h^2 = 0, \qquad (16)$$

where $\psi$ may be assumed to depend on $x$, $y$, $z$ only. (We omit changing the notation of the dependent variable, which we really ought to do.)

[5./6. E. Schrödinger, „Annalen der Physik", and „The Physical Review"]

# Explanation of alpha decay (G. Gamow 1928)






**Zur Quantentheorie des Atomkernes.**

Von **G. Gamow,** z. Zt. in Göttingen.

Mit 5 Abbildungen. (Eingegangen am 2. August 1928.)

Es wird der Versuch gemacht, die Prozesse der $\alpha$-Ausstrahlung auf Grund der Wellenmechanik näher zu untersuchen und den experimentell festgestellten Zusammenhang zwischen Zerfallskonstante und Energie der $\alpha$-Partikel theoretisch zu erhalten.

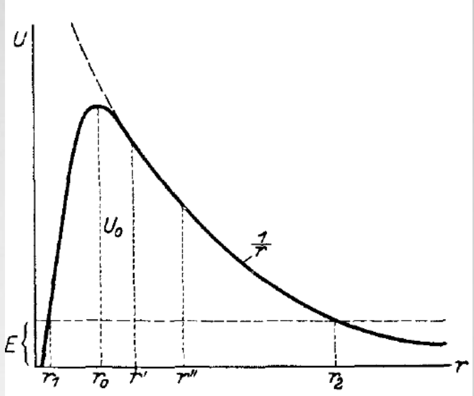



Fig. 1.

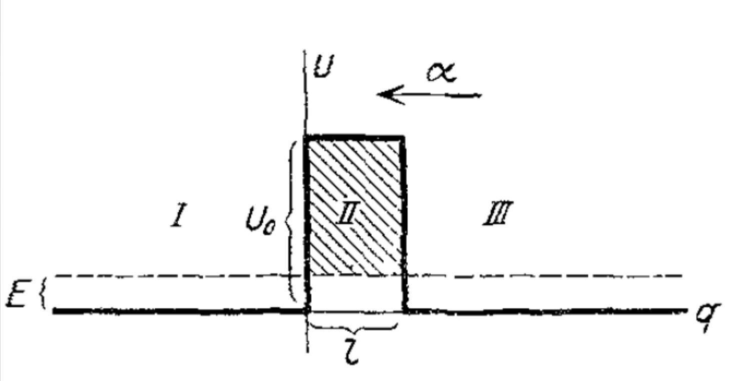



Fig. 2.

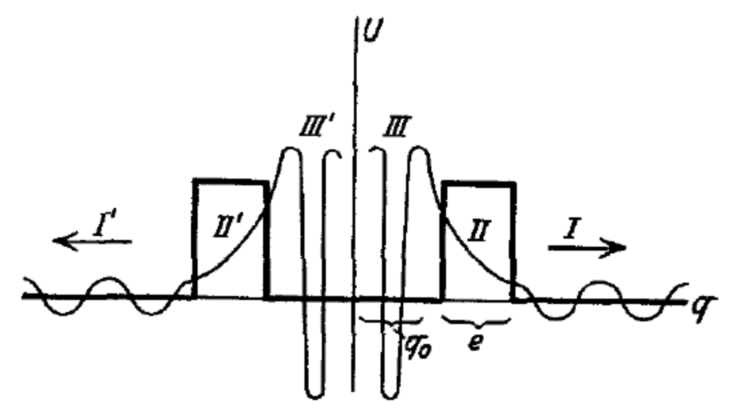



Fig. 3.

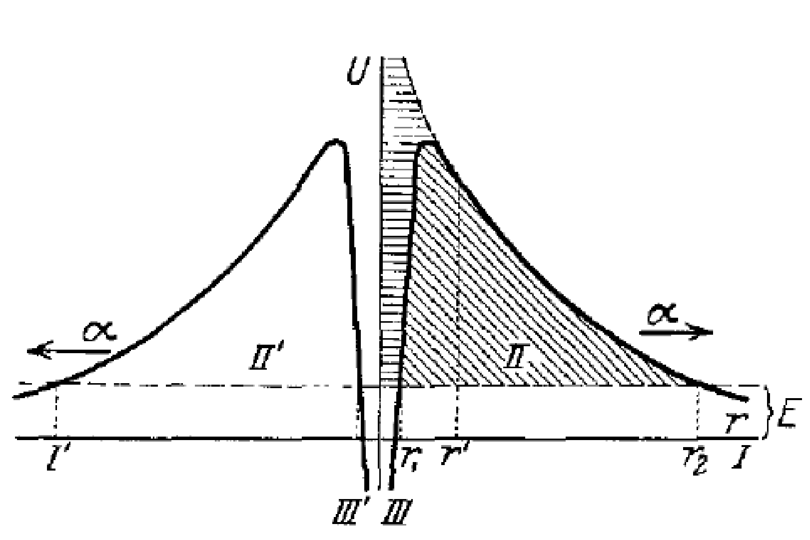



Fig. 4.

[7. G. Gamow, „Zur Quantentheorie des Atomkernes“]

# Tunneling



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

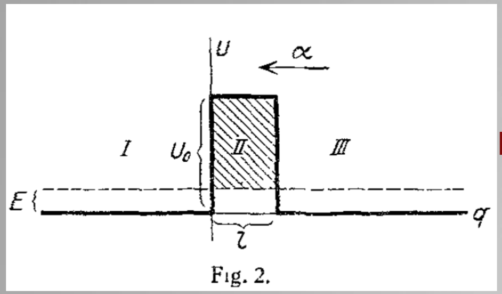
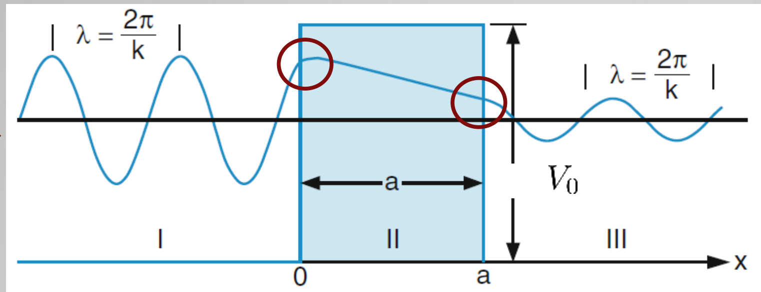



Fig. 2.

[7. G. Gamow, „Zur Quantentheorie des Atomkernes“]




[10. Demtröder, „Atoms, Molecules and Photons“]

Ansatz:

$$\Phi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\Phi_{\mathrm{I}}(x) = e^{ikx} + Re^{-ikx} \qquad \Phi_{\mathrm{II}}(x) = \alpha e^{\kappa x} + \beta e^{-\kappa x} \qquad \Phi_{\mathrm{III}}(x) = Te^{ikx}$$

Use Schrödinger Equation / $\Phi_{\mathrm{I}}(0) = \Phi_{\mathrm{II}}(0)$ / $\Phi_{\mathrm{II}}(a) = \Phi_{\mathrm{III}}(a)$

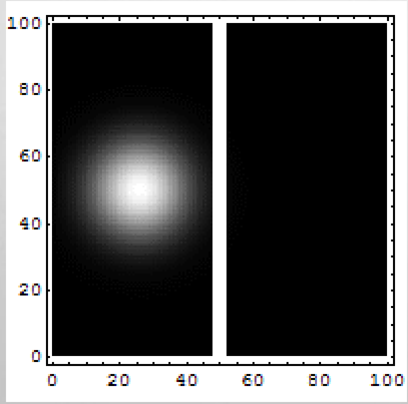
/ $\frac{d\Phi_{\mathrm{I}}(0)}{dx} = \frac{d\Phi_{\mathrm{II}}(0)}{dx}$ / $\frac{d\Phi_{\mathrm{II}}(a)}{dx} = \frac{d\Phi_{\mathrm{III}}(a)}{dx}$

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$T = \frac{1-E/V_0}{(1-E/V_0)+(V_0/4E)\sinh^2(a\kappa)}$$

$$\sinh(a\kappa) \approx \frac{1}{2}e^{a\kappa}$$

$$|T|^2 + |R|^2 = 1$$




[9. Wikipedia, „Tunneleffekt“]

$$T \approx \frac{16E}{V_0^2}(V_0 - E)e^{-2a\kappa}$$

# WKB-approximation and Gamow factor



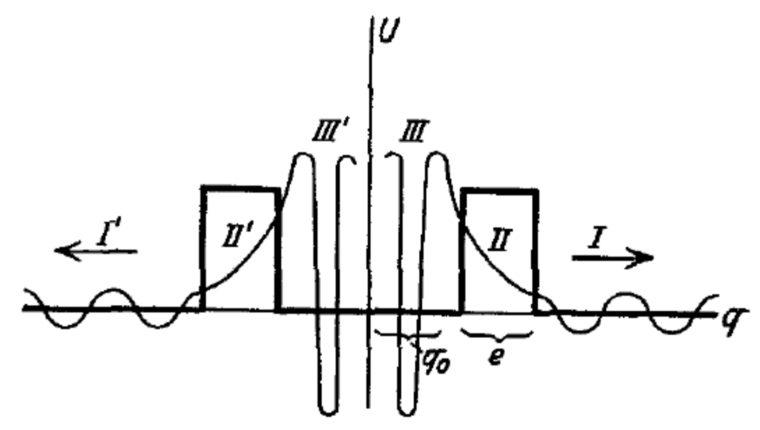



Fig. 3.

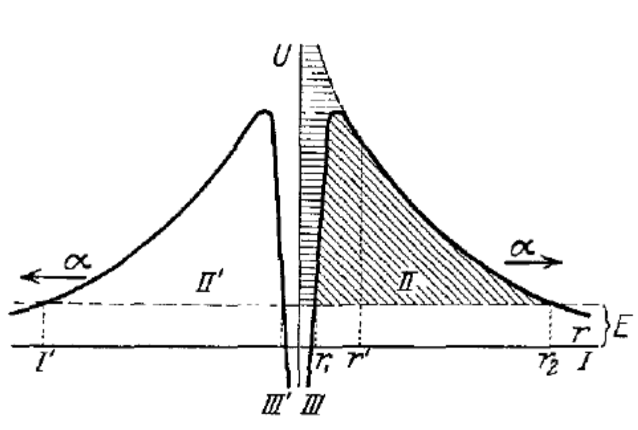



Fig. 4.

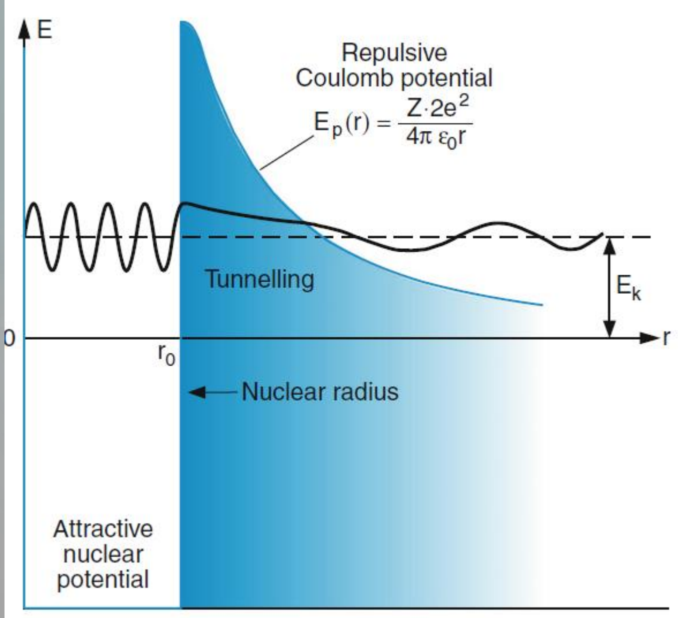
[7. G. Gamow, „Zur Quantentheorie des Atomkernes“]

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

Box potential

$$\kappa(r) = \sqrt{\frac{2m}{\hbar^2}(V(r) - E)}$$

$$T \approx \frac{16E}{V_0^2}(V_0 - E)e^{-2a\kappa}$$




[10. Demtröder, „Atoms, Molecules and Photons“]

$$T = \exp(-2G)$$

$$G = \int_{r_1}^{r_2} \sqrt{\frac{2m}{\hbar^2}(V(r) - E)}\mathrm{d}r$$

Gamow factor

# Correct prediction of alpha decay

parallele Gerade. Die empirische Formel lautet:

$$\lg \lambda = \text{Const} + b\,E,$$

wo ***b*** eine allen radioaktiven Familien gemeinsame Konstante ist.

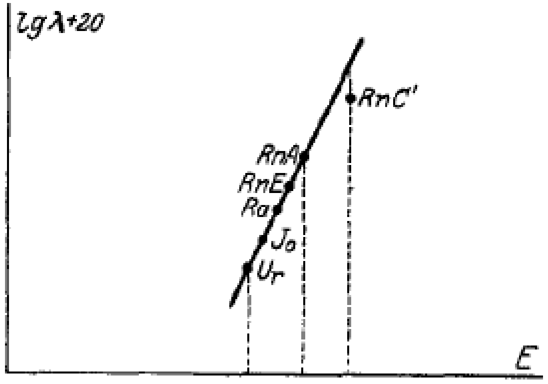



Fig. 5.

Der experimentelle Wert von ***b*** (aus **Ra A** und **Ra** berechnet) ist

$$b_{\text{exper.}} = 1{,}02\,.\,10^{+7}.$$

Wenn wir aber in unsere Formel den Energiewert für Ra A einsetzen, so gibt die Rechnung

$$b_{\text{theor.}} = 0{,}7\,.\,10^{+7}\,*.$$

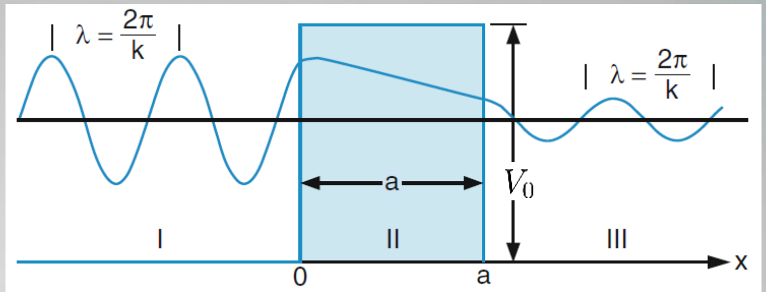
Die Übereinstimmung der Größenordnung zeigt, daß die Grundannahme der Theorie richtig sein dürfte. Nach unserer Theorie müssen

[7. G. Gamow, „Zur Quantentheorie des Atomkernes“]

Particles are tunneling through Potential barriers

# A few numbers






[10. Demtröder, „Atoms, Molecules and Photons"]

$T \approx e^{-2\kappa a}$ $\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

$E = V_0/2$ $a = \lambda_{dB}/2\pi$ ➡ $\kappa a = 1$ $T \approx 0.14$

$E = V_0/2$ $a = \lambda_{dB}$ ➡ $\kappa a = 2\pi$ $T \approx 10^{-6}$

Macroscopic tunneling? ➡ It's not going to happen!

[11. Wikimedia Commons, „Fly on insect net"]

# But he was not actually the first…

# Molecular spectral lines (F. Hund 1926/27)



**Zur Deutung der Molekelspektren. III.**

**Bemerkungen über das Schwingungs- und Rotationsspektrum bei Molekeln mit mehr als zwei Kernen.**

Von **F. Hund** in Göttingen.

Mit 7 Abbildungen. (Eingegangen am 28. Mai 1927.)

Im Falle, daß eine vier- oder mehratomige Molekel zwei spiegelbildlich gleiche Anordnungen tiefster potentieller Energie hat, sind diese in jedem stationären Zustand in gleicher Weise vorhanden. Dem Übergang aus der einen Anordnung in das Spiegelbild entspricht eine Frequenz. Diese Tatsache steht mit der

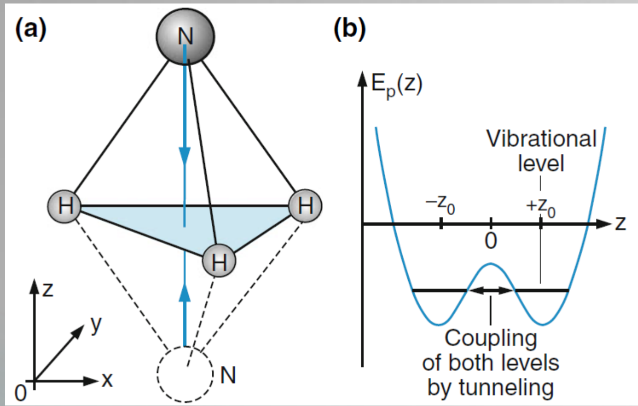
- If quantum objects can tunnel through potential barriers, they can also be in superposition of several states that are separated by a potential.
- Coupling through tunneling.

Wir können also sagen: Wenn bei einer Molekel zwei einander spiegelbildlich entsprechende und verschiedene Anordnungen der Kerne möglich sind, so sind die stationären Zustände nicht Bewegungen in der Nähe einer der beiden Gleichgewichtsanordnungen. Jeder stationäre Zustand ist vielmehr aus Rechts- und Linksanordnungen gleichmäßig zusammengesetzt. Bei den höher angeregten Schwingungen ist die mitt-

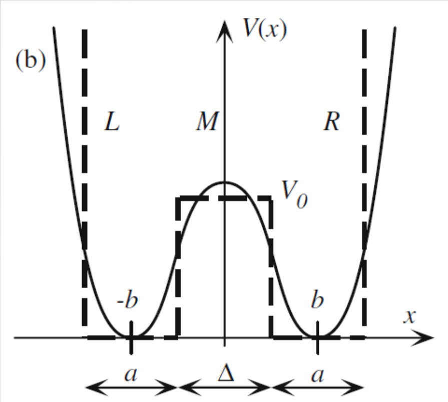
[8. F. Hund, „Zur Deutung der Molekelspektren III“]

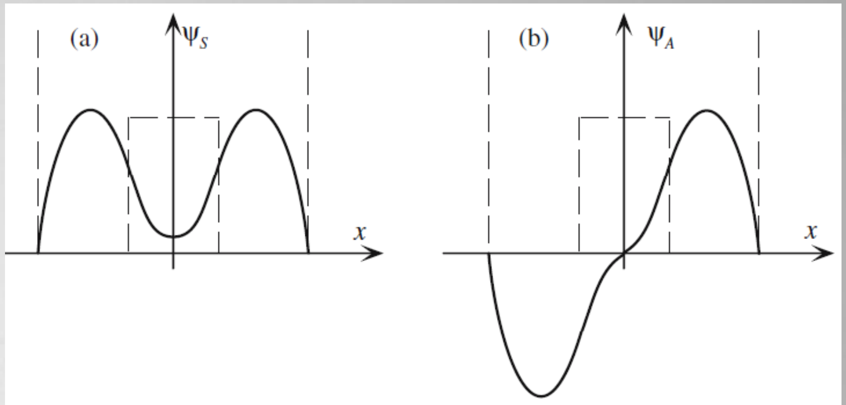
# Example: Ammonia



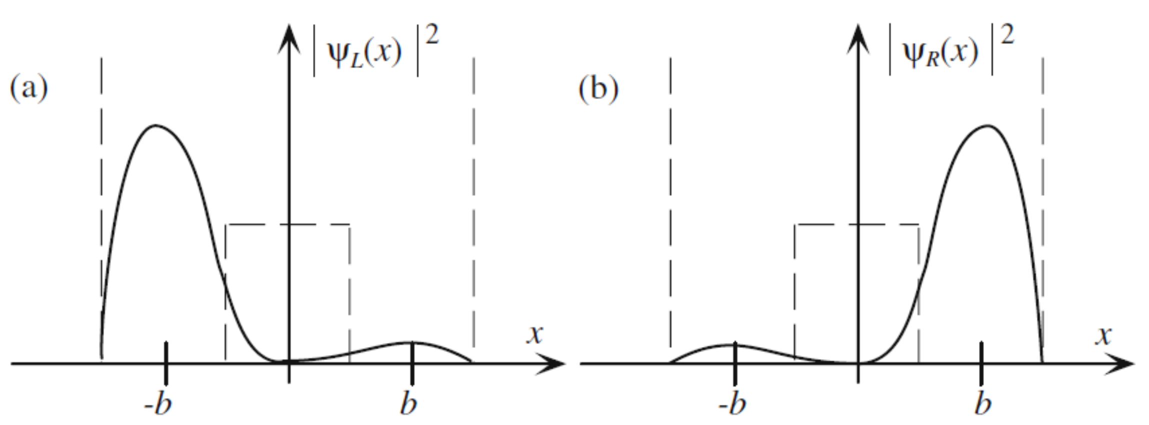



[10. Demtröder, „Atoms, Molecules and Photons“]




$$\psi_L = (\psi_S - \psi_A)/\sqrt{2} \qquad \psi_R = (\psi_S + \psi_A)/\sqrt{2}$$




[12. J.-L. Basdevant/J. Dalibard, „Quantum Mechanics“]

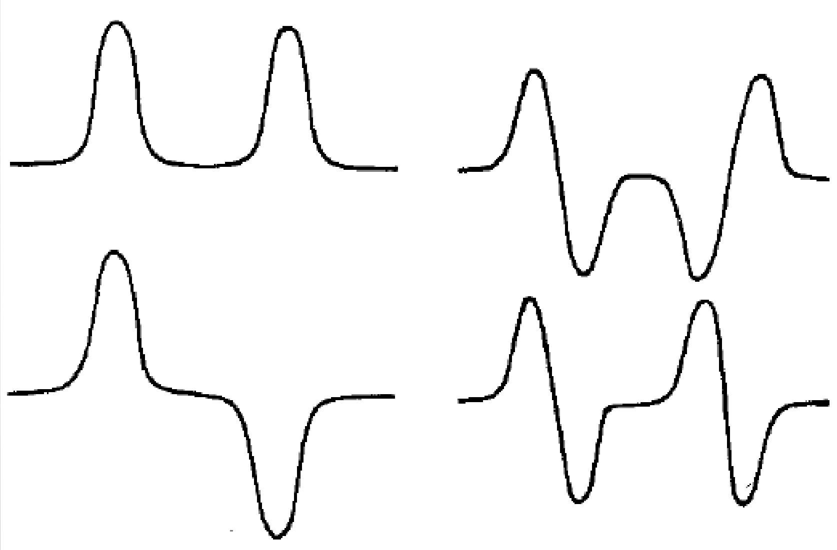


Fig. 1.

[8. F. Hund, „Zur Deutung der Molekelspektren III“]

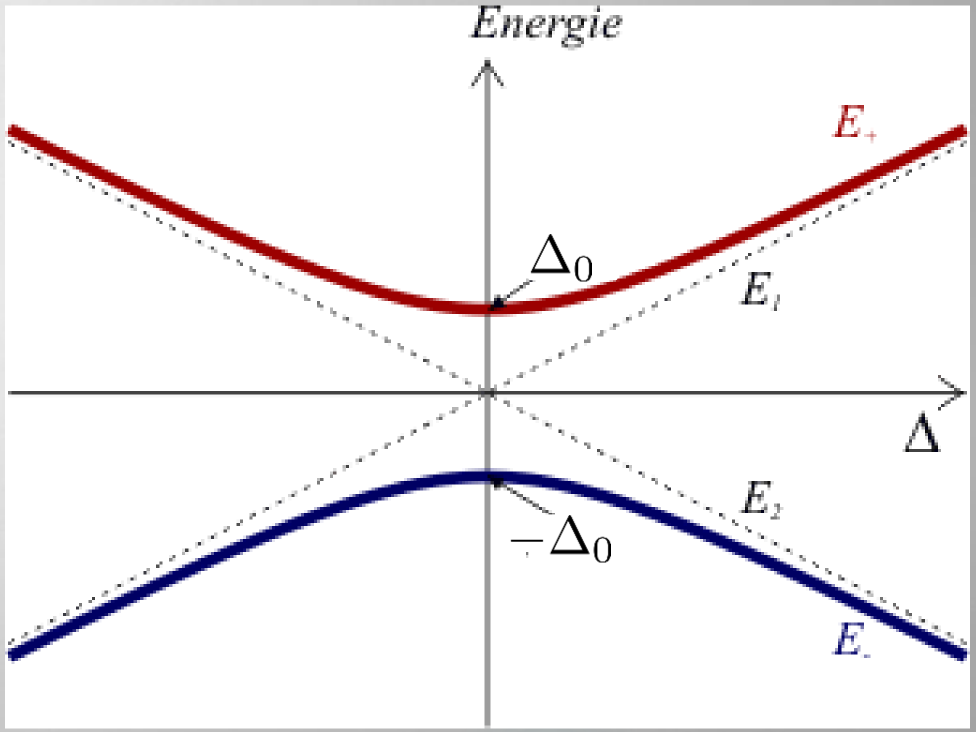
# Two-State quantum system



$$\Delta = E_1 - E_2$$

$$H = \begin{pmatrix} E_1 & \Delta_0 \\ \Delta_0 * & E_2 \end{pmatrix} \rightarrow E_\pm = \frac{1}{2}[(E_1 + E_2) \pm \sqrt{(E_1 - E_2)^2 + 4\Delta_0^2}]$$

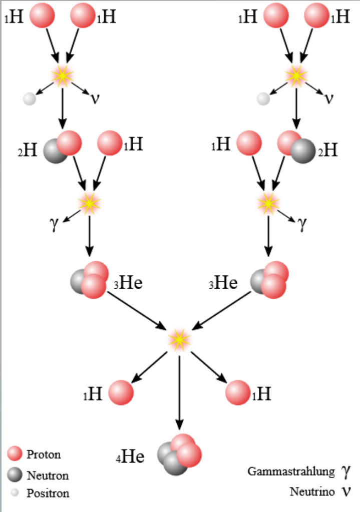
- Dipole moment
- Interaction with external em-field




[13. Wikipedia, „Zweizustandssystem“]

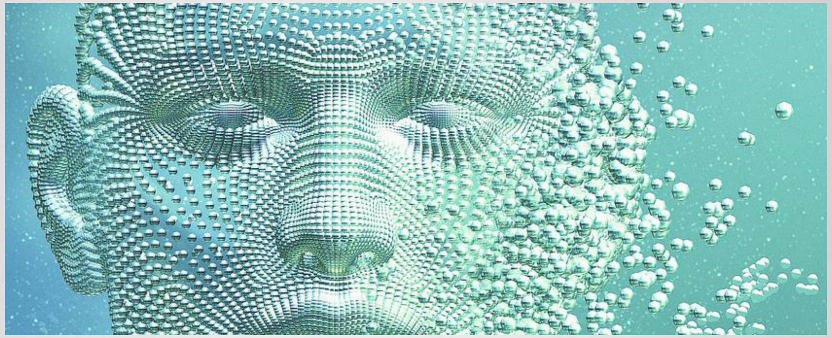
# Tunneling is everywhere






[14. Wikipedia, „Nuclear Fusion"]

Nuclear fusion

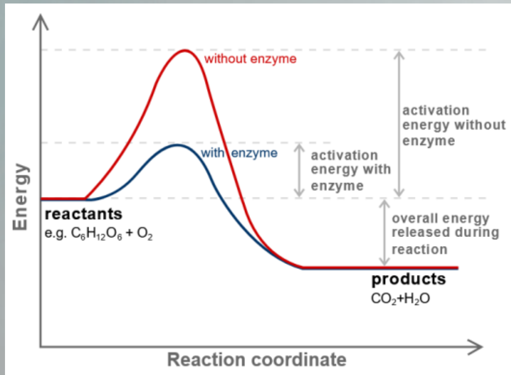


[16. Spektrum der Wissenschaft, „Leben in der Quantenwelt"]

Quantum biology

DNA-mutations

Photosynthesis

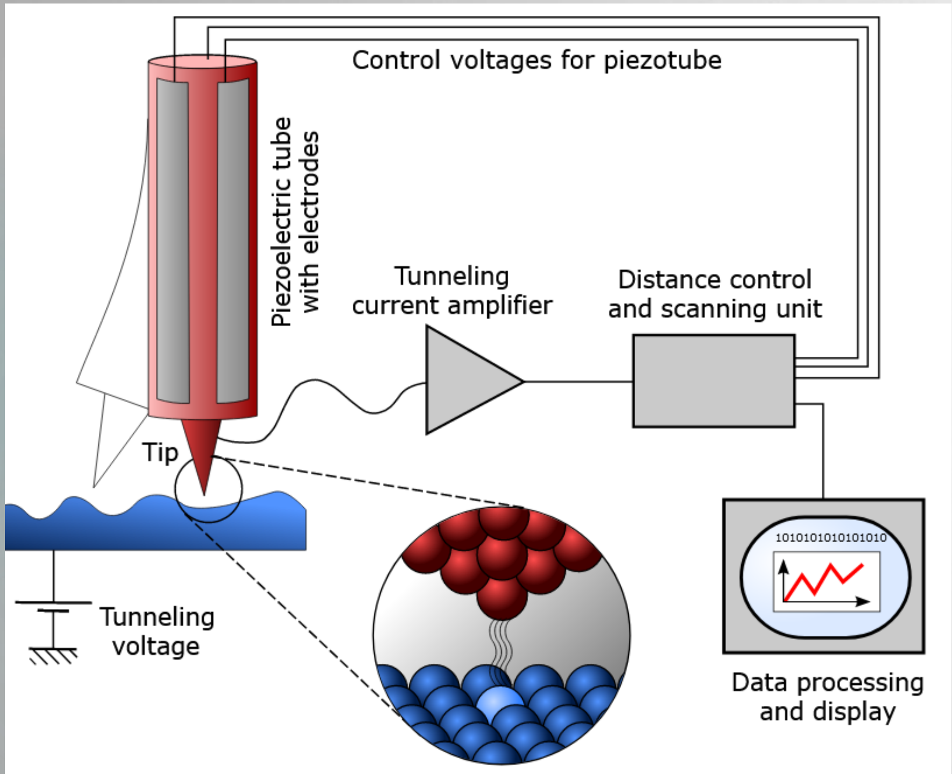


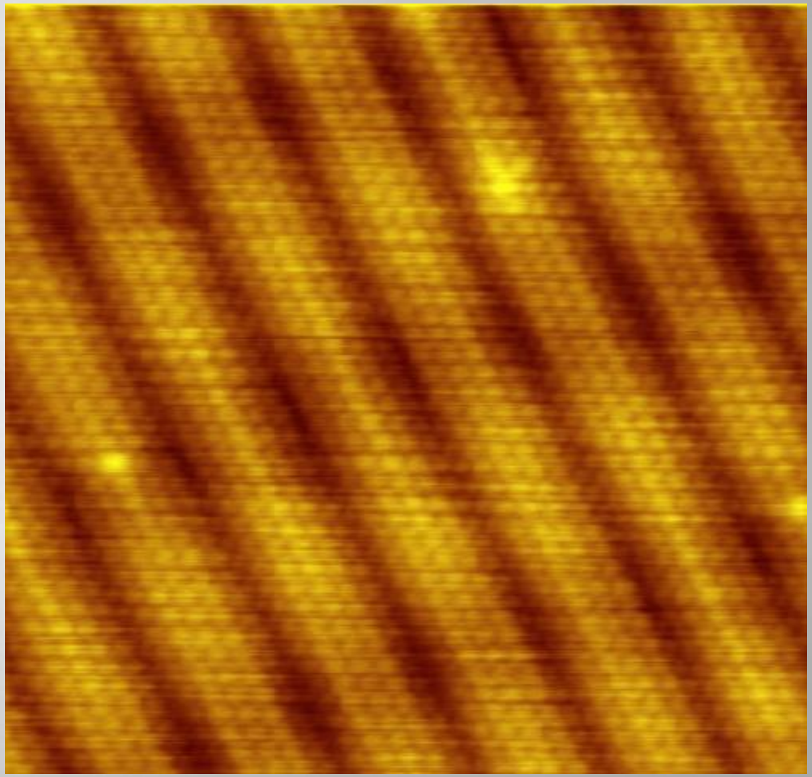

[15. Wikipedia, „Activation Energy"]

Chemical reactions

# Technical applications: Scanning tunneling microscope



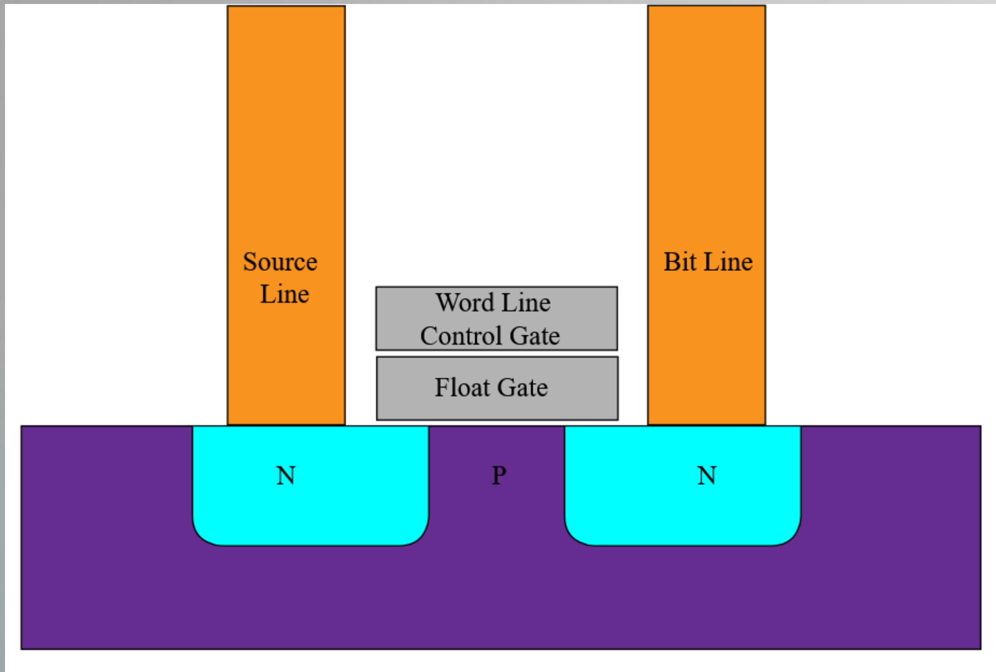


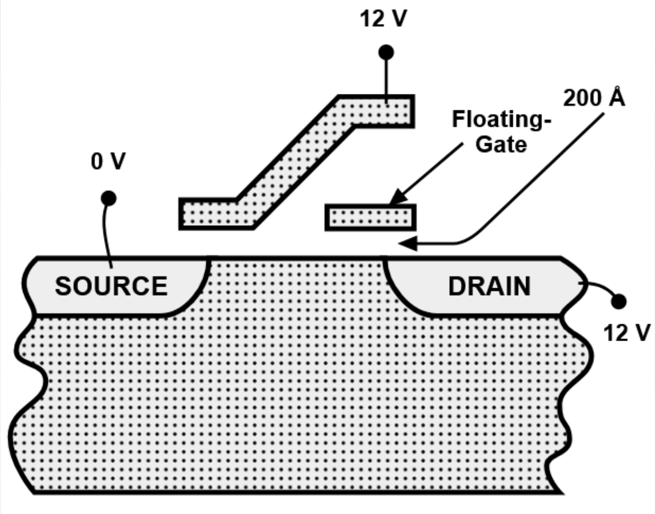
[Wikipedia, „Scanning tunneling micoroscope"]

# Technical applications: Flash memory

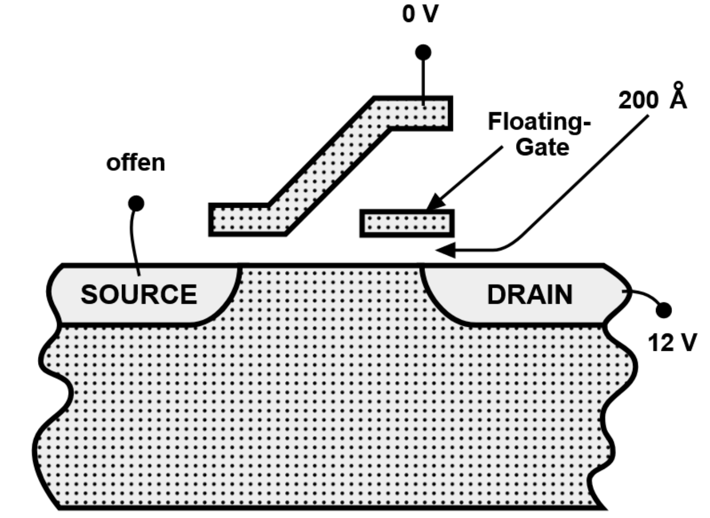





Programming




Erasing




Charge in floating gate determines bit value ➡ Can only be changed through tunneling by applying high voltage

[17. Wikipedia, „Flash memory“]

# Amorphous and crystalline Quartz

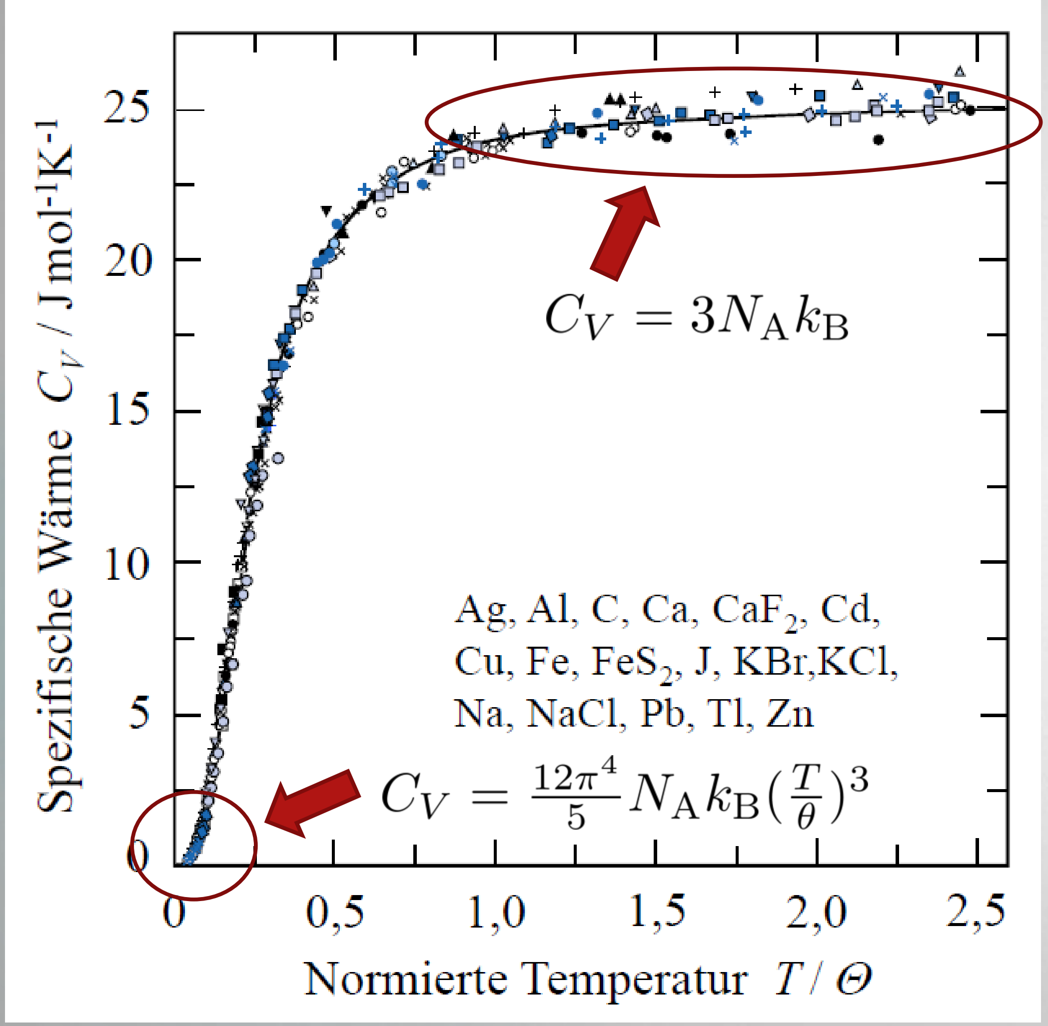


$SiO_2$

[2. Wikipedia, „Quarz"]

# Debye model






[18. S. Hunklinger, „Festkörperphysik"]

High temperature regime: Dulong-Petit law

Specific heat constant for all solids

$$C_V \sim \text{const}$$

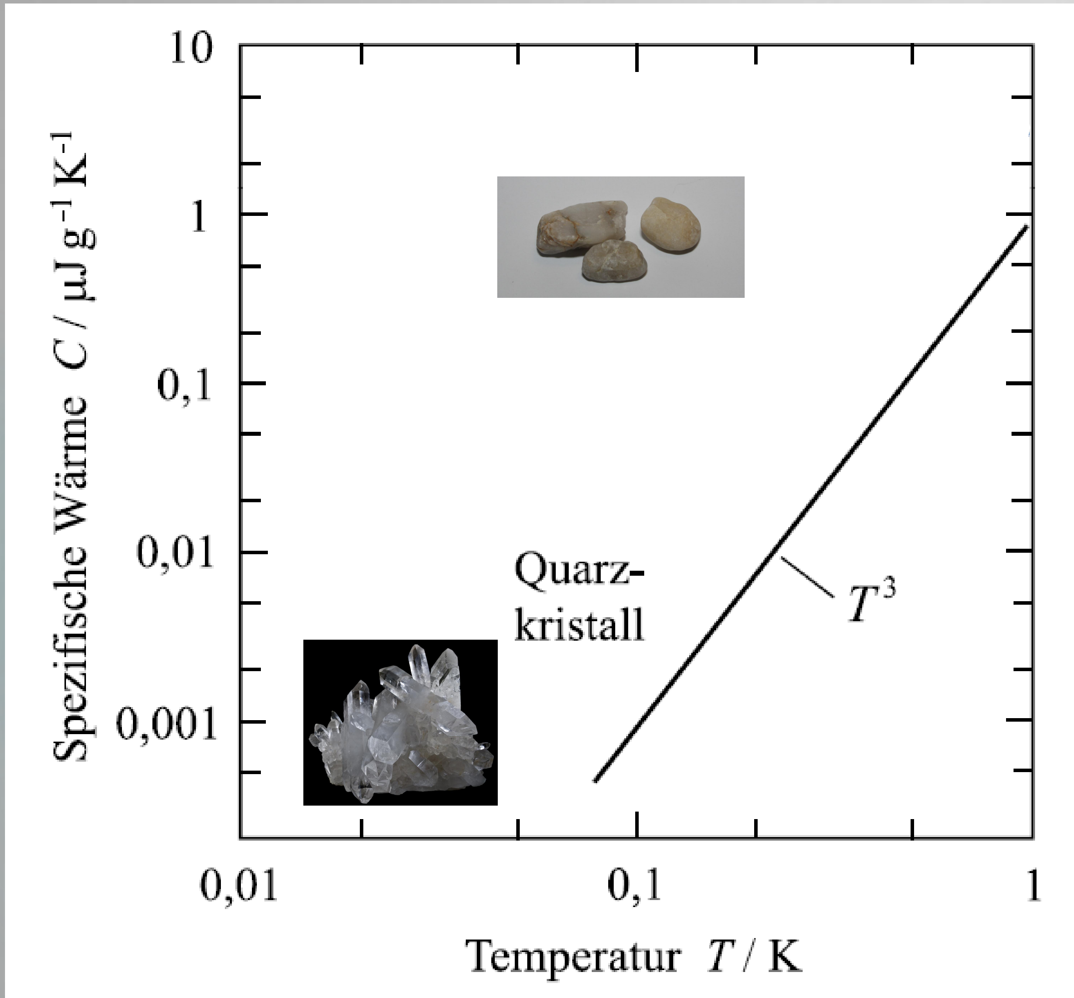
Low temperature regime: Debye model

Specific heat temperature dependent

$$C_V \sim T^3$$

# And at very low temperatures?





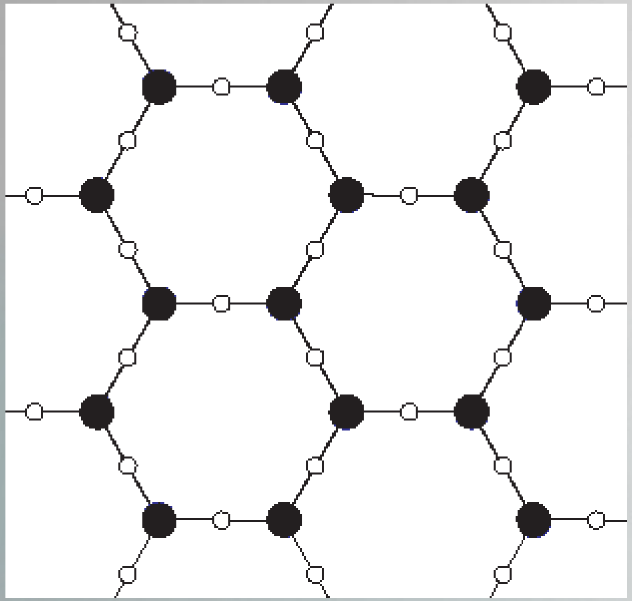

$C_V \sim T$ How is this possible?

➡ Density and composition are identical

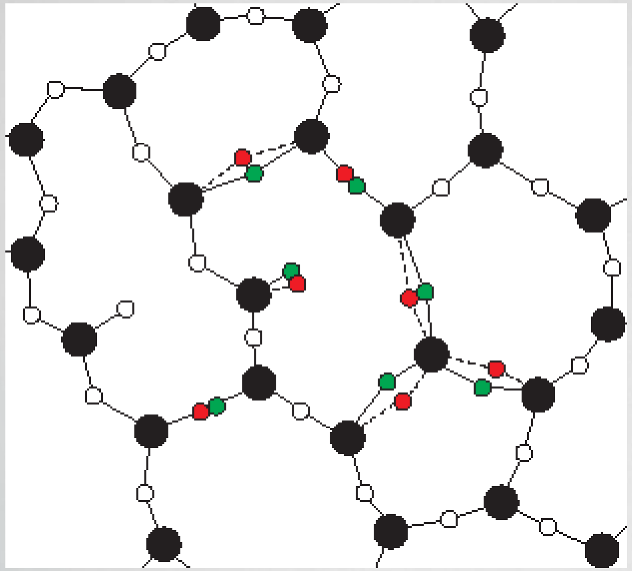
➡ All that's left is the structure itself

[18. S. Hunklinger, „Festkörperphysik"]

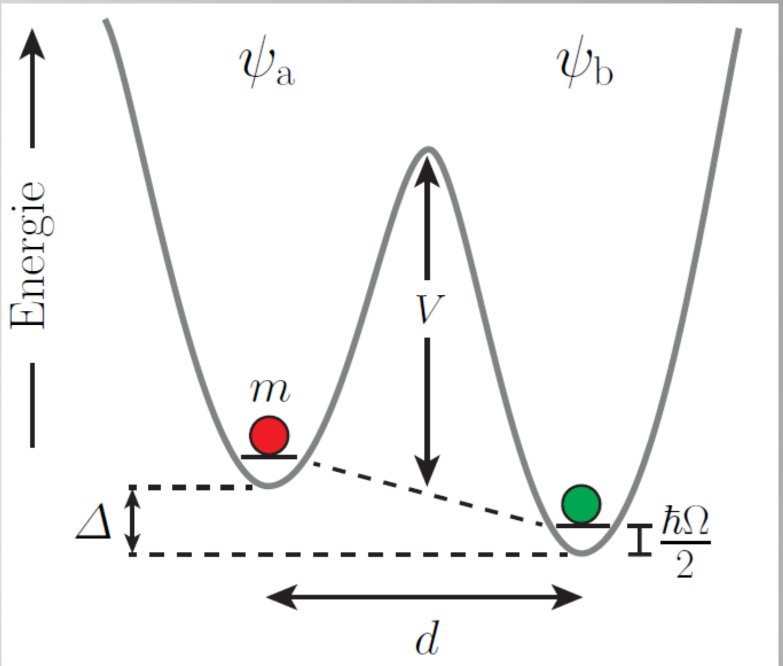
# Tunneling systems in amorphous solids



Crystal



Amorphous Solid (Glass)




Two energetically similar states

→ Two-state system

$$E_{\pm} = \frac{1}{2}\left(\hbar\Omega \pm \sqrt{\Delta^2 + \Delta_0^2}\right)$$

[18. S. Hunklinger, „Festkörperphysik“]

# Calculation of specific heat



Energy of two-state system

$$E = E_+ - E_- = \sqrt{\Delta^2 + \Delta_0^2}$$

Tunneling parameter

$$\lambda^2 = mVd^2/2\hbar^2$$

Distribution function

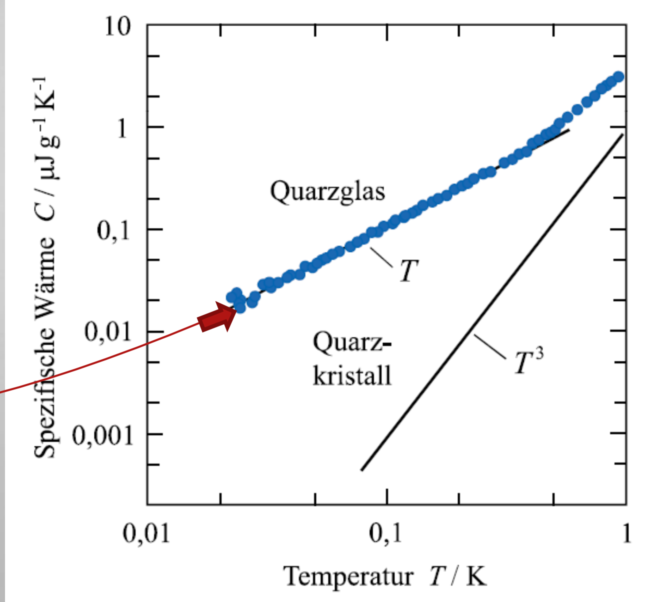
$$P(\Delta,\lambda)\mathrm{d}\Delta\mathrm{d}\lambda = \overline{P}\mathrm{d}\Delta\mathrm{d}\lambda$$

Density of states ➡ $D(E) = \int_0^{\lambda_{\max}} P(E,\lambda)\mathrm{d}\lambda = \overline{P}\lambda_{\max}\ln\frac{\hbar\Omega}{2E} \approx D_0 = const$

Internal energy ➡ $U = \int_0^{\infty} D(E)Ef(E,T)\mathrm{d}E = \frac{\pi^2 D_0 k_B^2 T^2}{12}$

Density of states | Energy | Fermi-Dirac distribution

Specific heat ➡ $C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{1}{6}\pi^2 D_0 k_B^2 T$




[18. S. Hunklinger, „Festkörperphysik“]

# Summary



## Alpha decay through tunneling

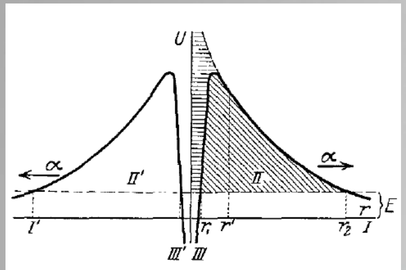
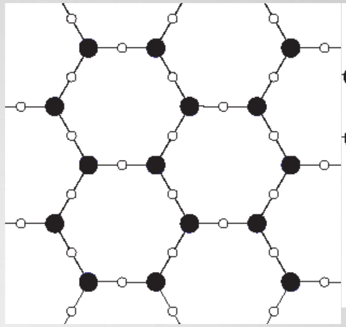


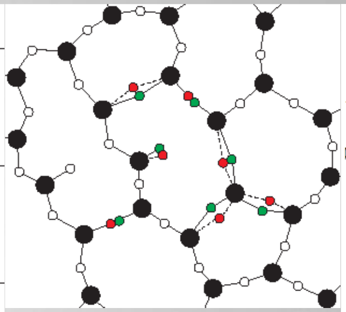
Fig. 4.

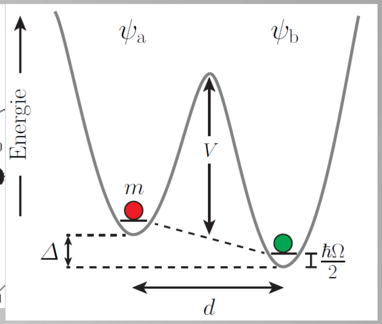
$$T \approx \frac{16E}{V_0^2}(V_0 - E)e^{-2a\kappa}$$

$$\kappa(r) = \sqrt{\frac{2m}{\hbar^2}(V(r) - E)}$$

## Amorphous and crystalline solids



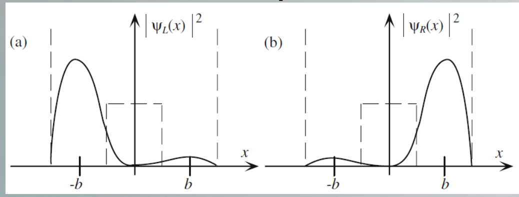





## Tunneling systems

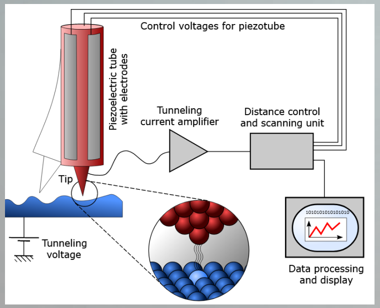
$$C_V \sim T^3 \Rightarrow C_V \sim T$$

## Two-State systems




$$E_\pm = \frac{1}{2}[(E_1 + E_2) \pm \sqrt{(E_1 - E_2)^2 + 4\Delta_0^2}]$$

## Technical applications ⟷ Quantum world




# Sources (1)




- 1. The man who could walk through walls; The Short Story Project; Marcel Aymé https://www.shortstoryproject.com/story/the-man-who-could-walk-through-walls/ [last visit 01.05.21]
- 2. Quartz; Wikipedia; https://de.wikipedia.org/wiki/Quarz [last visit 01.05.21]
- 3. Alpha decay; Wikipedia; https://en.wikipedia.org/wiki/Alpha_decay [last visit 01.05.21]
- 4. The STM […] The forgotten contribution of Robert Francis Earhart to the discovery of quantum tunneling.; Thomas Mark Cuff; https://www.researchgate.net/publication/294260678 [2016]
- 5. Annalen der Physik, Vierte Folge, Band 80; Erwin Schrödinger [1926]
- 6. The Physical Review, An Undulatory Theory of the Mechanics of Atoms and Molecules; E. Schrödinger [1926]
- 7. Zur Quantentheorie des Atomkernes; G. Gamow [1928]
- 8. Zur Deutung der Molekelspektren III; F. Hund [1927]
- 9. Tunneleffekt; Wikipedia; https://de.wikipedia.org/wiki/Tunneleffekt [last visit 01.05.21]
- 10. Atoms, Molecules and Photons; Springer; Third Edition; Wolfram Demtröder [2018]
- 11. Fly on insect net; Wikimedia Commons https://commons.wikimedia.org/wiki/File:Fly_on_insect_net_20060621_002.jpg [last visit 01.05.21]
- 12. Quantum Mechanics; Second Edition; Springer; J.L. Basdevant/ J. Dalibard [2002]
- 13. Zweizustandssystem; Wikipedia https://de.wikipedia.org/wiki/Zweizustandssystem [last visit 01.05.21]
- 14. Nuclear Fusion; Wikipedia https://en.wikipedia.org/wiki/Nuclear_fusion [last visit 01.05.21]

# Sources (2)



- 15. Activation energy; Wikipedia https://en.wikipedia.org/wiki/Activation_energy [last visit 01.05.21]
- 16. Leben in der Quantenwelt; Spektrum der Wissenschaft; Vlatko Vedral https://www.spektrum.de/magazin/leben-in-derquantenwelt/1116464 [2011]
- 17. Flash memory; Wikipedia https://en.wikipedia.org/wiki/Flash_memory [01.05.21]
- 18. Festkörperphysik; S. Hunklinger; 5. Auflage [2018]