

2D kvantová jáma s rotační symetrií

$$-\frac{\hbar^2}{2\mu} \nabla^2 \Psi + V\Psi = E\Psi$$

↓

v polárních souřadnicích

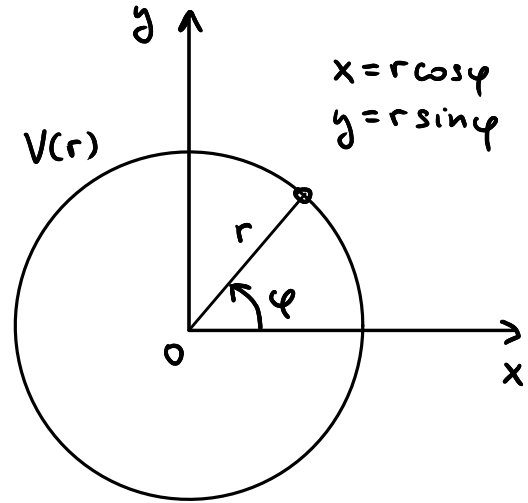
$$-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right) \Psi + V(r)\Psi = E\Psi$$

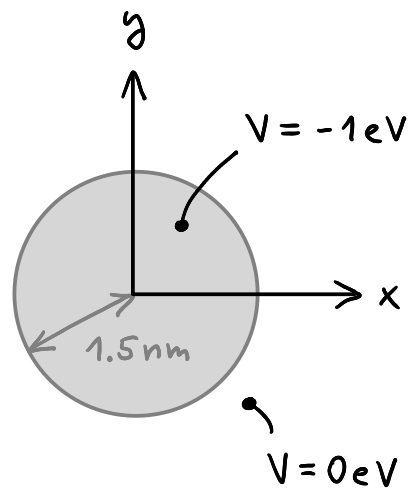
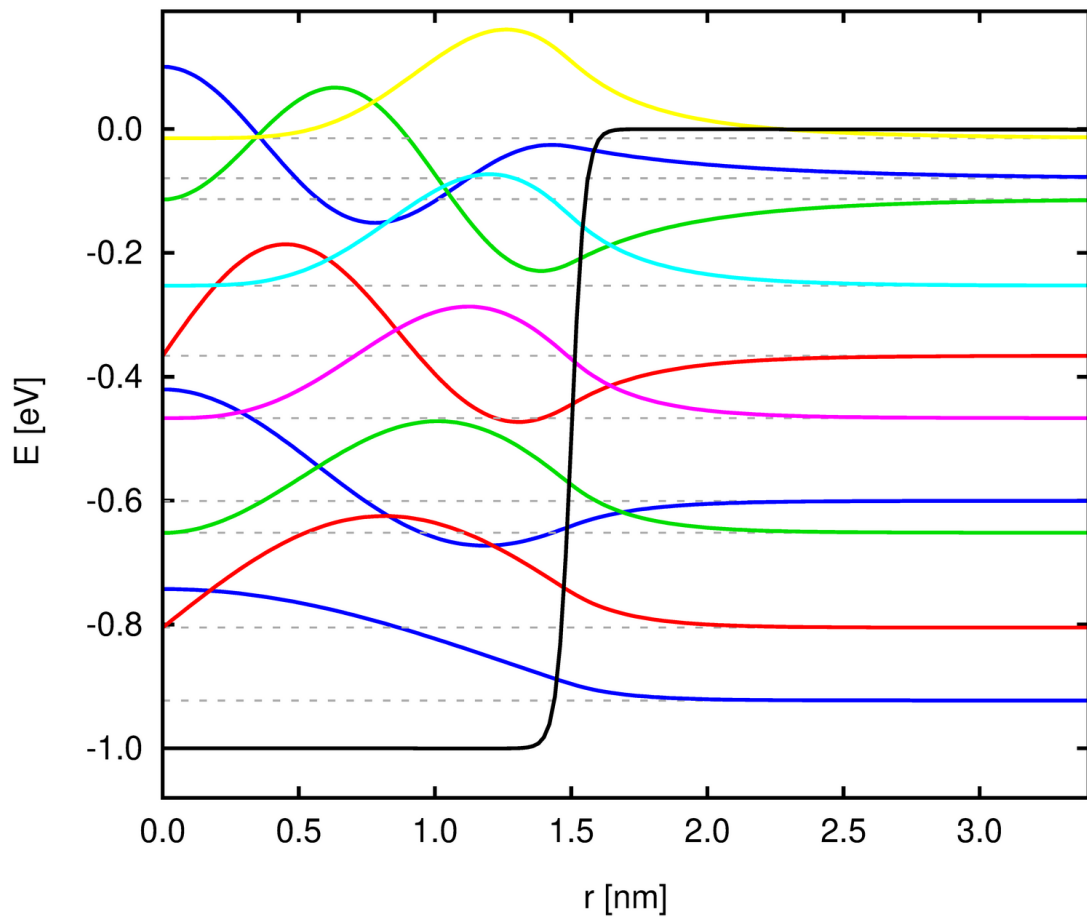
separace proměnných vede na

$$\Psi(r, \varphi) = R(r) e^{im\varphi} \quad m \in \mathbb{Z} \quad \text{vlastní stav } \hat{L}_2: \hat{L}_2 \Psi = \hbar m \Psi$$

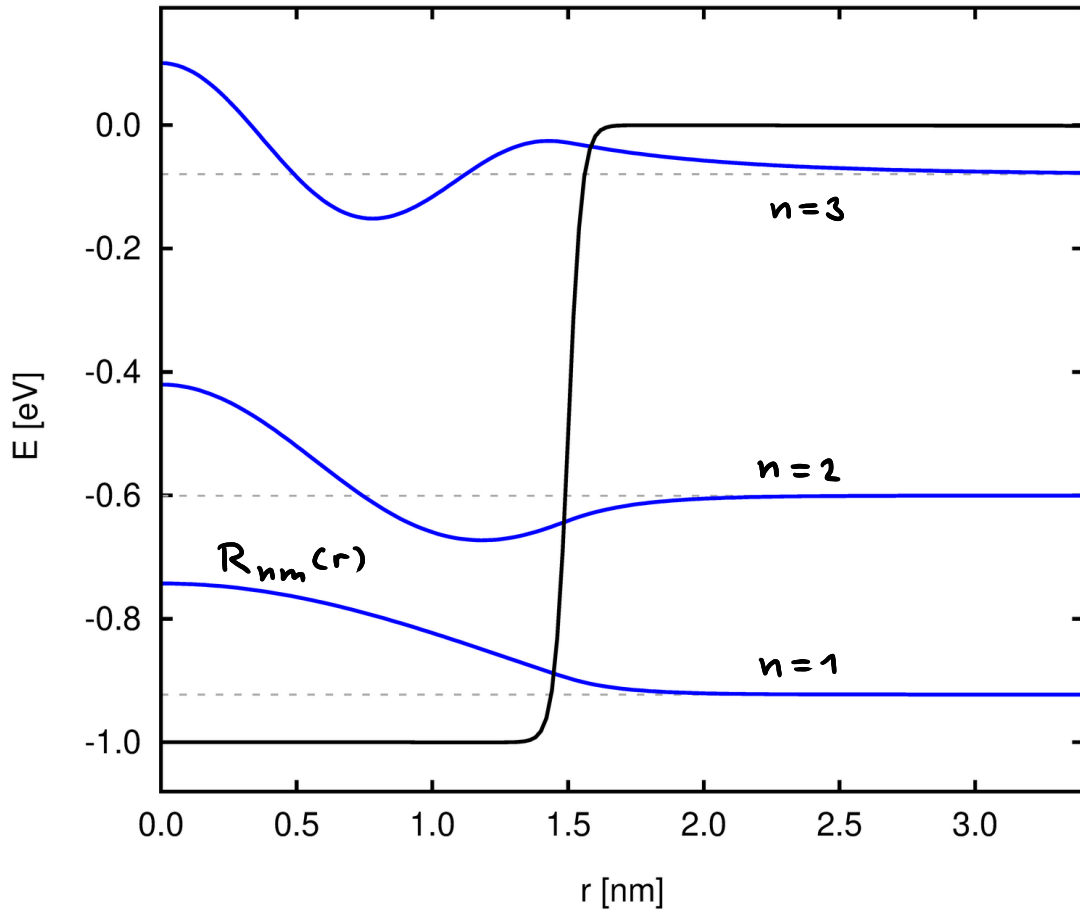
a radiální rovnici pro $R(r)$

$$-\frac{\hbar^2}{2\mu} \left(\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} \right) + \left[V(r) + \frac{(\hbar m)^2}{2\mu r^2} \right] R = ER$$

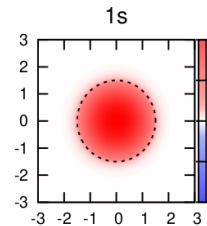
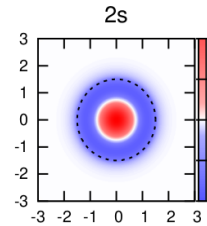
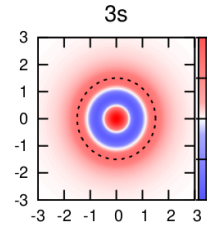




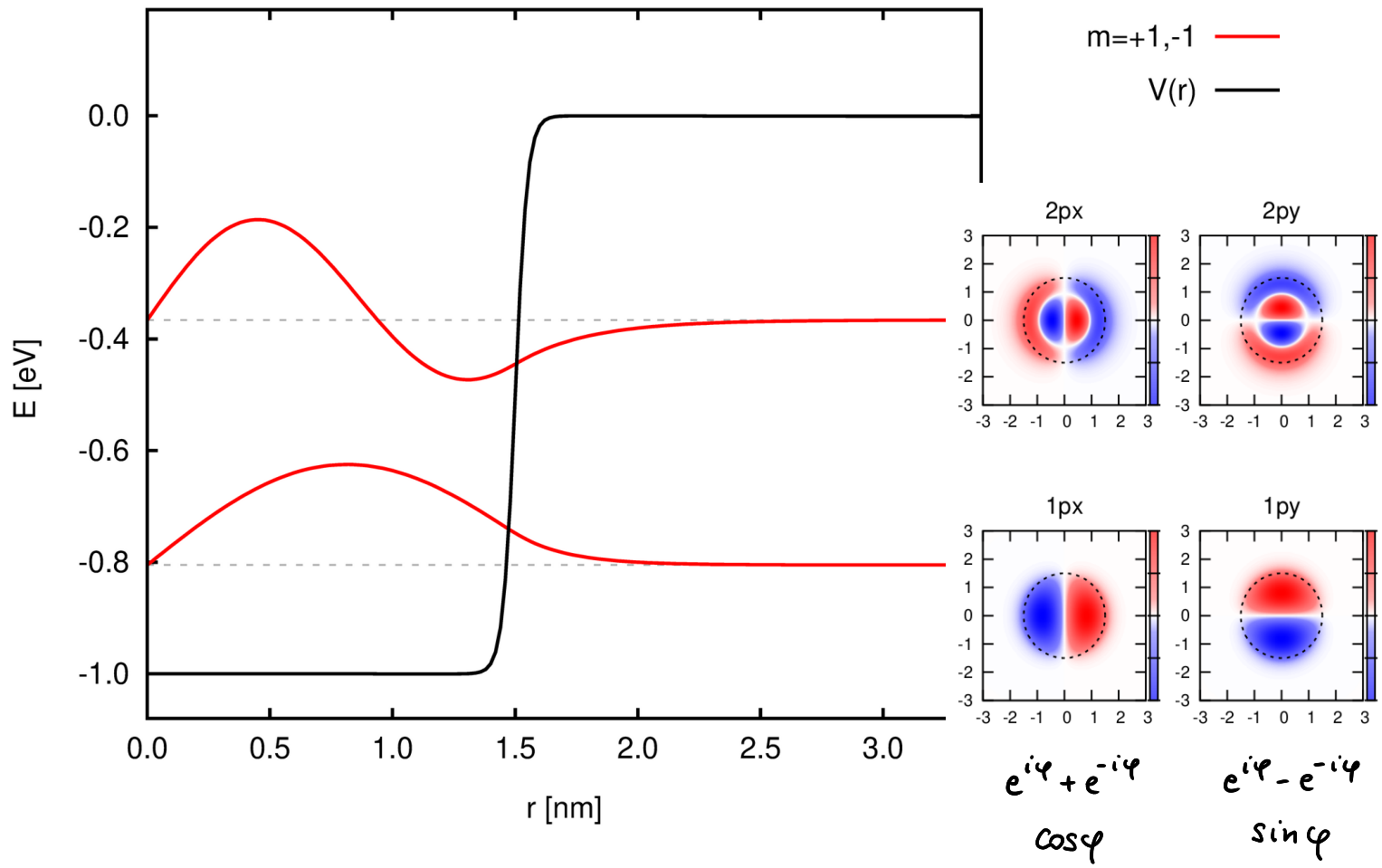
$m=0$ s-orbitally $\Psi(r,\varphi) = R_{n0}(r)$



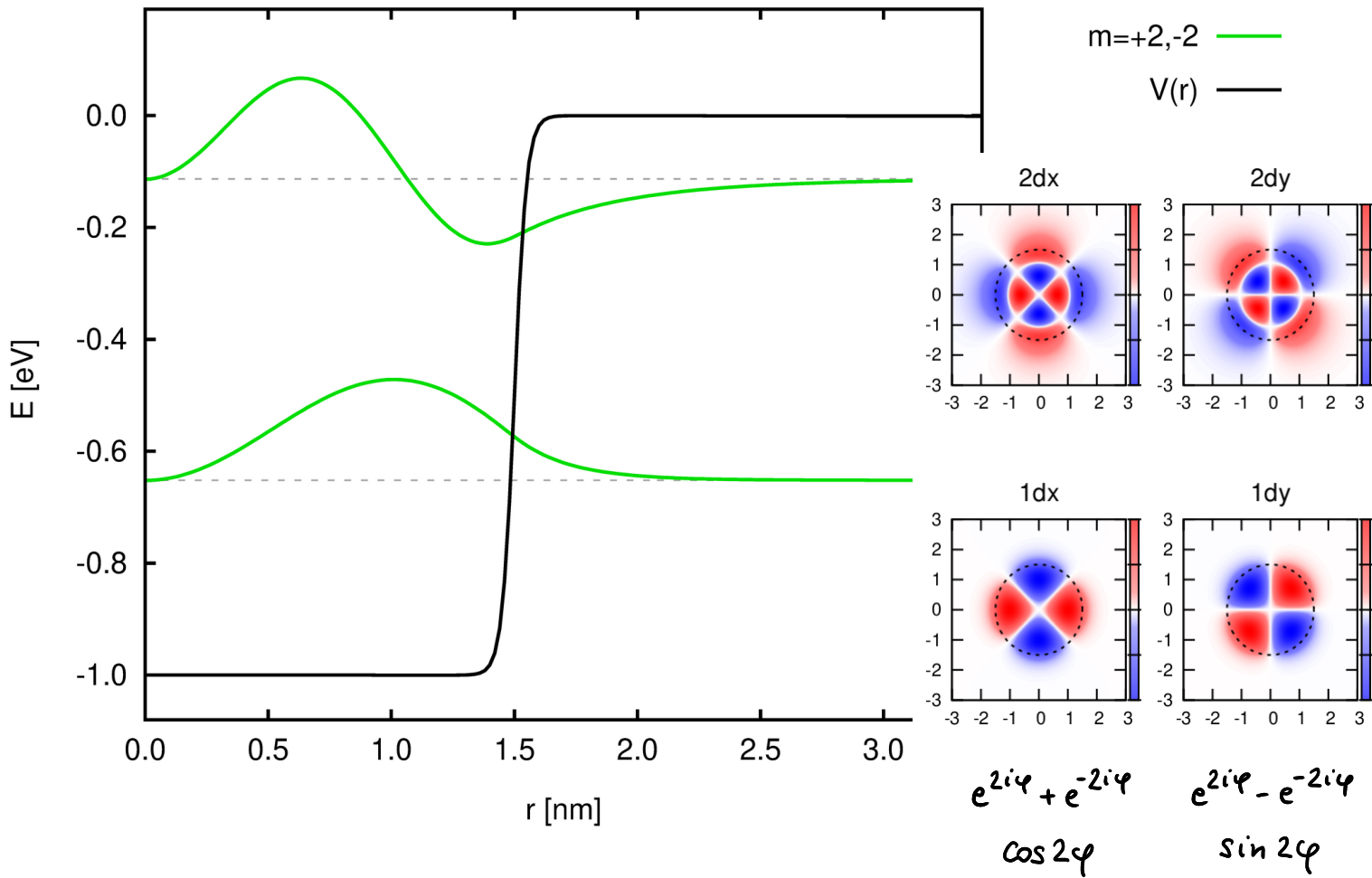
$m=0$ — blue line
 $V(r)$ — black line



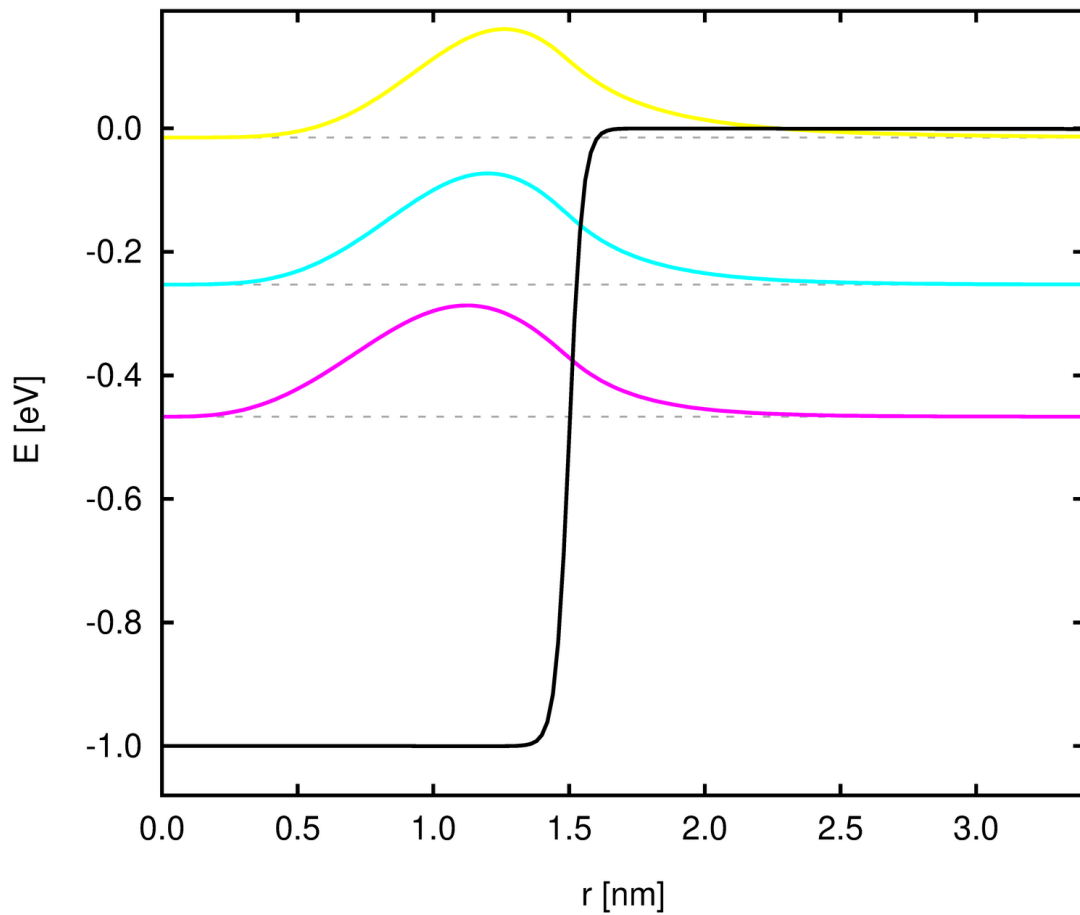
$m = \pm 1$ p-orbitals $\Psi(r, \varphi) = R_{n1}(r) e^{\pm i\varphi}$



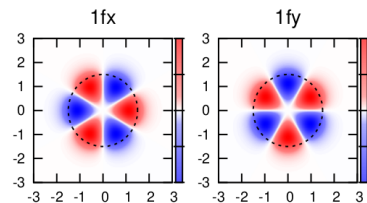
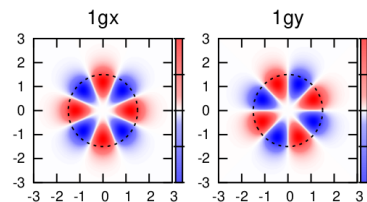
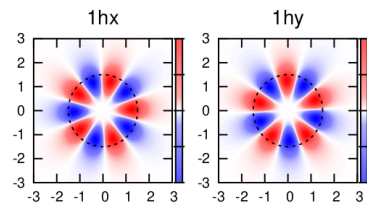
$m = \pm 2$ d-orbitally $\Psi(r, \varphi) = R_{n2}(r) e^{\pm 2i\varphi}$



$m = \pm 3, 4, 5$ Fig. h-orbitals



$m = +3, -3$ —
 $m = +4, -4$ —
 $m = +5, -5$ —
 $V(r)$ —

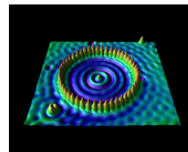
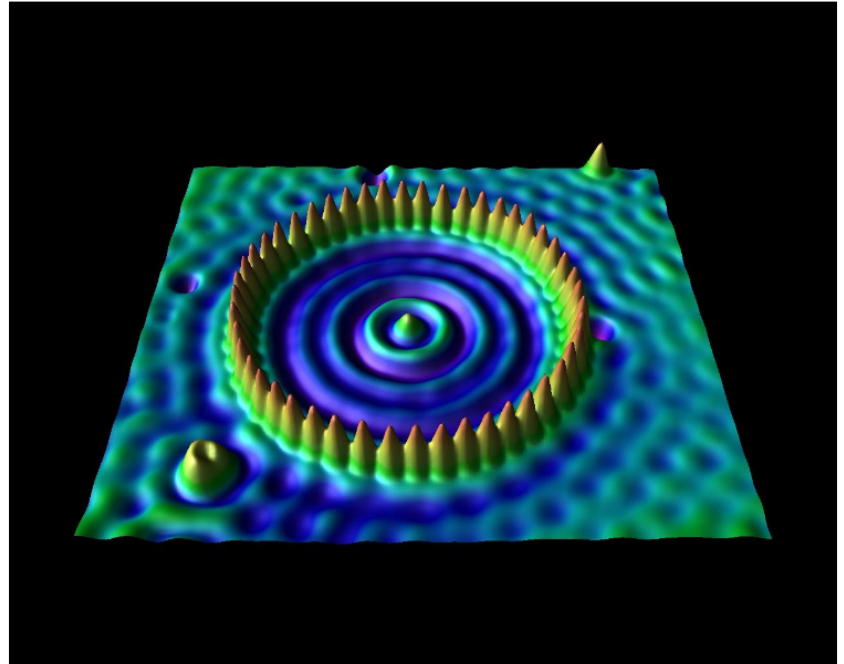


Kvantové korály

■ DESCRIPTION

The corral is an artificial structure created from 48 iron atoms (the sharp peaks) on a copper surface. The wave patterns in this scanning tunneling microscope image are formed by copper electrons confined by the iron atoms. Don Eigler and colleagues created this structure in 1993 by using the tip of a low-temperature scanning tunneling microscope (STM) to position iron atoms on a copper surface, creating an electron-trapping barrier. This was the first successful attempt at manipulating individual atoms and led to the development of new techniques for nanoscale construction.

- **SIZE:** The radius of the corral is about 7 nm.
- **IMAGING TOOL:** Scanning tunneling microscope



Confinement of Electrons to Quantum Corrals on a Metal Surface

M. F. Crommie, C. P. Lutz, D. M. Eigler

A method for confining electrons to artificial structures at the nanometer lengthscale is presented. Surface state electrons on a copper(111) surface were confined to closed structures (corrals) defined by barriers built from iron adatoms. The barriers were assembled by individually positioning iron adatoms with the tip of a 4-kelvin scanning tunneling microscope (STM). A circular corral of radius 71.3 Å was constructed in this way out of 48 iron adatoms. Tunneling spectroscopy performed inside of the corral revealed a series of discrete resonances, providing evidence for size quantization. STM images show that the corral's interior local density of states is dominated by the eigenstate density expected for an electron trapped in a round two-dimensional box.

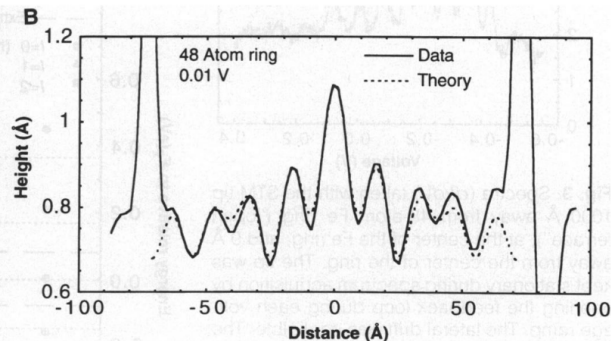
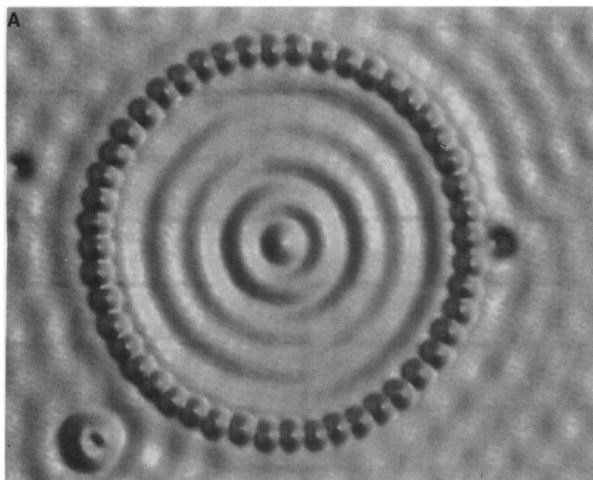


Fig. 2. Spatial image of the eigenstates of a quantum corral. **(A)** 48-atom Fe ring constructed on the Cu(111) surface ($V = 0.01$ volt, $I = 1.0$ nA). Average diameter of ring (atom center to atom center) is 142.6 Å. The ring encloses a

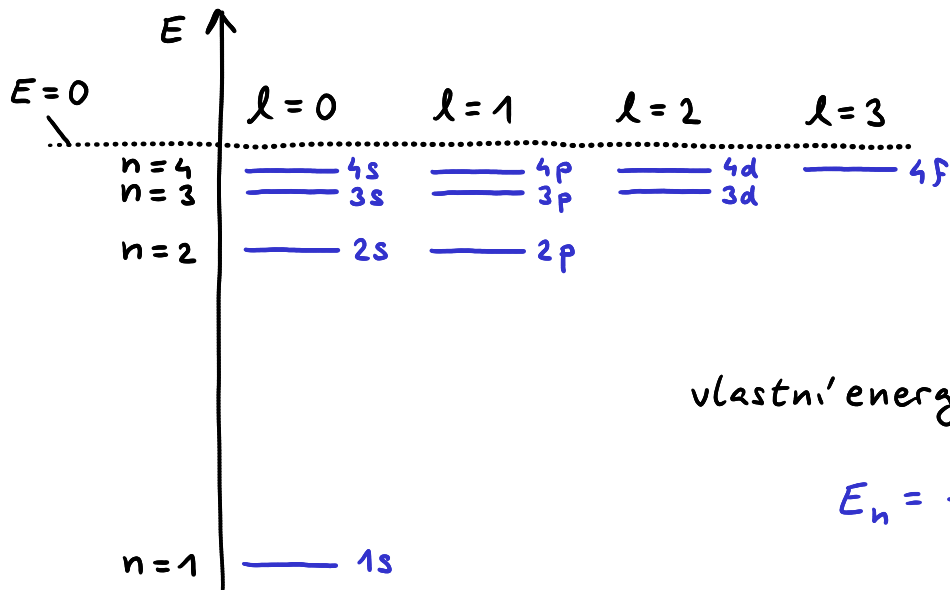
defect-free region of the surface. **(B)** Solid line: cross section of the above data. Dashed line: fit to cross section using a linear combination of $|5,0\rangle$, $|4,2\rangle$, and $|2,7\rangle$ eigenstate densities.

Atom vodíku

radia'lní Schrödingerova rovnice

odpovídá' odstředivý' potenciál'

$$-\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{d^2}{dr^2} (rR) + \left[\frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] R = ER$$



vlastní energie

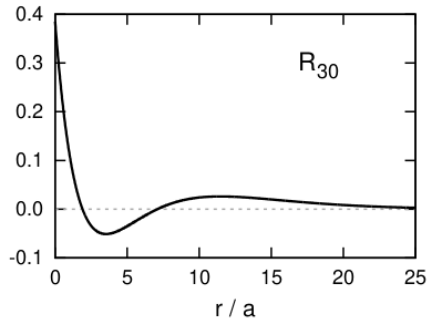
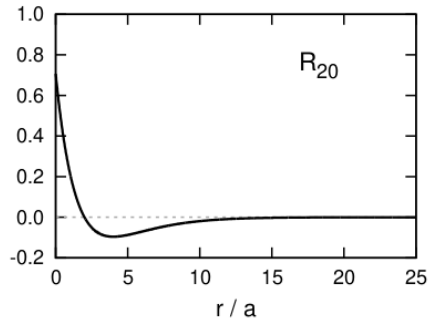
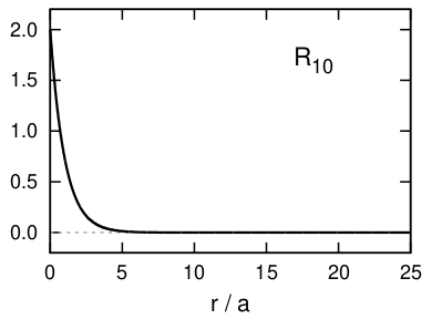
$$E_n = - \frac{me^4}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2}$$

$n = 1$

$n = 2$

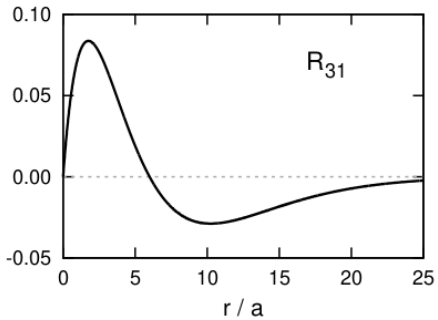
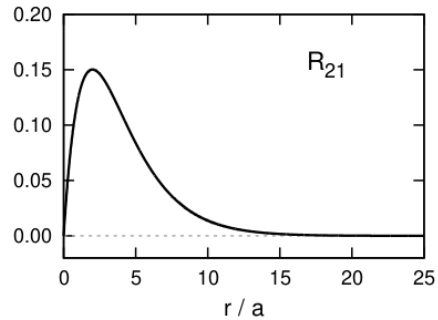
$n = 3$

$l = 0$



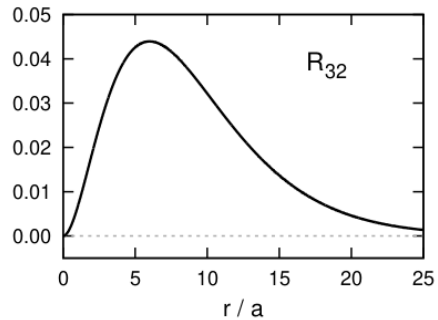
$l = 1$

$R_{nl}(r)$



$l = 2$

Bohrův poloměr $a = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$

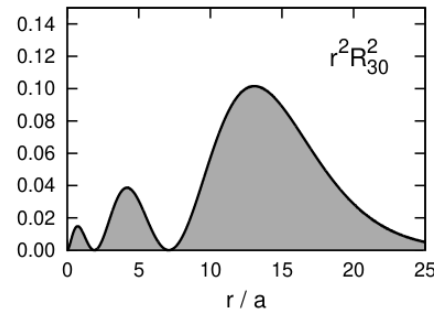
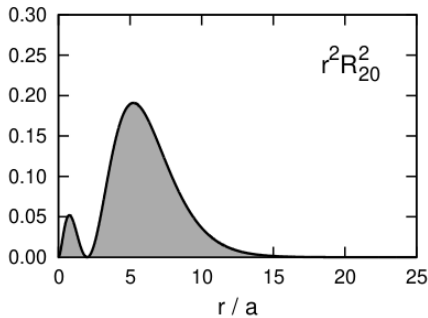
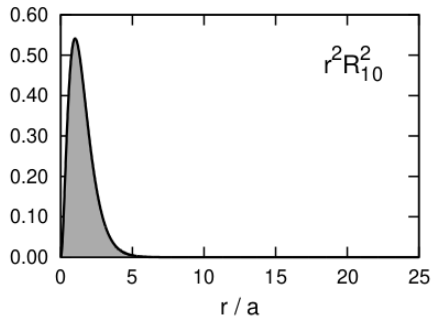


$n = 1$

$n = 2$

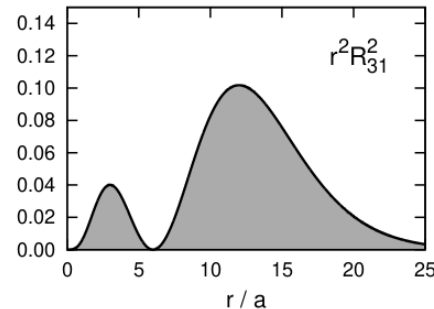
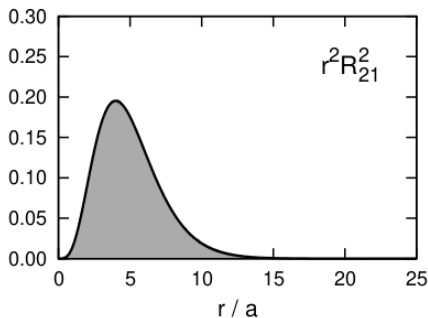
$n = 3$

$l = 0$

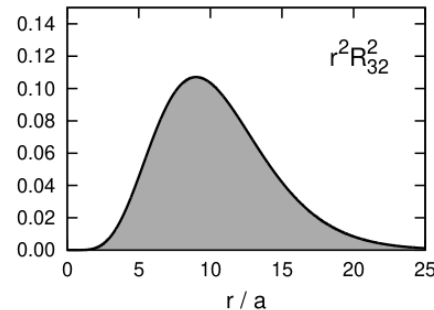


$l = 1$

$r^2 R_{nl}^2(r)$

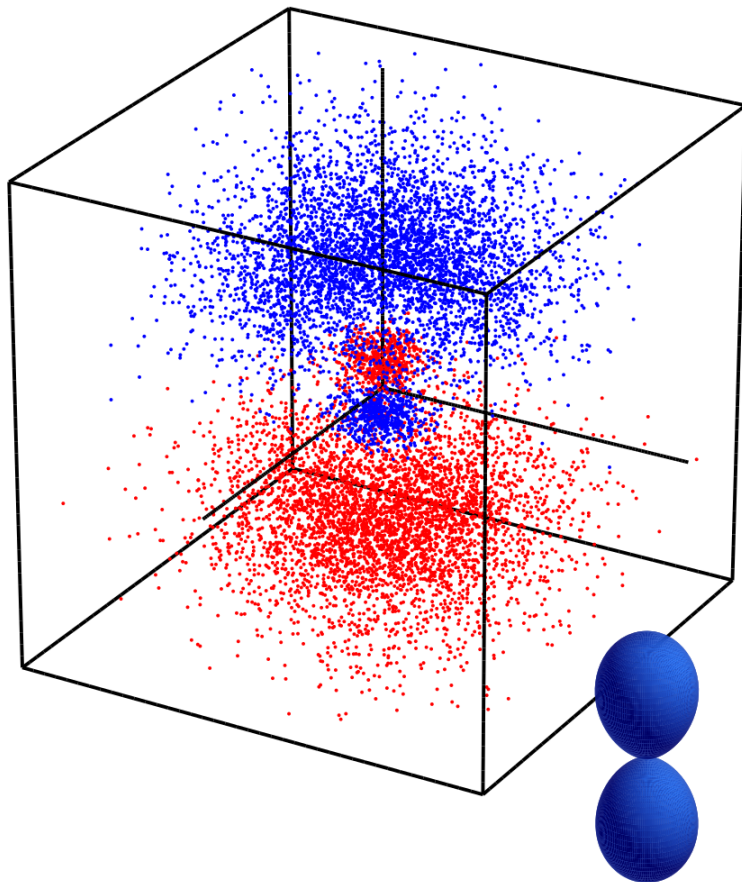


$l = 2$

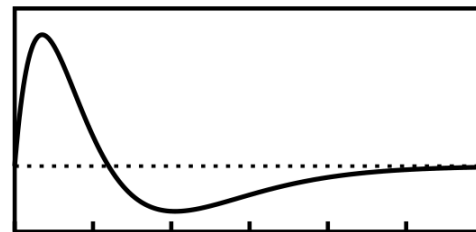


Bohrův poloměr $a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$

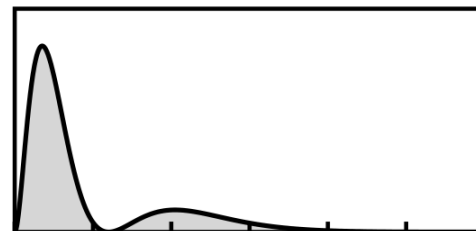
$3p_z$



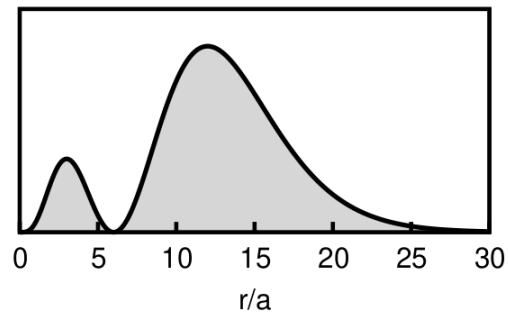
$R_{nl}(r)$



$|R_{nl}(r)|^2$



$r^2|R_{nl}(r)|^2$



Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik.

Von W. Pauli jr. in Hamburg.

(Eingegangen am 17. Januar 1926.)

Es wird gezeigt, daß sich die Balmerterme eines Atoms mit einem einzigen Elektron aus der neuen Quantenmechanik richtig ergeben und daß die in der bisherigen Theorie aus den Zusatzverboten von singulären Bewegungen entstehenden Schwierigkeiten, die insbesondere im Falle der gekreuzten Felder zutage treten, in der neuen Theorie verschwinden. Auch die Beeinflussung des Wasserstoffspektrums durch äußere elektrische und magnetische Kraftfelder wird vom Standpunkt der neuen Quantenmechanik aus diskutiert. Die Berücksichtigung der Relativitätskorrekturen sowie die Berechnung der Übergangswahrscheinlichkeiten (Intensitäten) bleibt jedoch zunächst noch außer Betracht.

§ 1. Die Grundlagen der neuen Quantenmechanik. Kürzlich ist von Heisenberg¹⁾ eine Formulierung der Prinzipien der Quantentheorie gegeben worden, [die gegenüber der bisherigen Theorie der mehrfach periodischen Systeme einen großen Fortschritt darstellt. Gemäß dieser Heisenbergschen Fassung der Quantentheorie wird auf eine mechanisch-kinematische Veranschaulichung der Bewegung der Elektronen in den stationären Zuständen des Atoms gänzlich verzichtet, und

¹⁾ W. Heisenberg, ZS. f. Phys. **33**, 879, 1925.

Kmity molekuly chlorovodíku

$$m_H = 1.674 \cdot 10^{-27} \text{ kg}$$

$$m_{Cl} = 58.9 \cdot 10^{-27} \text{ kg}$$

$$\mu = \frac{m_H m_{Cl}}{m_H + m_{Cl}} \approx m_H$$

Morseův potenciál

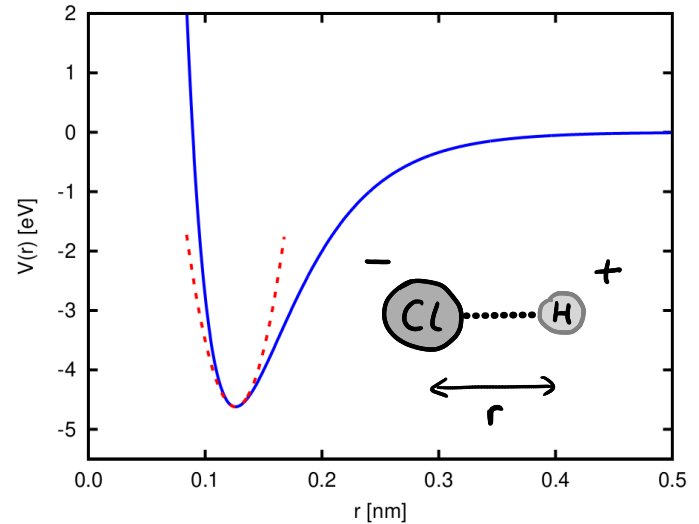
$$V(r) = D(e^{-2\alpha\zeta} - 2e^{-\alpha\zeta})$$

$$\zeta = \frac{r-r_0}{r_0}, \quad r_0 = 0.126 \text{ nm}, \quad D = 4.62 \text{ eV}, \quad \alpha = 2.38$$

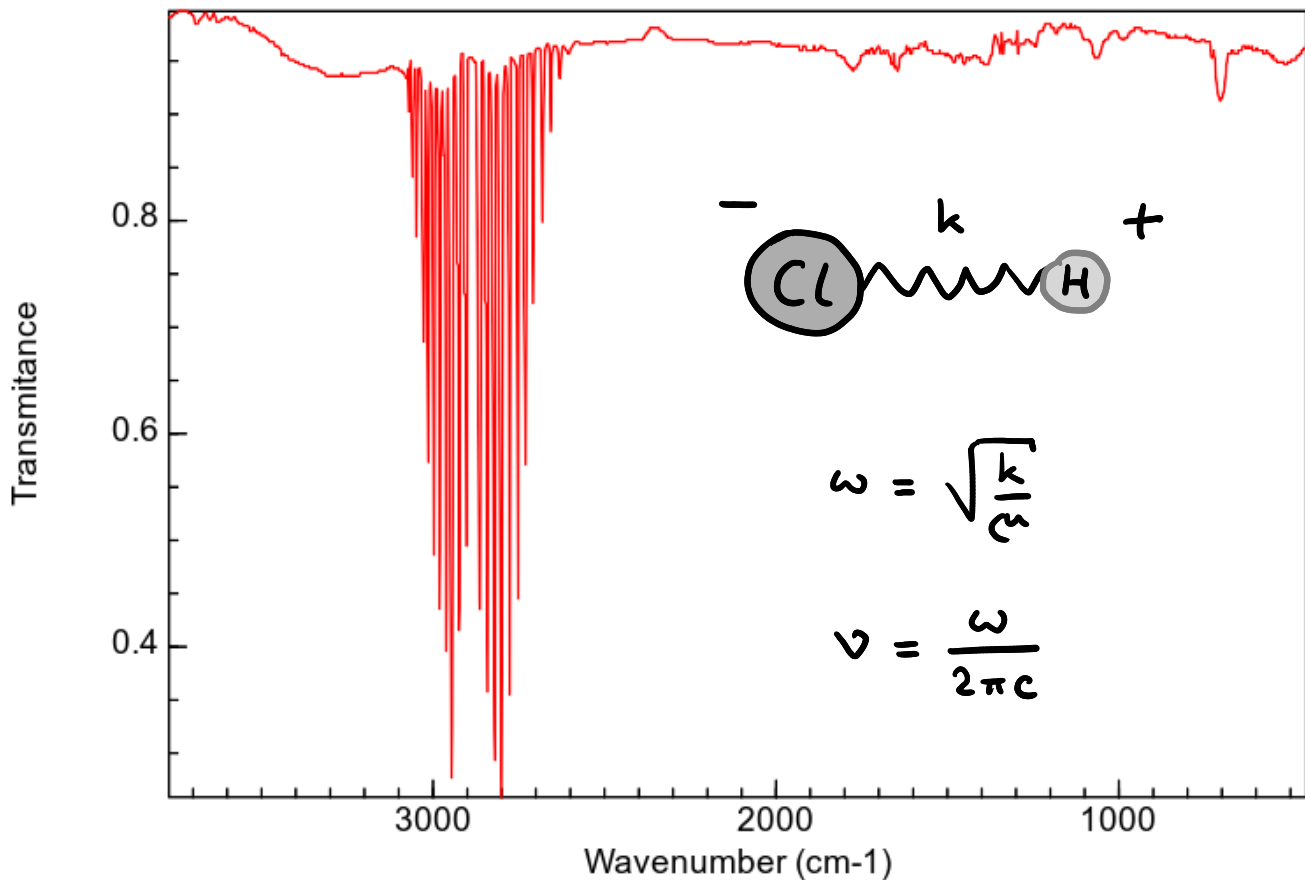
harmonická aproximace

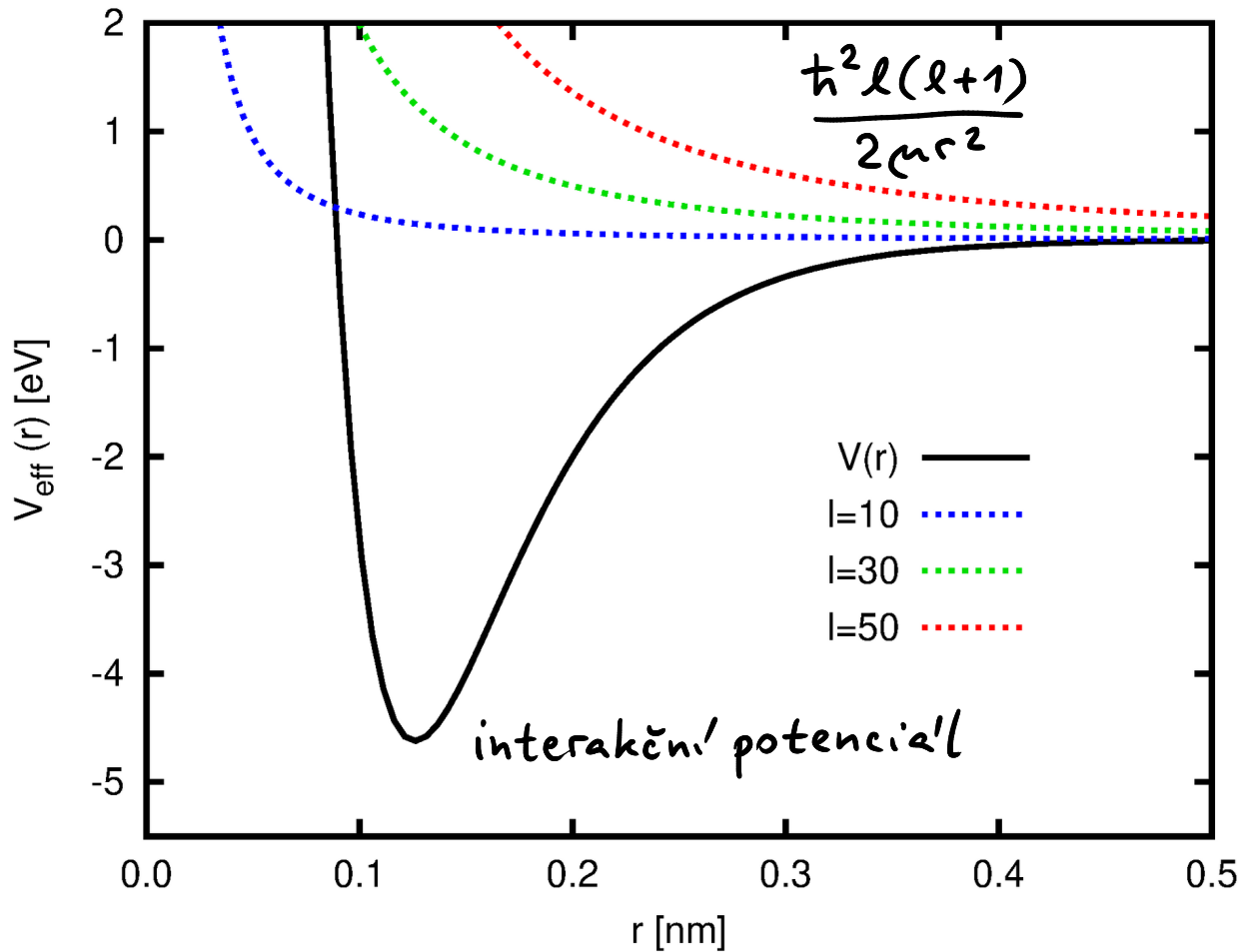
$$V(r) \approx V(r_0) + \frac{1}{2} \frac{d^2V}{dr^2} \Big|_{r=r_0} (r-r_0)^2$$

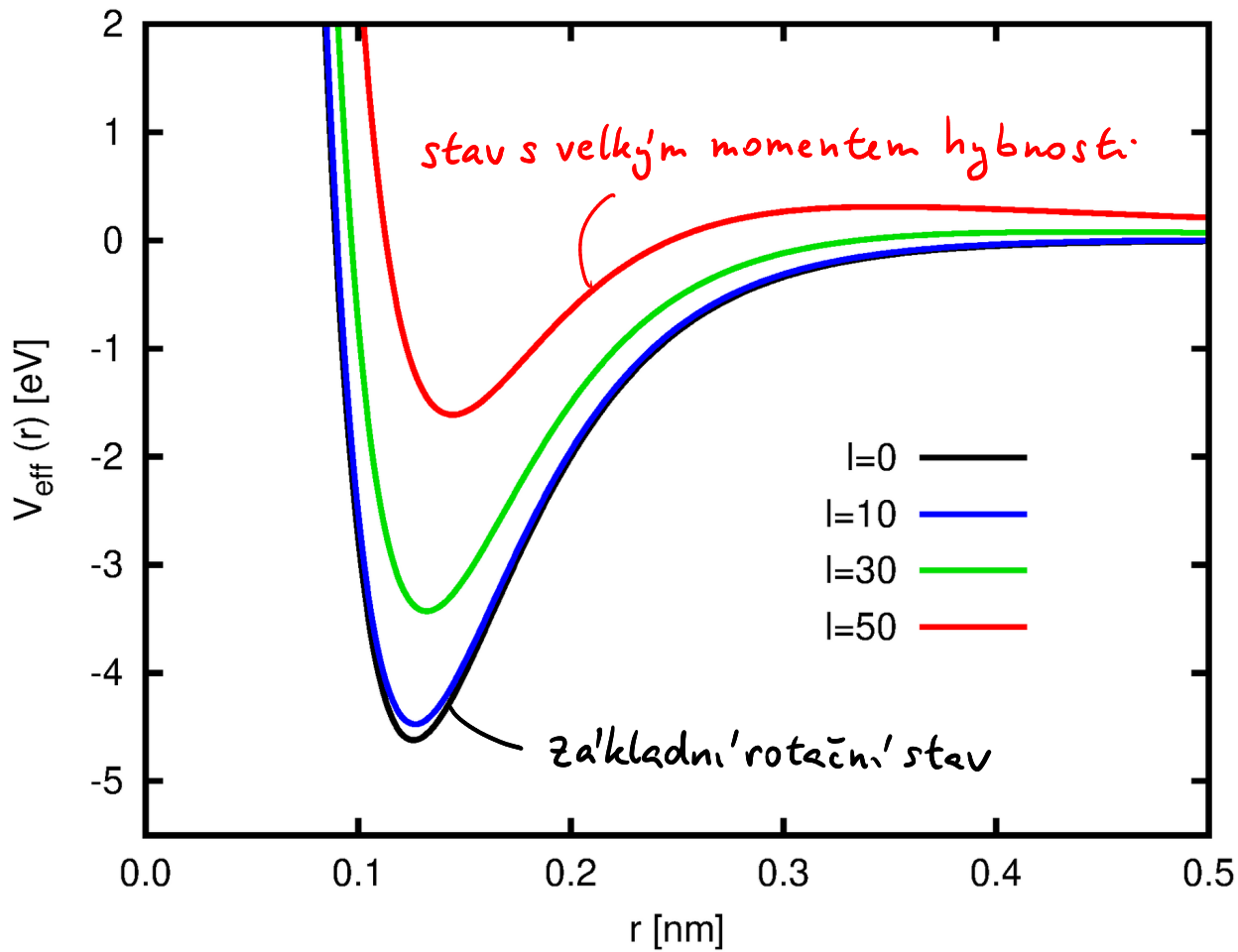
$$k = m\omega^2 = \frac{2D\alpha^2}{r_0^2} \quad \rightarrow \quad \omega = \sqrt{\frac{2D\alpha^2}{m r_0^2}}$$

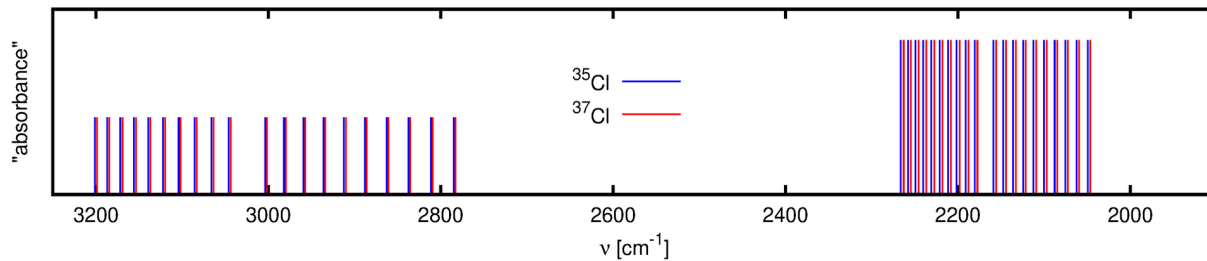
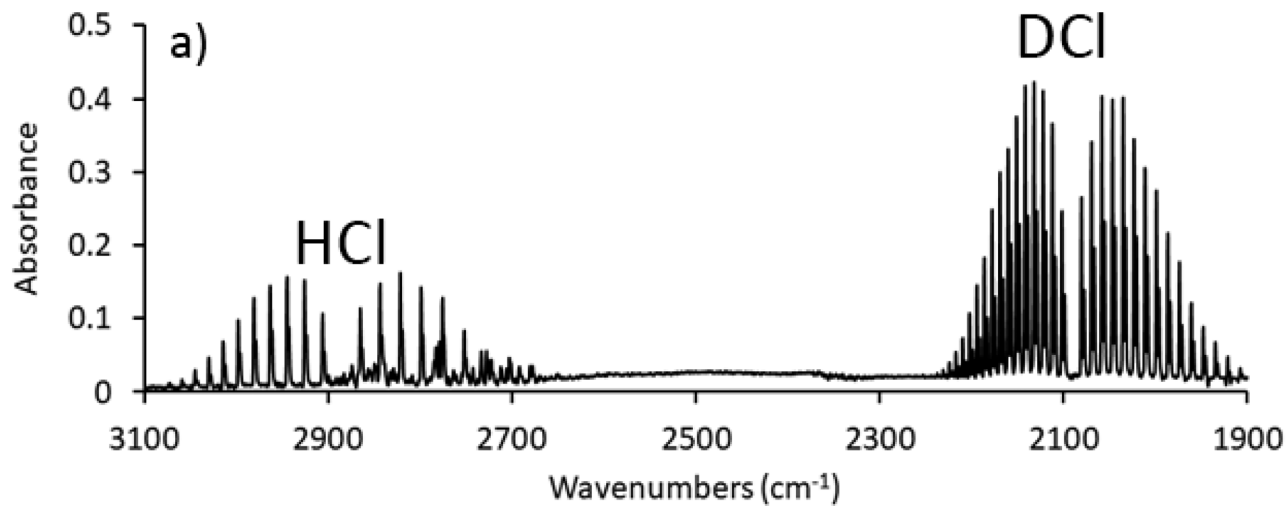


HYDROGEN CHLORIDE INFRARED SPECTRUM

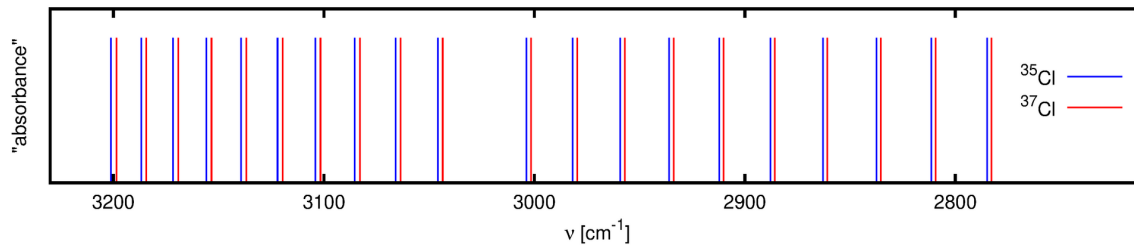
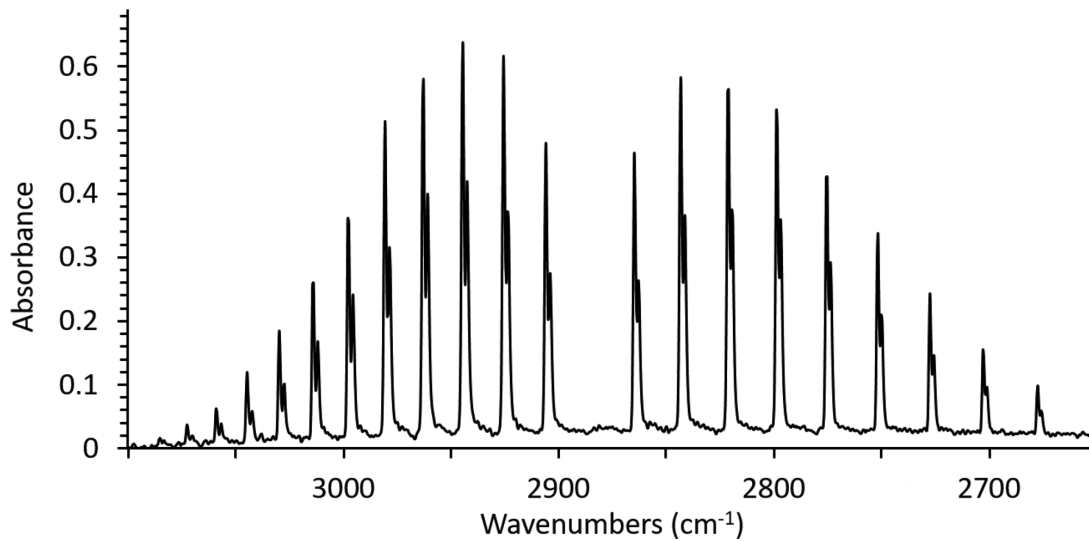


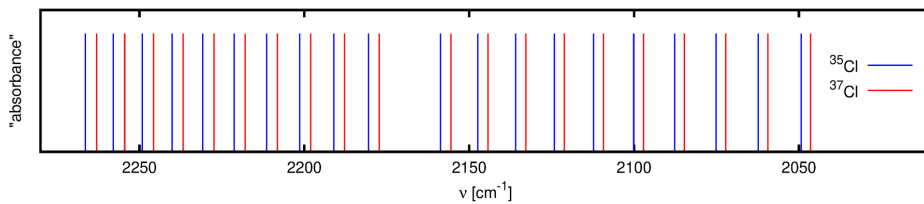
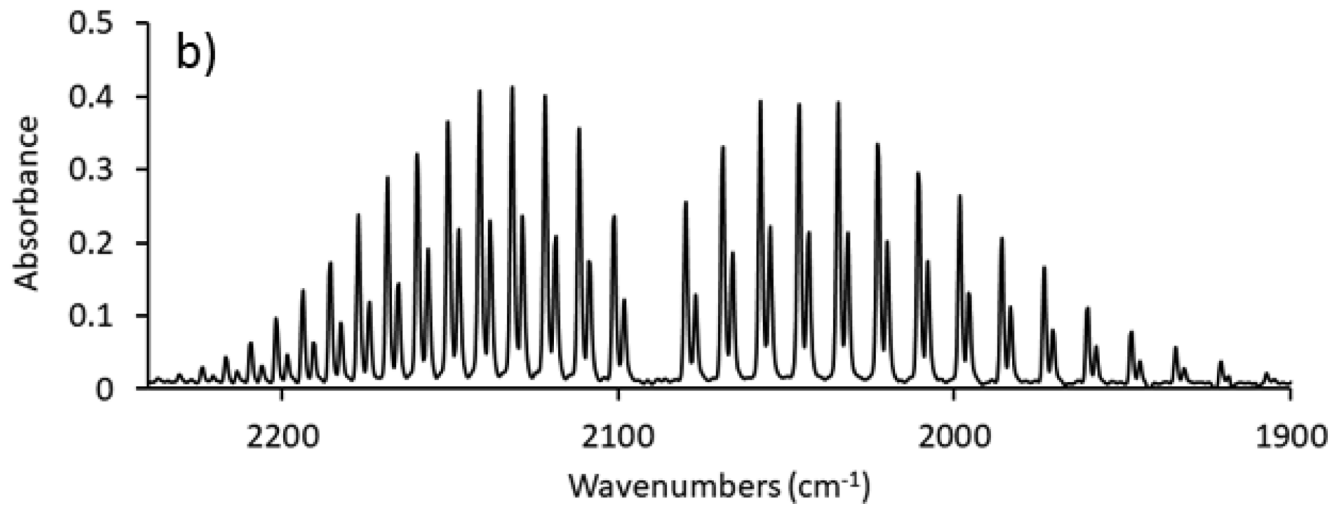
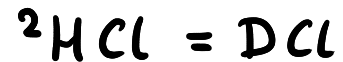






^1HCl





Die Rotations-Schwingungsbanden nach der Quantenmechanik.

Von Lucy Mensing in Göttingen.

(Eingegangen am 29. März 1926.)

Es wird das dem klassischen Modell des zweiatomigen Moleküls ohne Elektronenimpuls analoge Modell (rotierender anharmonischer Oszillator) nach der neuen Quantenmechanik durchgerechnet. Der reine Rotationsanteil der Energie wird proportional mit $j(j+1)$ ($j = 0, 1, 2 \dots$), womit der Ausfall der Nulllinie bei den Banden richtig herauskommt. — Die Übergangswahrscheinlichkeiten sind berechnet. Für die Intensitäten der einzelnen Bandenlinien ergeben sich die Formeln von Fowler.

Wir betrachten zweiatomige Moleküle. Wie bei klassischer Behandlung des Problems¹⁾ machen wir die Annahme, daß sich die beiden Atome als Kraftzentren auffassen lassen, die mit einer nur von der Entfernung abhängigen Kraft aufeinander wirken. — Ein Elektronenimpuls soll nicht vorhanden sein.

Die Hamiltonsche Funktion dieses Modells ist:

$$H = \frac{1}{2m_0} \{ p_x^2 + p_y^2 + p_z^2 \} + U(r),$$

wo

$$\frac{1}{m_0} = \frac{1}{m_1} + \frac{1}{m_2}$$

(m_1, m_2 Atommassen).

Die Matrix r ist definiert durch $r^2 = x^2 + y^2 + z^2$. $U(r)$ ist die potentielle Energie.

Wir fügen noch eine mit dem Parameter λ proportionale Störung hinzu (z. B. ein homogenes Magnetfeld), durch welche die Entartung aufgehoben wird; dabei soll die z -Achse eine Symmetrieachse für das System bleiben, so daß die zu z parallele Komponente M_z des Drehimpulses konstant ist. Wir beschäftigen uns jedoch zunächst nur mit dem Grenzfall $\lambda = 0$. Nach der Quantenmechanik²⁾ ist dann M_z sowohl als auch $M^2 = M_x^2 + M_y^2 + M_z^2$ eine Diagonalmatrix. Man kann den einzelnen Termen des nichtentarteten Systems ($\lambda \neq 0$) zwei Quantenzahlen m, j (magnetische und innere bzw. Rotations-Quantenzahl) zuordnen, derart, daß

$$M_z = \frac{h}{2\pi} m, \quad M^2 = \left(\frac{h}{2\pi}\right)^2 j(j+1).$$

¹⁾ Vgl. z. B. M. Born, Vorlesungen über Atommechanik. § 20.

²⁾ M. Born, W. Heisenberg, P. Jordan, ZS. f. Phys. **35**, 557, 1926.

Lucy Mensing

Lucy Mensing (also Lucie), later Mensing-Schütz or Schütz, (11 March 1901 - 28 April 1995) was a German physicist and a pioneer of [quantum mechanics](#).

Scientific career [[edit](#)]

Mensing studied mathematics, physics and chemistry at the [University of Hamburg](#). During her studies she specialized in theoretical physics. In 1923/24 she wrote a thesis in which she applied the older quantum hypothesis based on Bohr-Sommerfeld's theory, which assumes electron trajectories, to diatomic molecules. This work was published in the [Zeitschrift für Physik](#) in 1925.^[1] In 1925 she received her doctorate under [Wilhelm Lenz](#) with a thesis on the influence of electric fields on the width of spectral lines.^[2]

After her doctorate, she got the opportunity to come to [Göttingen](#) and take part in the development of [quantum mechanics](#), where she was advised by [Pascual Jordan](#). She studied the rotational spectrum of diatomic molecules using the methods of [matrix mechanics](#).^[3]

After [Wolfgang Pauli](#)'s treatment of the hydrogen atom, this was one of the first applications of the new quantum mechanics to physical systems.^[4] In the course of this work she was the first to find the permissible values for the quantum mechanical orbital angular momentum.^{[5][6]} The results were published in the [Zeitschrift für Physik](#) in 1926.^[7]

In Hamburg she worked together with [Wolfgang Pauli](#) on the calculation of the electrical polarizability of gases from diatomic molecules with the help of matrix mechanics. The result was also published in 1926 in the [Physikalische Zeitschrift](#).^[8] This work was another milestone in the application of quantum mechanics.^{[5][9]}

She then published in 1926 on the matrix mechanics applied to the partial Paschen-Back effect^[10] in continuation of the work of [Werner Heisenberg](#) and [Pascual Jordan](#).

In 1926, [Alfred Landé](#) offered her a position in [Tübingen](#), which she accepted. There she considered the scattering of slow electrons on atoms, about which she wrote a publication in 1927.^[11]

She published her last journal article in 1930 on the broadening of spectral lines.^[12]



OQC @OxfordQCCircuits · Nov 30, 2021
 OQC's latest system,

Lucy, an 8 QPU quantum computer,

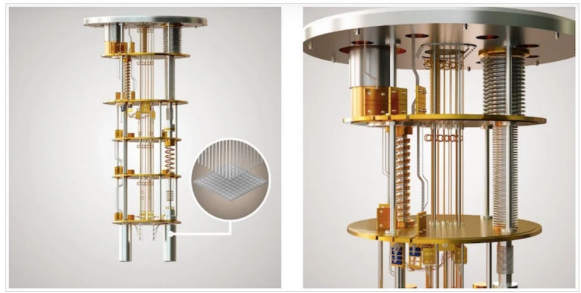
will debut on Amazon Braket and will be available to customers from February 2022 🇬🇧



1 5 17

Amazon Taps Into the "Lucy" Quantum Computer

Earlier this year, OQC made its 8-qubit Lucy quantum computer available via [Amazon Braket](#), a cloud-based quantum computing service that allows users to run both quantum and classical workloads. Lucy is named after Lucy Mensing, a pioneer in quantum mechanics and physics. OQC's Lucy machine is the [first quantum computer located in Europe](#) that is available on [Amazon Braket](#).



A rendering of OQC's 8-qubits processor Lucy. Image used courtesy of [Oxford Quantum Circuits](#)



OQC
 @OxfordQCCircuits

All our quantum computers are named after groundbreaking [#women](#) in STEM

Our upcoming Amazon Braket system honours Lucy Mensing: a German physicist and pioneer of quantum mechanics.

[en.wikipedia.org/wiki/Lucy_Mens...](https://en.wikipedia.org/wiki/Lucy_Mensing)



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