Q.M. in molecules and solids, the laser

| 9,10,11—Molecular and solid bonding, lasers | 9.5 and 9.6 only. All sections of both Chaps. 10 and 11, plus supplementary reading on molecular electronic wave functions and molecular orbitals (at website) | Probs. in Chap. 9: 21, 27, 28
Questions in Chap. 10: 2,6 (But do for H$_2$ and D$_2$)
Probs. in Chap. 10: 3,6,18,21 [Just make use of the result from Chap. 9 that the rms spread in emission frequency due to atomic motion relative to the observer will be given by:
\[ \Delta f = \frac{f_0}{c} \sqrt{\frac{kT}{m}} \].,
22, 25, 26, 32, 60(66)
S1: Show that the selection rule for vibrational transitions in a diatomic molecule is valid for excitations from the $v = 0$ state to the $v = 1$ and $v = 2$ states by directly calculating the relevant integrals. Use symmetry in dealing with the integrands to simplify your work. Questions in Chap. 11: 1, 9, 12, 14
Probs. in Chap. 11: 2, 12(14), 16, 31(33) |
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**9HE Quiz 2 Results**

- Mean: 69
- Median: 68
- Std. Dev.: 9

![Histogram showing Quiz 2 grades with mean 69, median 68, and standard deviation 9.](image-url)
The quantum mechanics of covalent bonding in molecules: \( \text{H}_2^+ \) with one electron

\[
\phi_+ = \phi_{\text{bonding}} \approx \phi_{1\text{sa}} + \phi_{1\text{sb}}
\]

\[
\phi_- = \phi_{\text{antibonding}} \approx \phi_{1\text{sa}} - \phi_{1\text{sb}}
\]

**FIGURE 10.2** The net potential energy curve, showing the equilibrium separation and binding energy.

**FIGURE 8.4** (a) Potential energy of an electron in the electric field of two nearby protons. The total energy of a ground-state electron in the hydrogen atom is indicated. (b) Two nearby protons correspond quantum-mechanically to a pair of boxes separated by a barrier.
Bonding in $H_2^+$: a linear combination of atomic orbitals (LCAO) or tight-binding (TB) picture

The bonding state
Bonding in $\text{H}_2^+$: a linear combination of atomic orbitals (LCAO) or tight-binding (TB) picture

The anti-bonding state
Bonding in $H_2^+$: a linear combination of atomic orbitals (LCAO) or tight-binding (TB) picture

The energies involved

$E(He^{+} 2p) = - \frac{(2)^2e^2}{8\pi\varepsilon_0 a_o(2)^2}$

$= -13.6 \text{ eV}$

$E(He^{+} 1s) = - \frac{(2)^2e^2}{8\pi\varepsilon_0 a_o(1)^2}$

$= -54.4 \text{ eV}$

$E(H1s) = - \frac{(1)^2e^2}{8\pi\varepsilon_0 a_o(1)^2} = -13.6 \text{ eV}$

Corrected

Figure 8.7: Electron, proton repulsion, and total energies in $H_2^+$ as a function of nuclear separation $R$ for the symmetric and antisymmetric states. The antisymmetric state has no minimum in its total energy.
13.3 THE HYDROGEN MOLECULE ION

An exactly soluble problem

We now begin the study of the electronic energies of molecules. We will use the Born–Oppenheimer approximation, keeping the nuclei fixed while we solve, as best we can, the Schrödinger equation for the motion of the electrons. We will usually be considering an isolated molecule, ignoring intermolecular interactions. Our results will be most applicable to molecules in the gas phase at low pressure.

We start with diatomic molecules, the simplest of which is $\text{H}_2^+$, the hydrogen molecule ion, consisting of two protons and one electron. ($\text{H}_2^+$ was discovered by J. J. Thomson in cathode rays.) Just as the one-electron hydrogen atom serves as a starting point in the discussion of many-electron atoms, the one-electron hydrogen molecular ion furnishes many ideas useful for discussing many-electron diatomic molecules. The electronic Schrödinger equation for $\text{H}_2^+$ is separable, and we can obtain exact solutions for the eigenfunctions and eigenvalues.

Figure 13.2 shows $\text{H}_2^+$. The nuclei are at $a$ and $b$; $R$ is the internuclear distance; $r_a$ and $r_b$ are the distances from the electron to nuclei $a$ and $b$. Since the nuclei are fixed, we have a one-particle problem whose Hamiltonian is [Eq. (13.5)]

\[
\psi = L(\xi)M(\eta)\Phi(\varphi) = L(\xi)M(\eta) \frac{1}{\sqrt{2\pi}} e^{i\sigma} \text{ where } m = 0 = \sigma, \pm 1 = \pi, \pm 2, \pm 3,...
\]

Make real in the usual way $L(\xi)$ and $M(\eta)$ are infinite series!
$2\sigma^*_u$

$2\sigma^*_g$

$1\sigma^*_u$

$1\sigma^*_g$

**H$_2^+$** -- The exact wavefunctions

* = anti-bonding  
No * = bonding  
g = even parity  
u = odd parity

Plus other images at:  
http://www.falstad.com/qmmo/
$\text{H}_2^+ -- \text{The exact wavefunctions}$

$3\sigma^*_u$

$1\pi^*_g$

$3\sigma_g$

$1\pi_u$

Fig. 6-2 (2), p. 217
The LCAO or tight-binding picture for $H_2$:

**III. MOLECULAR ORBITAL DRAWINGS**

1. Hydrogen

Symmetry: $D_{coh}$

**Bonding**

$$\psi_{bonding}^{MO} \approx \phi_{1sa} + \phi_{1sa}$$

$\varepsilon = -0.5944$ a.u. = -16.16 eV

(Compare – 13.61 for H atom 1s)

**Anti-Bonding**

$$\psi_{anti}^{MO} \approx \phi_{1sa} - \phi_{1sa}$$

$\varepsilon = 0.2656$ a.u. = +7.21 eV

$\varepsilon$ positive (unoccupied)

$\varepsilon$ negative (occupied)
Compare the approximate, but often-used linear combination of atomic orbitals picture

Filling these with 2 electrons in each (spin up and spin down) from bottom up to describe first-row homonuclear diatomics.

For example, $O_2$:

2 x 8 = 16 electrons

\[
[\sigma 1s]^2 \ [\sigma*1s]^2 \ [\sigma 2s]^2 \\
[\sigma*2s]^2[\sigma 2p_x]^2 \ [\pi 2p_y]^2 \\
[\pi 2p_z]^2 \ [\pi*2p_y]^1 \ [\pi*2p_z]^1
\]

Total spin = $\frac{1}{2} + \frac{1}{2} = 1$

Paramagnetic

1 electron in each of $2p_y$ and $2p_z$ to minimize e-e repulsion and with spins parallel again to minimize repulsion through the Fermi hole of antisymmetric wave fn.
The Hydrogenic Atom

Schroedinger Equation: Spherical Polar Coordinates

Classically:

\[ \mathbf{L} = \mathbf{r} \times \mathbf{p} \]

\[ V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r} \]

\[ \mu = \text{reduced mass} \]

\[ \mu = \frac{m_e}{1 + \frac{m_e}{M_n}} \]

Quantum mechanically:

\[ K = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \]

\[ \hbar^2 = \frac{\mu r^2}{2\mu r^2} \]

\[ \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = -\cos\theta \int_0^r r \times 2\pi = 4\pi \]

Polar angle = \( \theta = \arccos(z/r) \)

Azimuthal angle = \( \phi = \arctan(y/x) \)

Converting to new coordinates

Center of mass

\[ \psi \text{ H-ATOM SCHR. EQN. IS:} \]

\[ \hat{H}\psi(r,\theta,\phi) = \hat{K}\psi(r,\theta,\phi) - \frac{Ze^2}{4\pi\varepsilon_0 r} \psi = E\psi \]
The rotating diatomic molecule, with just a few simplifications:

Classically:

\[ \mathbf{r} \rightarrow \mathbf{R} \text{ (fixed)} \]

\[ \mathbf{L} = \mathbf{r} \times \mathbf{\dot{p}} \]

is conserved

\[ \mu = \text{reduced mass} \]

\[ \frac{\mu}{M_1} = \frac{1}{1 + \frac{M_1}{M_2}} \]

Quantum mechanically:

Polar angle = \( \theta = \text{arc cos}(z/r) \)

Azimuthal angle = \( \phi = \text{arc tan}(y/x) \)

\[ \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi = -\cos \theta \int_0^r r \times 2\pi = 4\pi \]

Converting to new coordinates

\[ \mu \hat{\mathbf{L}} = \frac{\mu}{2\mu r^2} \]
The Bohr Formula!

\[ \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \]

\( \Theta(\theta) \equiv f(\theta) & \Phi(\phi) \equiv g(\phi) \) in text

- **Use Separation of Variables:**

\[ \frac{d^2 \Phi}{d \phi^2} + \frac{1}{\sin \theta} \frac{d}{d \theta} \left( \sin \theta \frac{d \Theta}{d \theta} \right) + \left[ \frac{\lambda^2 - \frac{m^2}{\sin^2 \theta}}{\sin^2 \theta} \right] \Theta = 0 \]

- **Solving for \( \Theta \) with (2)**

\[ \Theta_m(\theta) = \text{assoc. Legendre polynomials} \]

\[ \Theta_m(\theta) \text{ in } (\cos \theta) - \text{real} \]

\[ L = 0, 1, 2, 3, \ldots \infty \]

\[ m = -L, -L+1, \ldots 0 \ldots + L-1, +2 \]

\( 2L+1 \)

- **Solving for \( R \) with (3)**

\[ R_{lm}(r) = \text{assoc. Laguerre functions} \]

\[ e^{-zr/\alpha} - \text{real} \]
Diatomic molecules have electronic as well as vibrational and rotational energies, wave functions, and selection rules.

\[ \Psi(\vec{r}_i, \vec{s}_i, i = 1..N; \vec{R}_1, \vec{R}_2) \approx \Psi_{\text{elec}}(\vec{r}_i, \vec{s}_i)\Psi_{\text{vib}}(\vec{R}_1, \vec{R}_2)\Psi_{\text{rot}}(\vec{R}_1, \vec{R}_2) \]

\[ E \approx E_{\text{elec}} + E_{\text{vib}} + E_{\text{rot}} \text{, another separation of variables!} \]

\[ \Psi_{\text{vib}}(x) = \Psi_n(x) = H_n(x)e^{-\alpha x^2/2} \]

\[ E_{\text{vib}} = (n + 1/2)\hbar \omega_{\text{vib}}, \quad n = 0, 1, 2, ... \]

\[ \omega_{\text{vib}} = \sqrt{\frac{K}{\mu}} \text{; Selection rule : } \Delta n = \pm 1 \]

The same basic functions as in atoms

\[ \Psi_{\text{rot}}(\theta, \phi) = Y_{JM_J}(\theta, \phi) = \Theta_{JM_J}(\theta) \frac{1}{\sqrt{2\pi}} e^{iM_J \phi} \]

\[ E_{\text{rot}} = \frac{\hbar^2 J(J + 1)}{2I}, \quad J = 0, 1, 2, ..., M_J = -J, -J + 1, ..., J - 1, J \]

\[ I = \mu R^2 \text{; Selection rule : } \Delta J = \pm 1 \]
The allowed transitions in absorption: diatomic molecule.

The rotational structure of the $v = 0 \rightarrow v = 1$ vibrational transitions in a diatomic molecule. There is no line at $v = v_0$ (the Q branch) because of the selection rule $\Delta J = \pm 1$. 

$$\Delta J = -1$$

$$\Delta J = +1$$
The resulting transitions in absorption for CO:

\[ \Delta J = -1 \quad P \text{ branch} \]

\[ \Delta J = +1 \quad R \text{ branch} \]

Microwave frequencies

\[ I_{\text{inc}} \rightarrow C-O(g) \rightarrow I_{\text{trans}} < I_{\text{inc}} \]

**FIGURE 8.17** The \( v = 0 \rightarrow v = 1 \) vibration-rotation absorption band in CO under high resolution. The lines are identified by the value of \( J \) in the initial rotational state.
THE ELECTROMAGNETIC SPECTRUM

Cellphones 0.8 to 1.9 x 10^9

(Well, blogs.nytimes.com/2011/02/22/cellphone-use-tied-to-changes-in-brain-activity/)

(Just a small change in temperature? No clinical significance?)
The Microwave Oven

Microwave ovens operate at about $2.45 \times 10^9$ Hz → 12 cm wavelength: watch water dance rotationally @ http://www.colorado.edu/physics/2000/applets/h2o.html

Water Molecule in a Microwave Field

Adjust the power of the microwave field to see how it affects the water molecule.
Zoom in and out with the zoom slider.

Click here to see this applet in a Physics 2000 context.
The randomized study, conducted in 2009, asked 47 participants to undergo positron emission tomography — or PET — scans, which measure brain glucose metabolism, a marker of brain activity.
The LCAO or tight-binding picture for CO:

Chemist's picture (no core): $\overset{x}{C} \overset{x}{\cdot} \cdot \cdot \overset{x}{O}$

1s $E = 20.00$ a.u. (1 a.u. = 27.2 eV)

1s $E = 10.88$

3σ $E = 6.8$

4σ $E = 8.038$

5σ $E = 14.5$

1πₓ

1πᵧ

3σ

4σ

5σ

Atoms A Orbitals i

\[ \varphi_j \text{MO}(\vec{r}) = \sum C_{A,j} \varphi_{AI} \text{AO}(\vec{r}) \]
+Vibrational (and rotational) excitations

\[ \text{CO} \quad \text{Carbon Monoxide} \]

UV PHOTOELECTRON SPECTRUM OF CO

\[ \text{C-O} \quad \text{e}^- \quad \text{C-O}^+ \]

Photoelectric effect

\[ \text{Bonding} 5\pi \text{ MO} \]

\[ \text{Bonding} 4\pi \text{ MO} \]

\[ \text{Non-Bonding} 4\sigma \text{ MO} \]

\[ \text{e}^- @ \text{infinity} \]
THE ELECTRONS IN HF (OR HCl): ionic molecules

HF: F 1s² 2σ² 3σ² 1πₓ² 1πᵧ²

Chemist’s picture (no core):

\[ \text{HF} \quad \text{F 1s core} \]

H : : F : :

1σ²

1 e⁻
9 e⁻

1σ E = -25.6 a.u.
Shakespeare sonnets encoded in DNA

Genetic code molecules could keep data safe for decades

The Associated Press  Posted: Jan 24, 2013 8:58 AM ET  |  Last Updated: Jan 28, 2013 1:03 PM ET  ▣ 03

It can store the information from a million CDs in a space no bigger than your little finger, and could keep it safe for centuries.

Is this some new electronic gadget? No. It's DNA.

The genetic material has long held all the information needed to make plants and animals, and now some scientists are saying it could help handle the growing storage needs of today's information society.

Researchers reported Wednesday that they had stored all 154 Shakespeare sonnets, a photo, a scientific paper, and a 26-second sound clip from Martin Luther King Jr.'s "I Have a Dream" speech. That all fit in a barely visible bit of DNA in a test tube.

The process involved converting the ones and zeroes of digital information into the four-letter alphabet of DNA code. That code was used to create strands of synthetic DNA. Then machines "read" the DNA molecules and recovered the encoded information.

That reading process took two weeks, but technological advances are driving that time down, said Ewan Birney of the European Bioinformatics Institute in Hinxton, England. He's an author of a report published online by the journal Nature.

The ones and zeroes of digital data were converted into sequences using the four-letter alphabet of DNA. The sequences were then encoded into synthetic strands of DNA.

The Associated Press

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Andrew Tack/Reuters

DNA For Data Banks

2013/01/26 - Pt. 1 10:52

Mobile  Facebook  Podcasts  Twitter  Alerts  Newsletter
Digital production, transmission and storage have revolutionized how we access and use information but have also made archiving an increasingly complex task that requires active, continuing maintenance of digital media. This challenge has focused some interest on DNA as an attractive target for information storage because of its capacity for high-density information encoding, longevity under easily achieved conditions and proven track record as an information bearer. Previous DNA-based information storage approaches have encoded only trivial amounts of information or were not amenable to scaling-up, and used no robust error-correction and lacked examination of their cost-efficiency for large-scale information archival. Here we describe a scalable method that can reliably store more information than has been handled before. We encoded computer files totalling 739 kilobytes of hard-disk storage and with an estimated Shannon information of 5.23106 bits into a DNA code, synthesized this DNA, sequenced it and reconstructed the original files with 100% accuracy. Theoretical analysis indicates that our DNA-based storage scheme could be scaled far beyond current global information volumes and offers a realistic technology for large-scale, long-term and infrequently accessed digital archiving. In fact, current trends in technological advances are reducing DNA synthesis costs at a pace that should make our scheme cost-effective for sub-50-year archiving within a decade.
### Background for the laser: some statistical physics and the blackbody (revisited)

#### THE THREE STATISTICAL DISTRIBUTION FUNCTIONS

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<td>Identical, distinguishable particles</td>
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<td>Category of particles</td>
<td>Classical</td>
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<tr>
<td>Properties of particles</td>
<td>Any spin, particles far enough apart so wave functions do not overlap</td>
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<tr>
<td>Examples</td>
<td>Molecules of a gas</td>
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Distribution function (number of particles in each state of energy $\epsilon$ at the temperature $T$): $F_{MB} = A \exp\left(-E / k_b T\right)$

Properties of distribution: No limit to number of particles per state

A, $B_1$, and $B_2$ from requiring No. particles = integral over $E$ of degeneracy $g(E)$ at $E$ times $F(E)$
Background for the laser: some statistical physics and the blackbody (revisited)

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<td>Distribution function</td>
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<td>(number of particles in each state of energy $E$ at the temperature $T$)</td>
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$A$, $B_1$, and $B_2$ from requiring No. particles = integral over $E$ of degeneracy $g(E)$ at $E$ times $F(E)$
Figure 9.8 A comparison of the three distribution functions, each drawn as a function of energy over the same range. The normalization constants $A$, $B_1$, and $B_2$ have been set equal to 1 for convenience. The Bose-Einstein distribution is higher than the Fermi-Dirac distribution, because bosons do not obey the Pauli principle. At high energies, the three distributions are close enough so that the classical Maxwell-Boltzmann distribution can be used to replace either quantum distribution.
Temperature dependence of the Fermi-Dirac distribution function, e.g. for electrons in a solid.

Occupied

Unoccupied

\[ E_F = \text{highest occupied level} \]

\[ k_B(T = 300\text{K}) = 1/40 \text{ eV} \]

Distribution function for fermions at three different temperatures. (a) At \( T = 0\), all the energy states up to the Fermi energy \( E_F\) are occupied. (b) At a low temperature, some fermions will leave states just below \( E_F\) and move into states just above \( E_F\). (c) At a higher temperature, fermions from any state below \( E_F\) may move into states above \( E_F\).
Standing electromagnetic waves in a blackbody cavity: all frequencies \( \nu \) (and wavelengths \( \lambda = c/\nu \)) allowed

\[
I(\lambda, T) = n(\lambda) \bar{E}(\lambda, T) \frac{c}{4} = u(\lambda, T) \frac{c}{4}
\]

Classical picture—Rayleigh-Jeans

Via Maxwell-Boltzmann factor integral

Via Maxwell-Boltzmann factor sum

Quantized picture—Planck

- Standing wave energies quantized
- Emission and absorption only in units of \( h\nu \)

\[ E_{\text{quant.}} = \frac{\hbar \nu}{e^{\hbar \nu/k_B T} - 1} \]

\( \lambda \rightarrow 0 \) as \( \hbar \nu \rightarrow \infty \)

Bose-Einstein statistics:

\[
I(\lambda, T) = \frac{2\pi c^2 h}{\lambda^5} \left[ \frac{1}{e^{hc/\lambda k_B T} - 1} \right]
\]

\( h = 6.62 \times 10^{-34} \text{ J-s} \)

By fit to data!

\( k_B = \text{the Boltzmann constant} = 1.3807 \times 10^{-23} \text{ J-K}^{-1} \)
3 MODES OF LIGHT INTERACTION WITH 2 LEVELS:

THE LASER:

\[ E_2 - E_1 = h \nu \]

\[ n(\lambda) = \text{photon density at a given frequency and temperature (as in black body problem)} = n(\lambda)E_{\text{aver}}(\lambda) \]

\[ A_{21}, B_{12}, B_{21} = \text{constants involving transition rates (to be determined from dipole rules)} \]

\[ N_1 \text{ and } N_1 \text{ are nos. of each state present} \]
\( N_1 \) and \( N_1 \) are nos. of each state present

\[ u(\lambda, T) = \text{photon density at a given frequency and temperature} \]

(as in black body problem) = \( n(\lambda)E_{\text{ave}}(\lambda) \)

\( A_{21}, B_{12}, B_{21} = \text{constants involving transition rates (to be determined from dipole rules)} \)
Therefore: Stimulated Emission must occur!!
The physics of laser action:

Thermal equilibrium: Boltzmann

\[ \frac{N_2}{N_1} = e^{(E_2 - E_1)/kT - \frac{hv}{kT}} = e \]

But no. up (absorption) = no. down (emission) at equilibrium, so

\[ B_{12} U(v, T) N_1 = [B_{21} U(v, T) + A_{21}] N_2 \]

\[ \Rightarrow U(v, T) = \frac{A_{21}}{B_{12} e^{\frac{hv}{kT}} - B_{21}} = \frac{B_{12} e^{\frac{hv}{kT}}}{B_{21}} - 1 \]

But Planck's blackbody law says:

\[ U(v, T) = \frac{8\pi hv^3}{c^3} \frac{1}{e^{\frac{hv}{kT}} - 1} \]

Which implies that (at equilibrium or non-equilibrium):

\[ B_{21} = B_{12} e^B : \text{stimulated just as strong as absorption} \]

Large and non-equilibrium = "population inversion"

\[ \Rightarrow \text{strong stimulated emission} = \text{Laser, maser} \]

Therefore: Stimulated Emission must occur!!
**THE He-Ne LASER**:

\[ \text{He}^+ 1s^12s^1 + \text{Ne} \rightarrow 2p^6 \rightarrow \text{He} 1s^2 + \text{Ne}^* \rightarrow 2p^55s^1 \]

Collision

20.61 eV

\[ 1s^12s^1 \rightarrow 20.66 \text{ eV} \]

\[ 18.70 \text{ eV} \]

FORBIDDEN

\[ 2s \rightarrow 1s \]

e⁻-He COLLISIONS IN MICROWAVE DISCHARGE \( \rightarrow \text{He}^* \)

ALLOWED \( 5s \rightarrow 3p \)

BUT WEAK

(ALSO LASES) IN IR

632.8 nm VISIBLE

20.66 eV

\[ 2p^55s^1 \]

\[ E_2 \]

\[ 2p^53p^1 \]

\[ E_1 \]

\[ 2p^53s^1 \]

\[ E_4' \]

\[ 2p^6 \]

\( E_0 = \text{GND. STATE} \)

\[ \text{He} \]

\[ 1s^2 \]

\[ \text{Ne} \]

\[ 2p^6 \]
High photon density $u(\nu, T)$ inside $\rightarrow$ Strong stimulated emission
Making a hologram

Partially reflecting mirror

Coherent light beam → Reference beam → Object beam → Object

Illumination beam → Photographic plate

Making a hologram

Seeing a holographic image

Lasers and Holography
Holography: e.g. Young’s double slit experiment

Loci of constructive maxima: \( m = 0,1,2,... \)

![Diagram of holography](image1)

**Figure 10-2** The two-dimensional interference pattern caused by two point sources of waves of constant frequency. Each set of waves is moving away from its source at the same constant speed. Nevertheless, the overall interference pattern remains constant in time. The two point sources creating this pattern can be seen near the center, along a horizontal direction, about four centimeters apart.

No. of wavelengths difference: \( = m \)

![Diagram of holography](image2)

**Figure 10-6** Light from \( S \) interferes with light from \( S' \) and produces a three-dimensional pattern inside a “thick” medium such as photographic emulsion (the “holoplate”).

**Figure 10-7** When the developed emulsion (hologram) is illuminated by \( S \) alone, the virtual image of \( S' \) is observed.
Figure 9.20 (a) Schematic diagram of a setup used in split-beam holography. The hologram is produced on the photographic plate by the interference of the primary beam (reflected from mirror $M$) with light scattered to the plate by the object. (b) The appearance of a typical hologram does not suggest the wealth of information it contains. (Ronald Erickson.) (c) Photographs of the same holographic image taken from two different angles demonstrate the three-dimension character of the reconstructed image (Bell Telephone Laboratories.).

- TAKE OBJECT AWAY
- LOOK THROUGH HOLOGRAM: IT'S STILL THERE!
Bonding in solids/solid-state devices as an extension of that in molecules

Diatomic—E.g. $[\text{Li}\ 1s^22s]_2$ – 6 electrons

Multi-atom solid—E.g. $[\text{Li}\ 1s^22s]_N$ N atoms -> 3N electrons

Unpaired! Magnetism?

"Band" of states

Example: $N = 11$: 22 e\textsuperscript{-} in 1s-derived
11 e\textsuperscript{-} in 2s-derived
ELECTRONS IN SOLIDS:

+ Successive Approximations:

Forget the surfaces

Treat as free-particle in a box

Fig. 5.1 The evolution of the energy spectrum of $\text{O}_2$ from an atom (a), to a molecule (b), to a solid (c).
ELECTRONS IN SOLIDS:

+ Successive Approximations:

Forget the surfaces

Treat as free-particle in a box

Fig. 5.1 The evolution of the energy spectrum of $\lambda$ from an atom (a), to a molecule (b), to a solid (c).

Fig. 5.3 The crystal potential seen by the electron.

$E_{\text{kin}}(\vec{r})$ - faster @ cores
$\Psi_{\text{valence}}$, $\Psi_{\text{core orthogonality}}$

$\approx$ free $e^-$ in a box

N very large!
The free-electron solid at absolute zero

\[ E(\bar{k}) = \frac{\hbar^2 k^2}{2m_e} = 3.81(k(\text{in } \text{Å}^{-1}))^2 \text{ (in eV)} \]

\[ @ T = 0 \]

\[ F(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \]

\[ F(E, T) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \]
The free-electron solid at absolute zero

\[ E(\tilde{k}) = \frac{\hbar^2 k^2}{2m_e} = 3.81(k\text{ (in Å}^{-1})\text{)}^2 \text{ (in eV)} \]

\[ \rho = \frac{\text{number of e}^-/\text{unit volume}}{\text{Valence electrons}} \]

\[ \rho(E) = \frac{\hbar^2}{2m_e} (3\pi^2 n)^{2/3} = \frac{\hbar^2 k_F^2}{2m_e} \]

\[ \rho(E) = \int g(E) F(E) \text{d}E \]

\[ k_F = (3\pi^2 n)^{1/3} \]

\[ u_F = p_F/m_e = \hbar k_F/m_e = \hbar(3\pi^2 n)^{1/3}/m_e \]

In Energy Space

In k- or “Reciprocal” Space
Two nearly-free electron metals

Fermi velocities about 0.01c, pretty fast

<table>
<thead>
<tr>
<th>Element</th>
<th>$E_F$ (eV)</th>
<th>$T_F$ ($\times 10^4$ K)</th>
<th>$u_F$ ($\times 10^6$ m/s)</th>
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<tbody>
<tr>
<td>Li</td>
<td>4.74</td>
<td>5.51</td>
<td>1.29</td>
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<tr>
<td>Na</td>
<td>3.24</td>
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<td>K</td>
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<td>8.16</td>
<td>1.57</td>
</tr>
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<td>Ag</td>
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<td>Nb</td>
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<td>12.7</td>
<td>1.96</td>
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<tr>
<td>Zn</td>
<td>9.47</td>
<td>11.0</td>
<td>1.83</td>
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<tr>
<td>Ca</td>
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<td>1.92</td>
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<tr>
<td>In</td>
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<td>10.0</td>
<td>1.74</td>
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<tr>
<td>Tl</td>
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<td>9.46</td>
<td>1.69</td>
</tr>
<tr>
<td>Sn</td>
<td>10.2</td>
<td>11.8</td>
<td>1.90</td>
</tr>
<tr>
<td>Pb</td>
<td>9.47</td>
<td>11.0</td>
<td>1.83</td>
</tr>
<tr>
<td>Bi</td>
<td>9.90</td>
<td>11.5</td>
<td>1.87</td>
</tr>
<tr>
<td>Sb</td>
<td>10.9</td>
<td>12.7</td>
<td>1.96</td>
</tr>
</tbody>
</table>

Electronic bands and density of states for “free-electron” metals-
Rydberg = 13.605 eV

Lithium—bcc, \(a = 3.49 \, \text{Å}\)

\(1s^22s^1\)

\[
E(k_x) \approx \frac{\hbar^2 (k_x)^2}{2m}
\]

\(= 1.8 \, \text{Å}^{-1}\)
Electronic bands and density of states for “free-electron” metals—
Rydberg = 13.605 eV

**Aluminum**—fcc, \(a = 4.05 \text{ Å}\)

\(1s^22s^22p^63s^23p^1\)

Lithium—bcc, \(a = 3.49 \text{ Å}\)

\(1s^22s^1\)
Different directions in k-space: fcc crystal

$k = 0 \equiv \Gamma$
Comparing Li and Al on the same energy and k scales: pretty close
ELECTRONS IN SOLIDS:

+ Successive Approximations:

Forget the surfaces

In between: The Kronig-Penney Model

Treat as free-particle in a box

Fig. 5.1 The evolution of the energy spectrum of $La$ from an atom (a), to a molecule (b), to a solid (c).

Fig. 5.3 The crystal potential seen by the electron.
The Kronig-Penney Model: particle moving in periodic boxes with tunneling between

Periodic over \( L = NA = N(a+b), N \) very large

\[
\Psi_1 = [A e^{ikx} + Be^{-ikx}] e^{ikx}
\]

\[
\Psi_2(x) = [Ce^{kx} + Be^{-kx}] e^{ikx}
\]

Requiring continuity of \( \psi \) and its Derivative at 0 and \( a \) finally yields for a very narrow barrier (\( \kappa b << 1 \)):

\[
\frac{\kappa^2 b}{2k} \sin(ka) + \cos(ka) = \cos(Ka)
\]

\[|\Psi(x)|^2 = |\Psi(x + MA)|^2, M = 1, 2, ... N, N \text{ very large}\]

\[\Psi(x) = \Psi(x + MA) e^{i\alpha x}, \text{ with } e^{i\alpha x} \text{ an arbitrary phase factor}\]

Also, for continuity around ring:

\[\Psi(x) = \Psi(x + NA)\]

\[\Psi(x) = \Psi(x + NA) e^{i\alpha NA} \rightarrow \alpha NA = P2\pi, P = 0, \pm 1, \pm 2, \pm 3...\]

\[\alpha = \frac{2\pi P}{A} \equiv K_{PN}, \text{ with many allowed values: } \frac{2\pi}{A} \times \frac{\pm 1}{N}, \frac{\pm 2}{N}, ..., \frac{\pm P}{N}, ..., \frac{\pm N}{N}\]

\[\rightarrow \text{quasi-continuous}\]

Finally, for all states in solids:

\[\Psi_k(x) = u_k(x) e^{ikx}, \text{ where } u_k(x) = u(x + A) \rightarrow \text{a Bloch function}\]
Electrons in crystalline solids—are everywhere

For all states in crystalline (ordered) solids:

$$\psi_k(\vec{r}) = u_k(\vec{r})e^{iK \cdot \vec{r}}, \text{ where } u_k(\vec{r}) = u(\vec{r} + \vec{A})$$, this is a "Bloch function"

with probability density of

$$\psi_k^*(\vec{r})\psi_k(\vec{r}) = u_k(\vec{r})e^{-iK \cdot \vec{r}}u_k(\vec{r})e^{iK \cdot \vec{r}} = u_k(\vec{r})^2$$, the same on every atom!

A typical Bloch function:

Re or Im part of $e^{iK \cdot \vec{r}}$: $\cos Kr$ or $\sin Kr$

And its probability density:
The Kronig–Penney Model

The Kronig–Penney model is a simple, idealized quantum-mechanical system that consists of an infinite periodic potential that can lead to the formation of electronic energy bands and band gaps. This is shown in this Demonstration.
Electronic bands and density of states for a semiconductor—Germanium—

$$1s^22s^2\ 2p^63s^2\ 3p^63d^{10}4s^24p^2$$

Bonding (filled at $T = 0$)

Anti-Bonding (empty at $T = 0$)
### Properties of Semiconductors

<table>
<thead>
<tr>
<th>Compound</th>
<th>Structure</th>
<th>Bandgap (eV)</th>
<th>$e^-$ mobility (cm²/V-s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>Diamond</td>
<td>1.11 (I)</td>
<td>1,350</td>
</tr>
<tr>
<td>Ge</td>
<td>Diamond</td>
<td>0.67 (I)</td>
<td>3,900</td>
</tr>
<tr>
<td>AIP</td>
<td>Sphalerite</td>
<td>2.43 (I)</td>
<td>80</td>
</tr>
<tr>
<td>GaAs</td>
<td>Sphalerite</td>
<td>1.43 (D)</td>
<td>8,500</td>
</tr>
<tr>
<td>InSb</td>
<td>Sphalerite</td>
<td>0.18 (D)</td>
<td>100,000</td>
</tr>
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<tr>
<td>GaN</td>
<td>Wurtzite</td>
<td>3.4 (D)</td>
<td>300</td>
</tr>
</tbody>
</table>

Typical metals: bcc, fcc (Al, Cu)

$e^-$ drift velocity = ($e^-$ mobility) x (applied field)
Electronic bands and density of states for a transition metal-Copper

Fig. 7.12. Bandstructure $E(k)$ for copper along directions of high crystal symmetry (right). The experimental data were measured by various authors and were presented collectively by Courths and Hufner [7.4]. The full lines showing the calculated energy bands and the density of states (left) are from [7.5]. The experimental data agree very well, not only among themselves, but also with the calculation
Figure 11.6 Possible band structures: (a) a conductor with an unfilled valence band, (b) a conductor with overlapping valence and conduction bands (a semimetal), (c) an insulator due to its large band gap, and (d) a semiconductor (due to its small band gap).

(e)
Spin-down  Spin-up
Ferromagnetic
Conductor
(The exchange interaction)
The electronic bands and densities of states of ferromagnetic iron

\[ \mu_S = 2.2 \text{ Bohr magnetons} \]  
(Atomic iron: 2.0 Bohr magnetons)

\[ 4 \times \frac{1}{2} = 2 \]
Response of a ferromagnet to field and temperature

Net magnetization versus temperature for a ferromagnet. $T_C = \text{Curie Temp.}$
Nobel gas configuration ions, with long-range point-charge Coulomb attraction or repulsion, plus short-range nearest-neighbor repulsion:

\[ V = V_{Coul} + V_{Rep} = \sum_{i=1}^{\infty} \frac{(+ or -)n_i q_i e^2}{4\pi \varepsilon_0 r_i} + \lambda e^{-\frac{r_i}{\rho}} \]
Ionic solids—another limit: e.g. NaCl

Cl$^{-}$ $1s^2 2s^2 2p^6 3s^2 3p^6$

Na$^+$ $1s^2 2s^2 2p^6$

Nobel gas configuration ions, with long-range point-charge Coulomb attraction or repulsion, plus short-range nearest-neighbor repulsion:

$$V = V_{\text{coul}} + V_{\text{rep}} = \sum_{i=1}^{\infty} \frac{(+ \text{ or } -) n_i q_i e^2}{4\pi\varepsilon_0 r_i} + \lambda e^{-\frac{r_i}{\rho}}$$

as e.g., for NaCl: $\lambda = 1.05 \times 10^{-8}$ erg, $\rho = 0.321$ Angstroms

$$V = \frac{e^2}{4\pi\varepsilon_0} \left[ -\frac{6}{a^2} + \frac{12}{\sqrt{2}a^2} - \frac{8}{\sqrt{3}a^2} + \cdots \right] + 1.05e^{-\frac{r_i}{\rho}}$$

$$= \frac{e^2}{2\pi\varepsilon_0 a} \left[ -6 + \frac{12}{\sqrt{2}} - \frac{8}{\sqrt{3}} + \cdots \right] + 1.05e^{-\frac{(a/2)(\text{Ang.})}{0.321}}$$

$$= \alpha = \text{Madelung constant}$$
Ionic solids—another limit: e.g. NaCl

The band structure

Flat bands $\rightarrow$ Highly localized, immobile electrons

Na$^+$ $\ldots$ 2s$^2$2p$^6$ at even lower energies

Cl$^-$ $\ldots$ 3s$^2$3p$^6$
Figure 11.6 Possible band structures: (a) a conductor with an unfilled valence band, (b) a conductor with overlapping valence and conduction bands (a semimetal), (c) an insulator due to its large band gap, and (d) a semiconductor (due to its small band gap).

(e) Spin-down Spin-up
Ferromagnetic Conductor
(The exchange interaction)

(f) Ionic solid:
Very narrow atomic/ionic filled bands
Superconductivity

High-T\textsubscript{C} Superconductors

Normal "BCS" Superconductors

"High T\textsubscript{C}":

YBa\textsubscript{2}CuO\textsubscript{7-δ} = “YBCO”
Superconductivity is a widely occurring phenomenon—at low $T_s$, + high $P_s$. 

![Periodic Table of Superconducting Elements](image)
**Theory of superconductivity—the BCS model of Cooper pairs**

![Diagram](image)

**Figure 12.20** The basis for the attractive interaction between two electrons via the lattice deformation. Electron 1 attracts the positive ions, which move inward from their equilibrium positions (dashed circles). This distorted region of the lattice has a net positive charge, and hence electron 2 is attracted to it.

**Figure 12.21** A schematic diagram of a Cooper pair. The electron moving to the right has a momentum \( \mathbf{p} \) and its spin is up, while the electron moving to the left has a momentum \( -\mathbf{p} \) and its spin is down. Hence the total momentum of the system is zero and the total spin is zero.
Graphene - A very special 2D case

The Nobel Prize in Physics 2010
Andre Geim, Konstantin Novoselov
"for groundbreaking experiments regarding the two-dimensional material graphene"

Photoelectron spectroscopy

### Properties of Semiconductors

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<tr>
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<td>Wurtzite</td>
<td>3.4 (D)</td>
<td>300</td>
</tr>
</tbody>
</table>

**Typical metals**
- bcc, fcc (Al, Cu)
- Graphene: 2D hexagonal

\[
e^{-} \text{ drift velocity} = (e^{-} \text{ mobility}) \times \text{(applied field)}
\]
Figure 11.6 Possible band structures: (a) a conductor with an unfilled valence band, (b) a conductor with overlapping valence and conduction bands (a semimetal), (c) an insulator due to its large band gap, and (d) a semiconductor (due to its small band gap).

(e) Spin-down  Spin-up
Ferromagnetic Conductor
(The exchange interaction)

(f) Ionic solid:
Very narrow atomic/ionic filled bands

+Doping to create + or – charge carriers
Doping of semiconductors to create - or + charge carriers

**n doping:**
- electron carriers

E.g. -
\[ \begin{align*}
  Si & \; 1s^2 \; 2s^2 \; 2p^6 \; 3s^2 \; 3p^2 \\
  P & \; 1s^2 \; 2s^2 \; 2p^6 \; 3s^2 \; 3p^3
\end{align*} \]
(an extra e⁻)

A donor

For ref.: \( kT \) at 300K is \( 1/40 \text{ eV} = 0.025 \text{ eV} \)
Temperature dependence of the Fermi-Dirac distribution function, e.g. for electrons in a solid.

Distribution function for fermions at three different temperatures. (a) At $T = 0$, all the energy states up to the Fermi energy $E_F$ are occupied. (b) At a low temperature, some fermions will leave states just below $E_F$ and move into states just above $E_F$. (c) At a higher temperature, fermions from any state below $E_F$ may move into states above $E_F$.

$k_B(T = 300K) = 1/40$ eV
Doping of semiconductors to create - or + charge carriers

n doping:
- electron carriers

E.g. -
Si\(1s^2\) \(2s^2\) \(2p^6\) \(3s^2\) \(3p^3\)
(\text{an extra } e^-)
A donor

p doping:
+ hole carriers

E.g. -
Si\(1s^2\) \(2s^2\) \(2p^6\) \(3s^2\) \(3p^2\)
B \(1s^2\) \(2s^2\) \(2p^1\)
Al\(1s^2\) \(2s^2\) \(2p^6\) \(3s^2\) \(3p^1\)
(a missing \(e^-\))
An acceptor

For ref.: \(kT\) at 300K is \(1/40\) eV = 0.025 eV

From Harris “Non-Classical Physics”

http://www.youtube.com/watch?v=vJZL1ILco44
The p-n junction diode, and other applications derived from it:

The light-emitting diode \(\rightarrow\) laser

Fermi levels equal at equilibrium!
THE CLASSIC He-Ne LASER:

Bragg-reflection mirrors made of synthetic multilayer materials:

\[ n\lambda = 2d\sin \Theta \]

\[ \text{In back reflection: } \Theta = 90^\circ, \sin \Theta = 1, n = 1, d = \lambda/2 \]

THE LED LASER:

High photon density \( u(\nu, T) \) inside \( \rightarrow \) Strong stimulated emission

The light-emitting diode \( \rightarrow \) laser

The light-emitting diode

The light-emitting diode \( \rightarrow \) laser
Diamond is an electrical insulator well known for its exceptional hardness. It also conducts heat even more effectively than copper, and can withstand very high electric fields. With these physical properties, diamond is attractive for electronic applications, particularly when charge carriers are introduced (by chemical doping) into the system. Boron has one less electron than carbon and, because of its small atomic radius, boron is relatively easily incorporated into diamond; as boron acts as a charge acceptor, the resulting diamond is effectively hole-doped. Here we report the discovery of superconductivity in boron-doped diamond synthesized at high pressure (nearly 100,000 atmospheres) and temperature (2,500–2,800 K). Electrical resistivity, magnetic susceptibility, specific heat and field-dependent resistance measurements show that boron-doped diamond is a bulk, type-II superconductor below the superconducting transition temperature $T_c \approx 4$ K. Superconductivity survives in a magnetic field up to $B_c(0) \approx 3.5$ T. The discovery of superconductivity in diamond-structured carbon suggests that Si and Ge, which also form the diamond structure, may similarly exhibit superconductivity under the appropriate conditions.

OTHER EFFECTS OF DOPING IN INSULATORS AND SEMICONDUCTORS:
SUPERCONDUCTIVITY AT ATMOSPHERIC PRESSURE

Silicon becomes a superconductor

Nov 22, 2006

Silicon -- the archetypal semiconductor -- has at long last been shown to demonstrate superconductivity. By substituting 9% of the silicon atoms with boron atoms, physicists in France have found that the resistance of the material drops sharply when cooled below 0.35 K (Nature 444 465).

Boron is widely added to silicon to make it a useful semiconductor, but rarely does it account for more than 0.002% of the total number of atoms. Because it has one fewer electron than silicon available for bonding with neighbouring atoms, boron incorporated into silicon leaves a positively charged "hole" at each site where boron's "missing" electron would be paired with one of silicon's. At room temperature these holes can move around, making boron-doped silicon a "p-type" semiconductor, but at low temperatures, the holes remain bound in orbitals to the boron nuclei. It has long been known that at boron concentrations of around 0.01% these low-temperature orbitals overlap, making metal-like conductivity possible. However, until now all attempts to make silicon superconducting have failed.

Busterret Etienne at the Centre National de la Recherche Scientifique in Grenoble and colleagues have now tried doping to even higher concentrations in a bid to witness the effect. Because silicon is normally reluctant to allow impurities into its structure, they had to employ a vigorous method called "gas immersion laser doping" that repeatedly melts and cools a thin silicon film using a pulsed laser. During each molten stage, atoms from boron gas diffuse into the film and remain there while it solidifies, ultimately replacing up to 9% of the silicon atoms. The researchers found that below a temperature of 0.35 K, this highly-doped silicon becomes superconducting.
Figure 1. Typical photolithographic processing steps necessary to pattern SiO$_2$ layer on a Si substrate. Key: A, thermal oxidation; B, photoresist deposition; C, resist exposure through photomask; and D, develop photoresist.
The IT workhorse: the metal-oxide-semiconductor field-effect transistor (MOSFET)

Electric field from gate pushes away p-type ‘holes’ and attracts/allows electrons from n-type inserts into channel.
The IT workhorse: the metal-oxide-semiconductor field-effect transistor (MOSFET)

Source (Emitter)  Drain (Collector)  Gate (Base)

Graph showing current (mA) vs. voltage (V) for different gate voltages ($V_G = 2$, $V_G = 3$, $V_G = 4$, $V_G = 5$ V). The graph illustrates the switching between "ZERO" and "ONE" states with varying gate voltages.
Some Basic Logic Circuits from Transistor: From Physics to the IT World

AND Gate

OR Gate

NAND Gate

NOR Gate

Complementary Metal-Oxide-Semiconductor (CMOS) logic mates each n-type gate with a p-type gate so the current flow is zero (sort of), cutting power consumption.

http://hyperphysics.phy-astr.gsu.edu/hbase/electronic/trangate.html
And the Shrink Goes On...

0.032 microns = 32 nm = 320 Å ('08) → 0.025 microns = 250 Å → 0.022 microns (2012)

~few atomic layers—currently 15 Å SiO₂

Some serious challenges

Cross section of a MOS transistor. Electron tunneling through the gate oxide (left inset) and high-concentration dopant interactions (right inset) are posing fundamental limitations to continuing historical transistor scaling trends.

High-k + Metal Gate Transistors

- Increases the gate field effect
- Allows use of thicker dielectric layer to reduce gate leakage
- Drive current increased >20% (>20% higher performance)
- Or source-drain leakage reduced >5x
- Gate oxide leakage reduced >10x

IBM Science 2001

- 10 µm – 1971
- 3 µm – 1975
- 1.5 µm – 1982
- 1 µm – 1985
- 800 nm – 1989
- 600 nm – 1994
- 350 nm – 1995
- 250 nm – 1997
- 180 nm – 1999
- 130 nm – 2002
- 90 nm – 2004
- 65 nm – 2006
- 45 nm – 2008
- 32 nm – 2010
- 22 nm – 2012
- 14 nm – 2014
- 10 nm – est. 2015
- 7 nm – est. 2017
- 5 nm – est. 2019
1959 — Richard P. Feynman
“There’s plenty of room at the bottom”

“We cannot write the entire 24 volumes of the Encyclopedia Brittanica on the head of a pin?”

It would be possible if you could print it with dots (= bits) that are 8 nanometers or about 32 metal atoms across, containing about 1000 atoms

+ Many visionary ideas:
  Miniaturization of computers
  Imaging and manipulation of single atoms or molecules
  http://www.zyvex.com/nanotech/feynman.html
1989—IBM, written with single xenon atoms, using a scanning tunneling microscope, but too slow for real data storage—so far
Current SiO₂ gate oxide thicknesses in the 1 nm range with high-k dielectrics, SiₜHfₓNᵧOₜ,… a few nm or more

Mixed oxides: Si⁺¹, Si⁺², Si⁺³, and coord. sites

Fig. 2 High resolution TEM cross section of 1.2nm physical SiO₂ gate oxide at the 90nm logic technology node. → 65 nm technology → 45 nm → 32 nm → 22 nm → 14 nm
"Moore's Law" for magnetic storage

Now 170 Gbits/in² = 20 Gbytes/in²

→ each bit ~14 nm x 30 nm x 210 nm
≈ 4,000,000 atoms

Read 1 billion times per second (GHz)

More challenges to maintain this
Too few atoms lead to unstable magnetism
Magnetic Random Access Memory (MRAM - Non Volatile)

Some new directions with magnetic nanolayer structures--”spintronics”

Magnetic Random Access Memory (MRAM-Non Volatile)

Now in every hard drive

Crucial surfaces and buried interfaces everywhere

Up to 100 Mbit devices in R&D/future cell phone use
Nobel Prizes in Physics and Chemistry—2007-2010

Directly related to nanoscience/surface science

2010-Graphene, a 2D material

The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov “for groundbreaking experiments regarding the two-dimensional material graphene.”

2007-Nanoscale magnetism and surface physics

From Spinwaves to Giant Magnetoresistance (GMR) and Beyond

Peter Grünberg held his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University. He was introduced by Professor Per Carlson, Chairman of the Nobel Committee for Physics.

The Origin, the Development and the Future of Spintronics

Albert Fert delivered his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University. He was introduced by Professor Per Carlson, Chairman of the Nobel Committee for Physics.

Reactions at Solid Surfaces: From Atoms to Complexity

Gerhard Ertl delivered his Nobel Lecture on 8 December 2007, at Aula Magna, Stockholm University, where he was introduced by Professor Gunnar von Heijne, Chairman of the Nobel Committee for Chemistry.

2000-The Integrated Circuit

The Nobel Prize in Physics 2000 was awarded “for basic work on information and communication technology” with one half jointly to Zhores I. Alferov and Herbert Kroemer “for developing semiconductor heterostructures used in high-speed and opto-electronics” and the other half to Jack S. Kilby “for his part in the invention of the integrated circuit.”
By JOHN MARKOFF
Australian and American physicists have built a working transistor from a single phosphorus atom embedded in a silicon crystal. The group of physicists, based at the University of New South Wales and Purdue University, said they had laid the groundwork for a futuristic quantum computer that might one day function in a nanoscale world and be orders of magnitude smaller and quicker than today’s silicon-based machines.

In contrast to conventional computers that are based on transistors with distinct "on" and "off" states, quantum computers are built from devices called qubits that exploit the quirky properties of quantum mechanics. Unlike a transistor, a qubit can represent a multiplicity of values simultaneously.

That might make it possible to factor large numbers more quickly than with conventional machines, thereby undermining modern data-scrambling systems that are the basis of electronic commerce and data privacy. Quantum computers might also make it possible to simulate molecular structures with great speed, an advance that holds promise for designing new drugs and other materials.

"Their approach is extremely powerful," said Andreas Heinrich, a physicist at IBM. "This is at least a 10-year effort to make very tiny electrical wires and combine them with the placement of a phosphorus atom exactly where they want them."

Dr. Heinrich said the research was a significant step toward making a functioning quantum computing system. However, whether quantum computing will ever be harnessed for useful tasks remains uncertain, and the researchers noted that their work demonstrated the fundamental limits to which today’s computers would be able to shrink.

"It shows that Moore’s Law can be scaled toward atomic scales in silicon," said Gerhard Klimeck, a professor of electrical and computer engineering at Purdue and leader of the project.

Figure 1 | Single-atom transistor based on deterministic positioning of a phosphorus atom in epitaxial silicon. a. Perspective STM image of the device, in which the hydrogen-desorbed regions defining source (S) and drain (D) leads and two gates (G1, G2) appear raised due to the increased tunneling current through the silicon dangling bond states that were created. Upon subsequent dosing with phosphine, these regions form highly phosphorus-doped co-planar transport electrodes of monatomic height, which are registered to a single phosphorus atom in the centre of the device. Several atomic steps running across the Si(100) surface are also visible. b. Close-up of the inner device area (dashed box in a), where the central bright protrusion is the silicon atom, which is ejected when a single phosphorus atom incorporates into the surface. c. Schematic of the chemical reaction to deterministically incorporate a single phosphorus atom into the surface. Saturation dosing of a three-dimer patch (I) at room temperature (RT) followed by annealing to 350°C allows successive dissociation of PH₃ (II-IV) and subsequent incorporation of a single phosphorus atom in the surface layer, ejecting a silicon adatom in the process (V).