

Chapter 1

ELECTRONS, BONDS, BANDS, AND HOLES

OBJECTIVES

- * Understand two fundamental electrical concepts**
 - Electrons
 - Holes

- * Understand two semiconductor materials models**
 - Bond Model (or Valence Bond Model)
 - Band Model (or Energy Band Model)

2 **FUNDAMENTALS OF SOLID-STATE ELECTRONICS – SOLUTION MANUAL**
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P100.1 Describe the two main physical causes that make classical Newtonian and classical statistical mechanics inadequate to describe the motion of electrons and atoms in a solid. What hypotheses, laws, principles, models, or methodologies are introduced in quantum mechanics and quantum statistical mechanics to overcome these limitations?

The explanations are given on pages 2-3 and 31-35 of FSSE. This question should be asked again and its answers thought through again at the end of chapter 3 when the students have learned the details of the fundamental physics concepts underlying the answers to this question. The detailed answers given below explain the fundamental reasons which the instructor can repeat in a class room discussion and the students can use as a review focus. The keyword-answers can be succinctly given in a few sentences which are underlined and could be adequate to receive full credit for the problem, provided the student understands the physics underlying the keywords as explained in the FSSE and summarized below. This presentation format (underlining) of the solutions is followed for some of the discussion and essay problems in this Solution Manual.

The two main physical causes are the large particle number (about 10^{23} particles in one cubic centimeter) and small interparticle distance (about one angstrom or 10^{-8} cm) in a solid. These combined, translate to high particle density which is a consequence rather than a cause.

The small interparticle distance means the force between two particles must be taken into account because for the charged particles (electrons and ionized atomic nuclei in a solid) the interparticle force is the long-range, $1/r$ dependent Coulomb force whose range is large compared with the interparticle spacing. (Actually, the Coulomb force has an 'infinite' range so the Coulombic interparticle force must be taken into account to analyze the particle motion of a many-particle system at all interparticle spacings, but the smaller spacings make the force more important. The particles cannot be treated as hard sphere with an infinite or large repulsive interparticle force at their radii and zero force when separated.)

The long-range interparticle force means that one must simultaneously solve the many Newton's equations of force and mass (10^{23} equations in one cm^3 of solid), one equation from each particle, which are coupled by the interparticle force. This coupling through the interparticle force that affects the trajectory of each particle is known as **scattering**. The small interparticle distance and the large number of particles mean that each particle experiences very many scattering events or deflections of their trajectories in an experimenter's observation time, about 10^{14} per second. It is obviously impossible

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to solve such a system of 10^{23} equations using any known computation equipment and methods. On the contrary, the motion (position and velocity at any given time) of celestial bodies are indeed obtained by solving simultaneously the Newton's equations, one for each body, which are coupled through the interbody gravitation force, but the solutions are readily obtained only for a partitioned or local celestial system that contains a few interacting bodies. For examples, earth, moon and sun is a three-body system; meteor composed of many small bodies clustered together is treated as one body when solving for its orbit around the sun; and similarly, the many electrons and atoms composing the earth (or sun or moon) are lumped together in one earth body in the three-body earth-moon-sun system.

A more practical reason in solid, unlike the celestial bodies, is that we cannot experimentally measure the motion (position and velocity) of each of the 10^{23} particles (electrons and atoms or nuclei) in a solid even with the sharpest electron or optical microscope to 'see' them or the most sensitive charge detection meter to 'feel' them, for two reasons: (i) electron or photon which is scattered off the particle during the process of 'seeing' the particle will have altered the position and velocity of the particle during the scattering, and (ii) the electrical properties of the solid we can measure with a meter or an oscilloscope are averaged properties over many particles and the motion of one particle among the 10^{23} is not relevant.

Thus, the classical mechanics of Newton is inadequate to analyze the many particle problem of a solid because there are too many equations, one for each particle, to be solved simultaneously and its solution, even if obtainable, is not what we observe and measure because the measuring particle (an x-ray photon or electron-microscope keV-electron) would have altered both the position and velocity of the particle being measured when scattered off the particle during the measurement.

Thus, there are two parts of the solid property problem to solve: (i) to describe the motion of a single particle whose position and velocity would have to be described in such a mathematical way in order to take into account that its motion would be changed by the measuring particle scattering off the measured particle, and (ii) to describe the motion of many interacting particles whose average properties are observed and measured in the laboratory. Both require the use of the probability concept.

First, we need a theory to describe the probability of finding a particle at a particular position (or in a finite volume element $\Delta x \Delta y \Delta z$ located at x , y , and z) with a particular velocity (or within a velocity range, v_x to $v_x + dv_x$, v_y to $v_y + dv_y$, and v_z to $v_z + dv_z$) and at a given time (or in a time interval, t to $t + dt$). A differential equation is the preference because it allows us to obtain the solutions for different initial (time) and boundary

(geometry) conditions and for different force laws. This is the Schrödinger partial differential equation proposed in 1925 whose solution is a wave-like function which is defined as the probability amplitude of finding the particle in $(\Delta x, \Delta y, \Delta z, \Delta t)$ at (x, y, z, t) . It is based on the wave-like properties of particles, hypothesized by deBroglie in 1924, and the particle-like properties of light or electromagnetic waves, hypothesized by Planck in 1900.

The single-particle solution of the Schrödinger equation must take up one further step to deal with the many particles in a solid since it is the average properties of the many particles we are observing and measuring in the laboratory or everyday life. The many particles means that the theory must be statistical in nature to allow calculation or prediction of the specific properties (electrical, mechanical, thermal, optical, ...) of the solid by averaging over the many particles contained in the solid. This theoretical scheme is known as statistical mechanics whose solution is the distribution function of the particle number. The distribution function is the probability of finding the particle in a particular range of velocity and direction, between (v_x, v_y, v_z) and $(v_x + dv_x, v_y + dv_y, v_z + dv_z)$, and in a corresponding range of kinetic energy between E and $E + dE$. This number probability distribution function then allows us to calculate or predict the velocity and kinetic energy of the system of particles averaged over the many particles of the system. The averaged velocity and kinetic energy are responsible for the observed properties of the solid and for the response of the solid to an externally applied force, such as a current by an applied voltage, or a displacement or contraction by an applied force or hydrostatic pressure. When the interparticle distance is large or the particle density is low, the identity or the spin of the particle is unimportant in the formulation of the statistical mechanics to find the velocity and energy distribution functions. This is known as the classical statistical mechanics and the distribution function is known as the Boltzmann distribution function. When the interparticle distance is small or the particle density is high, the particle identity, including the spin, must be taken into account to exclude (Pauli's exclusion principle proposed in 1925) two identical particles (including spin) from locating at the same point in the position-spin space. The additional dependence of the probability or wavefunction and energy on the spin is added to the Schrödinger equation for one or many particles. This statistical theory is known as the quantum statistical mechanics. The particle distribution function at the high particle density is known as the Fermi function for particles with odd integer multiplier of $1/2$ spin unit such as electron with spin of $1/2$, and the Bose function for particles with even integer multiplier of $1/2$ spin unit.

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Thus, the Schrödinger equation provides the probability of finding a particle at a specified velocity, position and time interval to take into account the uncertainty during measurement by scattering, and the Fermi-Bose distribution functions are the statistical distributions of the particles at high particle densities in solids to calculate and predict the solid's properties averaged over all the particles composing the solid.

P100.2 What distinguish(es) hypotheses from laws? When does a hypothesis become a law? Are the following rules hypotheses or laws and why: Newton, Coulomb, Ampere, Planck, de Broglie, Bohr atom, tunneling, Fermi distribution, Bose distribution, Shockley diode, MOSCV, SNS diode, Bethe diode, Mott-Schottky diode, NMOS, CMOS? (Answer those which you already know. Others will be described in detail in the following chapters. Do this problem again at the end of the semester.)

A law is a quantitative relationship that is deduced from observations in many similar and different experiments. In the unabridged Random House Dictionary of the English language, 2nd edition (Random House, New York, 1987), "in science . . . a statement of a relation or sequence of (experimental) phenomena invariable under the same conditions." A hypothesis is "a proposition, or set of propositions, set forth as an explanation for the occurrence of some specified group of phenomena, either asserted merely as a provisional conjecture to guide investigation or accepted as highly probable in light of established facts." A hypothesis becomes a law when it is shown by experiment to be a statement of an invariable relation.

Newton:	Law, deduced from experiment.
Coulomb:	Law, deduced from experiment.
Ampere:	Law, deduced from experiment.
Planck:	Hypothesis, conjecture supported by experiments.
de Broglie:	Hypothesis, conjecture supported by experiments.
Bohr atom:	Hypothesis, conjecture supported by existing experiments.
tunneling:	Law, deduced from experimental I-V and other measurements.
Fermi distribution:	Hypothesis, conjecture supported by experiments.
Bose distribution:	Hypothesis, conjecture supported by experiments.
Shockley diode:	Law, deduced from experimental I-V and other measurements.
MOSCV:	Law, deduced from experimental C-V measurements.

SNS diode:	Law, deduced from experimental I-V measurements.
Bethe diode:	Law, deduced from experimental I-V measurements.
Mott-Schottky diode:	Hypothesis, conjecture deduced from experiments but proven incorrect by later experiments and a correct theory by Bethe.
NMOS:	Circuit containing nMOST. The response of a specific NMOS circuit is a law and reproducible in repeated measurements. The response is predictable by theoretical (or circuit) analysis.
CMOS:	Circuit containing both nMOST and pMOST. The response of a specific CMOS circuit (with given transistors, resistors, capacitors, etc.) is a law and reproducible in repeated measurements. The response is predictable by theoretical (or circuit) analysis.

P110.1 What is the most important fundamental parameter that distinguishes solid, liquid and gas and what are its ramifications? (Hint: A length.)

The fundamental parameter that distinguishes solid, liquid, and gas is the correlation length. It defines the dimension of the region in which the material exhibits a regular arrangement or location-ordering of the atoms. A crystalline solid has long-range order, i.e. the location of many atoms in a large volume are on a periodic lattice, and hence the crystalline solid has a correlation length that is large compared with the interatomic separation, which is another way of saying that the atoms' spacings are constant and the atoms are located on a periodic lattice extending over a large if not the entire volume of the crystalline solid. The atomic density in the crystalline or noncrystalline solid is high, meaning the atoms are packed closely together. This tends to prevent the atoms in the solid from changing location and diffusing from one part of the solid to another so the atomic diffusivity is low. In a liquid, the atoms and molecules are far apart and more apt to change location because their interparticle Coulomb force at the large particle separations are too weak to keep the particles in fixed locations. But a few of the particles in the liquid are close to each other and form a nearly unique structure or geometry of ordered atomic arrangement. Thus, liquids have a short-range order and short correlation length which give them the liquidus properties. In gases, the atoms are very far part and so are moving very rapidly because of the weak interatomic or intermolecular binding forces at the large separations. The atoms or molecules change location rapidly from the random collision or scattering between them even though the interatomic and intermolecular separation is large but the close encounter collisions are

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still rampant. The ramifications of the correlation length are its relation to the rate at which atoms change location or diffuse, and to the attenuation of a disturbance (electrical, mechanical) by scattering and dissipation. For example, the rate of diffusion is low in crystalline solid but high in gas. Attenuation of an electrical signal is low in a crystalline semiconductor and higher in a noncrystalline or amorphous semiconductor due to the increased random scattering of the conduction or current-carrying electrons which randomizes the electron velocity (current is proportional to velocity in the current flowing direction) and the increased rate of dissipation of the kinetic energy of the current-carrying electrons during scattering. These are represented by the electrical resistance of the material.

P111.1 Review the classifications of solid and in what engineering areas are they used?

The classification schemes discussed in section 111 are grouped by: geometrical (crystallinity vs imperfection), purity (pure vs impure), electrical (electrical conductivity), and mechanical (binding force).

Geometrical (crystallinity vs imperfection): chemical engineering, material science and engineering including ceramic and metallurgy engineering, and electrical engineering (solid-state electronics).

Purity (pure vs impure): chemical engineering, electrical engineering (solid-state electronics), material science.

Electrical (electrical conductivity): electrical engineering.

Mechanical (binding force): mechanical engineering, civil engineering, chemical engineering, aeronautical engineering, materials science.

P120.1 Itemize the reasons why crystallinity and semiconductivity are needed to make transistors.

Reasons for crystallinity:

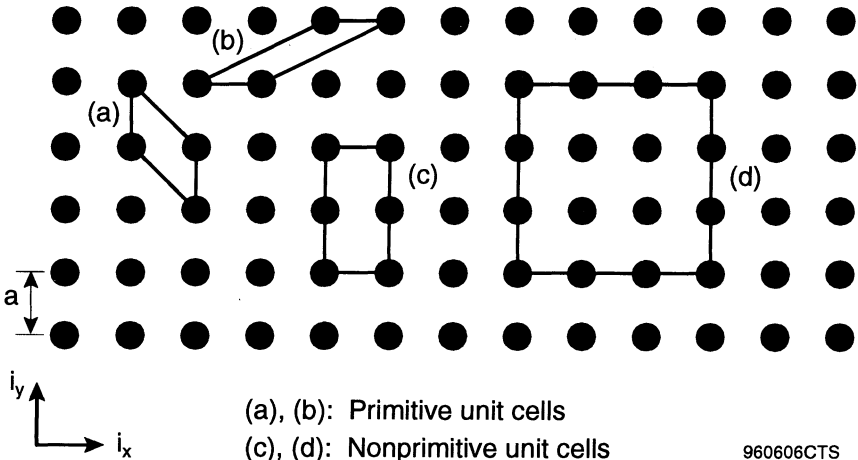
- Non-crystalline semiconductors contain physical defects.
- Physical defects are structural imperfections or displacement of host atoms.
- Physical defects are electron and hole traps.
- Electron and hole disappear when they recombine at traps.
- High trap density gives short electron-hole lifetime.

- Electrical signal carried by electron is attenuated if lifetime is short.
- Electrical attenuation reduces the transistor's current amplification factor.

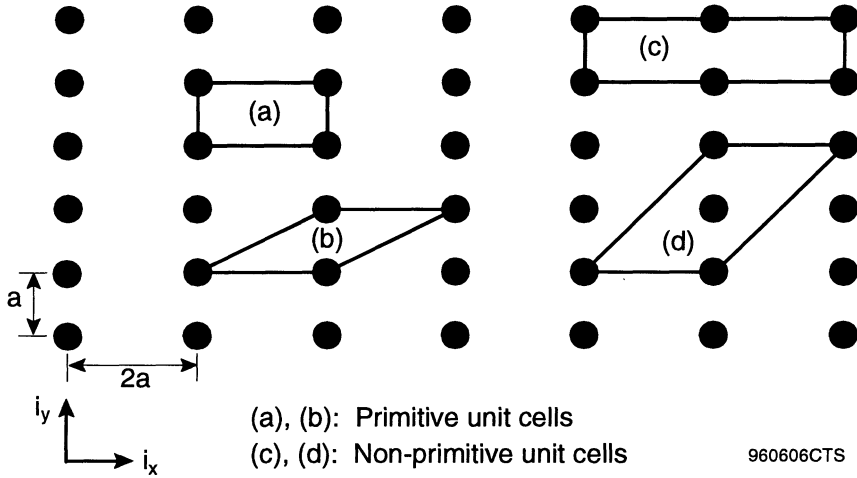
Reasons for semiconductivity:

- Impurities are added to semiconductors
 - * To control the magnitude of the electrical conductivity.
 - * To give two conductivity types:
 - n-type conduction by electrons.
 - p-type conduction by holes.
 - * Transistors require two conductivity types to form highly nonlinear rectifying p/n junctions.

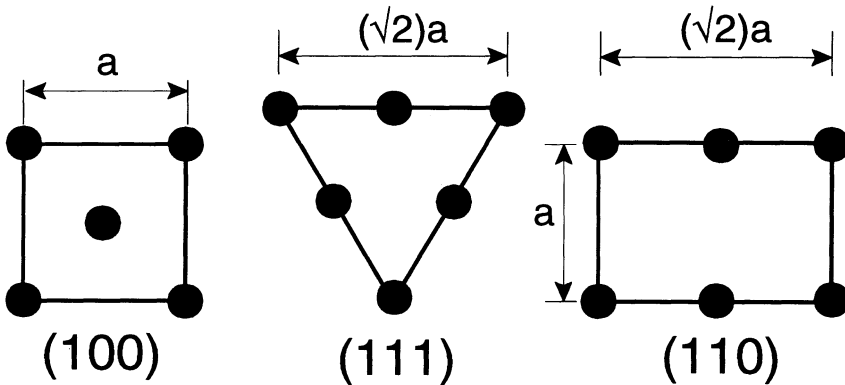
P131.1 Identify two primitive and two non-primitive cells of the two-dimensional square lattice which are not given in Fig. 131.1.



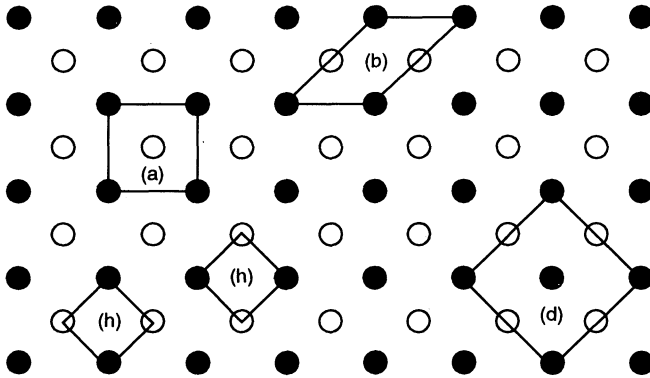
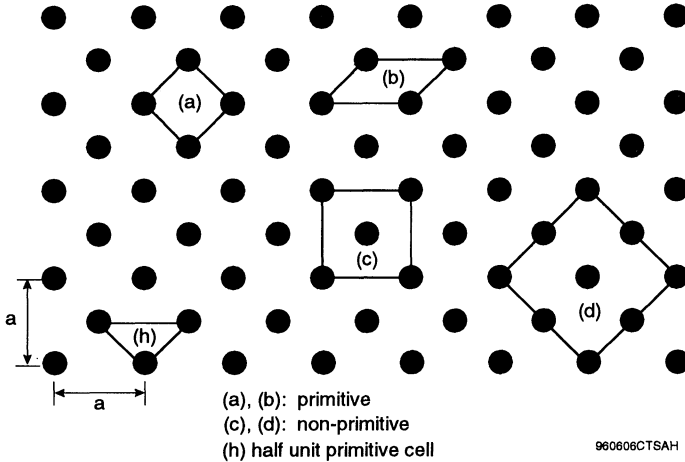
P131.2 Draw the two dimensional lattice whose primitive translation vector of the lattice is $2a\mathbf{i}_x + a\mathbf{i}_y$. Show two primitive and two non-primitive unit cells, one of each should be non-rectangular.



P132.1 Draw the (100), (110) and (111) planes of a face-centered cubic lattice.



P131.3 Identify two primitive and two non-primitive cells of a two-dimensional face-centered square lattice. Give the primitive unit vector and draw it on the figure. Is this a primitive lattice or a composite lattice of two simple lattices?



The upper figure shows a two-dimensional face-centered square lattice of one type of atoms which is just a simple square lattice turned 45° . However, if there are two kinds of atoms as shown in the lower figure, then it is a composite lattice of two simple square lattices. The primitive unit cells of the two lattices are different.

P133.1 Obtain the atomic density expression of the two-dimensional rectangular lattice given in P131.2 using four unit cells similar to those selected for the square lattice in Fig. 133.1.

Consider the four unit cells (a), (b), (c), and (d) shown in Figure P131.2. The results are tabulated below. It is evident that the atomic density is independent of the unit cell geometry selected as anticipated.

<u>Unit Cell Type</u>	<u>Cell Area</u>	<u>Number of Atoms per Cell</u>	<u>Atomic Density</u>
(a)	$2a^2$	1	$1/2a^2$
(b)	$2a^2$	1	$1/2a^2$
(c)	$4a^2$	2	$1/2a^2$
(d)	$4a^2$	2	$1/2a^2$

P133.2 Calculate the atomic density of Ga atom, As atom, and GaAs atom-pair in GaAs.

In a zinc blende semiconductor crystal lattice, one type of atom occupies a fcc lattice and the other type of atom occupies the other fcc lattice.

<u>Unit Cell Type</u>	<u>Cell Volume</u>	<u>Number of Atoms per Cell</u>
Ga atom FCC	a^3	8 corner atoms \times $1/8 = 1$ atom 6 face-centered atoms \times $1/2 = 3$ atoms Ga atom density = 4 atoms/ a^3
As atom FCC	a^3	8 corner atoms \times $1/8 = 1$ atom 6 face-centered atoms \times $1/2 = 3$ atoms As atom density = 4 atoms/ a^3
GaAs atom pair FCC	a^3	8 corner pairs \times $1/8 = 1$ pair 6 face-centered pairs \times $1/2 = 3$ pairs GaAs pair density = 4 pairs/ a^3

P133.5 Oxygen causes indirect problems in controlling the electrical properties of silicon transistors and integrated circuits as described in section 134. The segregation coefficient of oxygen in Si is unity. Can oxygen impurity be

removed from Si using the zone refining technique? How can oxygen be removed during the growth of a silicon crystal?

Because the segregation coefficient of oxygen in Si is unity, the oxygen concentration is the same in the solid and the melt. Therefore, the zone refining technique cannot be used to reduce the oxygen concentration. However, oxygen can be removed by heating the silicon in an inert gas (He, Ar) ambient or in vacuum (such as in vacuum float-zone crystal growth or zone-refining furnaces), causing outdiffusion of the oxygen in the solid silicon to the solid surface and evaporation into the gas phase or vacuum ambient which is then evacuated. Silicon crystal grown in vacuum ambient has much lower oxygen concentration ($\sim 10^{16} \text{cm}^{-3}$) than grown from Si melt in a fused quartz (SiO_2) crucible ($\sim 5 \times 10^{18} \text{cm}^{-3}$).

P140.1 Answer the question posed in Problem 110.1 again but this time, give a more detailed and less qualitative or more quantitative but concise (itemized) description of the fundamental reasons.

[What is the most important fundamental parameter that distinguishes solid, liquid and gas and what are its ramifications? (Hint: A length.)]

The fundamental factor discussed in Section 140 that distinguishes solid, liquid, and gas is the particle density.

The consequence of the high particle density in solid is: (1) interparticle distance is very small, about 2 angstroms, (2) the force on a single particle is due to all the other, $10^{23} - 1$, particles, and (3) the rate of collision between the particles is high.

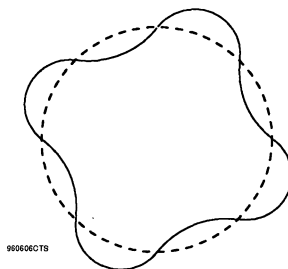
The small interparticle distance cited in (1) means that the instantaneous position of the particle can no longer be defined and the deterministic classical mechanics must be replaced by the probabilistic quantum mechanics.

The interaction between all of the surrounding particles cited in (2) and the high rate of collision cited in (3) indicate that the average motion of many particles is the quantity measured during experiment. Therefore, the statistical properties of a large number of particles are necessary to explain the measured electrical characteristics which is the realm of statistical mechanics.

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- P141.1** Bohr's first postulate in his hydrogen atom model states that the orbital angular momentum of the bound electron is quantized (or discrete). After (141.4) in the text, a statement is made that this has a very simple geometrical interpretation. Give the graphical demonstration for $n=1$ and $n=4$ (easier to draw than $n=1$) that is anticipated in the text.

The picture on the right depicts a standing sine wave drawn on the circle whose radius is the Bohr radius so that the circumference of the circle is exactly equal to four deBroglie wavelengths. The figure is a sketch of the standing wave whose wavelength is one fourth the circumference of the circle.



- P141.1** Show that Fig.141.5 is drawn correctly with respect to the text statements.

Page 46 states that electric field points in the x -direction of the (x,y,z) coordinates but does not specify positive or negative x -direction. Figure 141.5 shows $E_x < 0$ and a force on the electron in the $+x$ direction.

- P141.2** Are the kinetic and potential energies spatially constant for an electron bound at the n -th orbit with energy E_n in Bohr's hydrogen atom model? Are the answers valid in the wave model described by Schrödinger's equation in section 156?

The total energy or the sum of the kinetic and potential energies is a constant. The kinetic and potential energies may not be individually.

- P141.4** A ball of 2000 grams is moving at 150 meter/sec. A 3000 pound automobile is moving at 65 mile/hour. An oxygen molecule in our air is moving at 10^7 cm/s. What is the kinetic energy (in joule and electron-volt), de Broglie wavelength in meters, and Planck frequency in Hz of these moving objects? Which particle may require wave-quantum mechanics to explain its motion and why?

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Answers for similar problems are on p.13 of FSSE-SG and for this problem below.

Key equations:

$$KE = (1/2)mv^2 \quad \text{classical law}$$

$$\lambda = h/p \quad \text{de Broglie wavelength}$$

$$E = hf \quad \text{Planck's energy quantum of a wave}$$

(1) Ball

Given: $m = 2000\text{g} = 2\text{kg}$, $v = 150\text{ m/s}$

Computed:

$$KE = (1/2)(2\text{ kg})(150\text{ m/s})^2 = 2.25 \times 10^4\text{ J}$$

$$KE = (2.25 \times 10^4\text{ J})(1\text{ eV}/1.602 \times 10^{-19}\text{ J}) = 1.40 \times 10^{23}\text{ eV}$$

$$\lambda = (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) / [(2\text{ kg})(150\text{ m/s})] = 2.21 \times 10^{-36}\text{ m} = 2.21 \times 10^{-24}\text{ \AA}$$

$$f = (2.25 \times 10^4\text{ J}) / (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) = 3.40 \times 10^{37}\text{ Hz}$$

(2) Car

Given: $m = (3000\text{ lb})(1\text{ kg}/2.2\text{ lb}) = 1364\text{ kg}$

$$v = (65\text{ mile/hour})(1.609\text{ km/mile})(1000\text{ m}/1\text{ km})(1\text{ hr}/3600\text{ s}) = 29.058\text{ m/s}$$

Computed:

$$KE = (1/2)(1364\text{ kg})(29.058\text{ m/s})^2 = 5.76 \times 10^5\text{ J}$$

$$KE = (5.76 \times 10^5\text{ J})(1\text{ eV}/1.602 \times 10^{-19}\text{ J}) = 3.59 \times 10^{24}\text{ eV}$$

$$\lambda = (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) / [(1364\text{ kg})(29.058\text{ m/s})] = 1.67 \times 10^{-38}\text{ m} = 1.67 \times 10^{-28}\text{ \AA}$$

$$f = (5.76 \times 10^5\text{ J}) / (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) = 8.69 \times 10^{38}\text{ Hz}$$

(3) O₂ molecule

Given: $m_{\text{O}_2} = 2(16\text{ amu})(1.66 \times 10^{-24}\text{ g/amu})(1\text{ kg}/1000\text{ g}) = 5.3126 \times 10^{-26}\text{ kg}$

$$v = (10^7\text{ cm/s})(1\text{ m}/100\text{ cm}) = 10^5\text{ m/s}$$

Computed:

$$KE = (1/2)(5.3126 \times 10^{-26}\text{ kg})(10^5\text{ m/s})^2 = 2.66 \times 10^{-16}\text{ J}$$

$$KE = (2.6563 \times 10^{-16}\text{ J})(1\text{ eV}/1.602 \times 10^{-19}\text{ J}) = 1.66 \times 10^3\text{ eV}$$

$$\lambda = (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) / [(5.3126 \times 10^{-26}\text{ kg})(10^5\text{ m/s})]$$

$$= 1.25 \times 10^{-13}\text{ m} = 1.25 \times 10^{-3}\text{ \AA}$$

$$f = (2.66 \times 10^{-16}\text{ J}) / (6.6262 \times 10^{-34}\text{ J}\cdot\text{s}) = 4.01 \times 10^{17}\text{ Hz}$$

(4) O₂ molecule

Given: $m_{\text{O}_2} = 2(16\text{ amu})(1.66 \times 10^{-24}\text{ g/amu})(1\text{ kg}/1000\text{ g}) = 5.3 \times 10^{-26}\text{ kg}$

$$v = (10^4\text{ cm/s})(1\text{ m}/100\text{ cm}) = 10^2\text{ m/s}$$

Computed:

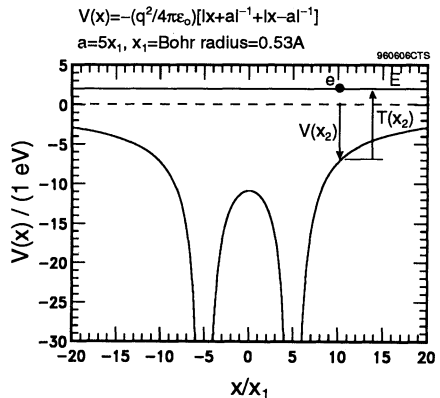
$$\begin{aligned} \text{KE} &= (1/2)(5.3126 \times 10^{-26} \text{ kg})(10^2 \text{ m/s})^2 = 2.66 \times 10^{-22} \text{ J} \\ \text{KE} &= (2.6563 \times 10^{-22} \text{ J})(1 \text{ eV}/1.602 \times 10^{-19} \text{ J}) = 1.66 \times 10^{-3} \text{ eV} \\ \lambda &= (6.6262 \times 10^{-34} \text{ J}\cdot\text{s}) / [(5.3126 \times 10^{-26} \text{ kg})(10^2 \text{ m/s})] \\ &= 1.25 \times 10^{-10} \text{ m} = 1.25 \text{ \AA} \\ f &= (2.66 \times 10^{-22} \text{ J}) / (6.6262 \times 10^{-34} \text{ J}\cdot\text{s}) = 4.01 \times 10^{11} \text{ Hz} \end{aligned}$$

The motion of the ball and car are adequately described by classical Newtonian mechanics since their body are very massive, their kinetic energy very large, and their deBroglie wavelength very small, compared with those of a measuring photon or particle which scatters off the massive body during measuring. The uncertainty in position determination during observation via scattering is of the order of λ from the uncertainty principle, $\Delta x \Delta p \sim h$, or $\Delta x \sim h/\Delta p \sim \lambda$, and hence negligible. The motion of the O_2 molecule with a high velocity in (3) can also be determined by Newtonian mechanics for the same reasons, however, the 1000-times slower moving O_2 molecule in (4) would require Schrödinger equation to give the probability of finding the O_2 for exactly the opposite reasons, large λ and small K.E.

P141.8 Draw the potential energy curve of an electron in the field of two motionless protons which are held at $x=-a$ and $x=+a$. Use $r=\infty$ as the reference potential energy. Label also the kinetic energy of the electron if its total energy is positive, $E > 0$.

The reference potential, $V(\infty) = V(-\infty) = 0$, is chosen since $1/r \rightarrow 0$ as $r \rightarrow \pm \infty$. The electron potential energy due to the proton at $x=-a$ and $x=+a$ are $V_{\text{proton1}}(x) = -q^2/(4\pi\epsilon_0|x-(-a)|)$ and $V_{\text{proton2}}(x) = -q^2/(4\pi\epsilon_0|x-a|)$. The total electron potential energy is the sum:

$$\begin{aligned} V(x) &= V_{\text{proton1}}(x) + V_{\text{proton2}}(x) \\ &= -q^2/(4\pi\epsilon_0|x+a|) - q^2/(4\pi\epsilon_0|x-a|) \\ &= -(q^2/4\pi\epsilon_0) \times (|x+a|^{-1} + |x-a|^{-1}) \end{aligned}$$



P141.9 In the two-proton problem above, do you expect the ground state energy of the electron to be more negative (more tightly bound) or more positive than the electron in the one-proton or hydrogen ground state? Why? Label the kinetic energy of the electron bound to the two-proton ground state.

More tightly bond because the two protons exert twice as much attractive force on the negatively charged electron, if the two protons are located at the same point in space or $a=0$. The separation of the two protons will reduce the attractive force from twice as much but it is still more than just the attractive force from one proton.

P141.10 The two lowest-energy wavefunctions of the electron bound to the two protons are symmetric and antisymmetric. Sketch and explain why one has a lower energy while the other has a higher energy.

The symmetric wavefunction peaks at the origin, $x=0$, to satisfy the space symmetry condition, $\psi_S(x) = +\psi_S(-x)$. The antisymmetric wavefunction must have null amplitude at the origin to satisfy the antisymmetry condition, $\psi_A(x) = -\psi_A(-x)$, thus, $\psi_A(x=0)=0$ and it peaks away from the origin. The potential energy at and around $x=0$ is large and negative where the symmetric electron spends more time. Thus, the total energy of the symmetric bound state wavefunction is larger (or more negative) than that of the antisymmetric wavefunction. The $\psi(x)$ vs x are similar to the lower two in Fig. 155.1(b). A similar result for a more complex problem of many electrons in a crystal is given in Fig. 181.3 and P181.8 for the same physical reason, i.e. the electrons concentrated at the atomic core are more tightly bond and hence with large and more negative total energy corresponding to those in the valence band.

P141.13 Can a true bound electron energy state exist in the potential energy given in Fig. 141.5? Why? (Hint: No, tunneling.)

True bound electron energy states cannot exist in Fig. 141.5 which is the potential energy diagram of an electron around a proton in the presence of an applied electric field because if the bound state exists, the bound electron will eventually tunnel out of the potential well and hence cannot be permanently bound, like an electron around a proton without the applied electric field, i.e. in hydrogen atom. Mathematically, a bound solution of the Schrödinger equation does not exist if the potential energy term consists of two terms, $Fx - A/r$, where Fx comes from the applied force or electric field along the

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x-direction. In practice, the electric field is small, and the classical-forbidden potential barrier is thick and the tunneling rate is so small that during any practical observation time, the electron is attached to the positive charge which gives the $-A/r$ Coulombic attractive potential. Since the Bohr ground state energy is 13.6eV and the Bohr radius is 0.52A, the electric field due to the proton is about $13.6/0.52 \times 10^{-8} \sim 10^9$ V/cm. So, the applied electric field has to be extremely high to cause rapid tunneling of the electron bound to the proton at the ground state of the hydrogen atom. Figure 141.5 shows to scale an electric field of $10V/20r_1 \sim 10^8$ V/cm which is about the practical upper limit that can be produced (100 Mega-Volt per centimeter) by the very reason that gas would ionize and the electrode atoms would be ripped off to prevent sustaining or even producing such a high electric field in the laboratory. The forbidden barrier thickness at -13.6eV estimated from extending the figure in the +x direction is $\sim 13.6/10^8$ or $a=13.6A$ and the barrier height is $E_{\text{Barrier}} = E_{\text{peak}} - (-13.6) \approx (-7) + 13.6 \approx 6.6\text{eV}$. This is a very thick and tall barrier, and the tunneling probability calculated from (153.11) assuming a square barrier, $\exp[-2(a/\hbar)\sqrt{2mE_B}]$ or (154.1A) assuming a triangular barrier is extremely small. The students may carry this estimate out by plugging in the numbers to determine the tunneling transition probability.

P142.1 Why do we pick the negative sign for **p** instead of positive sign?

In order that a traveling wave with positive velocity is traveling in the positive x-direction. See graphical solutions for the P142.5.

P142.4 Construct a traveling wave moving in the negative x direction.

$$y(x,t) = Y(0)\cos(\omega t + kx) \tag{P142.4A}$$

The velocity of this traveling wave is negative, i.e. the point of constant phase is moving in the negative direction with time as demonstrated by

$$\text{Phase} = \Theta = (\omega t + kx) = \text{constant.}$$

Thus, phase velocity is $dx/dt = -d\omega/dt < 0$.

One can also graphically illustrate this by drawing the cosine wave versus x at $t=0$ and a later time $t=t_1$ which is demonstrated in the next problem for a travelling wave moving in the positive x direction.

Other examples are the following wavepackets that could represent a group of electrons moving in the negative direction or positive direction (change the + sign to - sign below). The first does not decay while the second decays and spreads out.

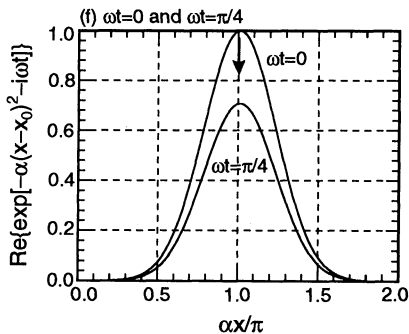
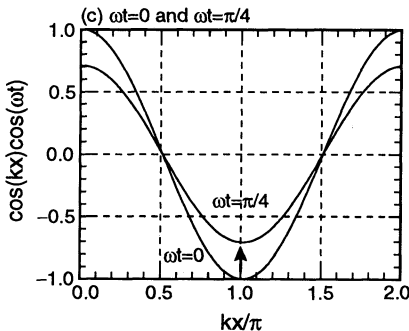
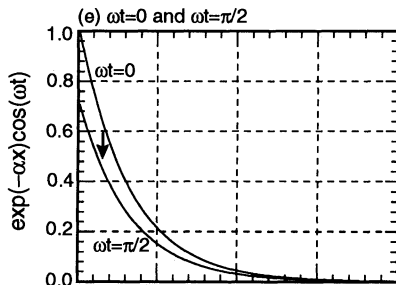
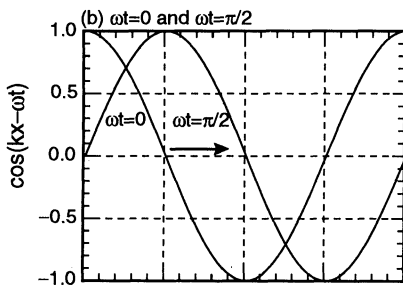
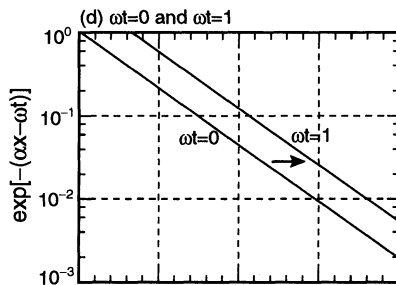
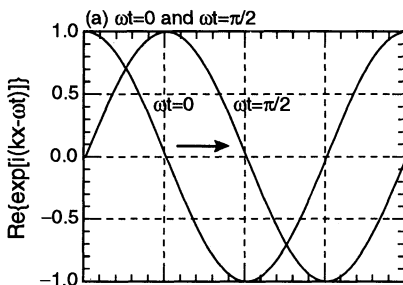
$$y(x,t) = Y(0)\exp[-(x+vt)^2/4Dt_0] \tag{P142.4B}$$

$$y(x,t) = Y(0)(t+t_0)^{-3/2}\exp[-(x+vt)^2/4Dt] \tag{P142.4B}$$

P142.5 Which of the following are traveling waves and standing waves? Use sketch at $t=0$ and $t=t_1$ to illustrate your answers. (a) $\exp[i(kx-\omega t)]$; (b) $\cos(kx-\omega t)$; (c) $\cos(kx)\cos(\omega t)$; (d) $\exp[-(\alpha x-\omega t)]$; (e) $\exp(-\alpha x)\cos(\omega t)$; (f) $\exp[-\alpha(x-x_0)^2-i\omega t]$. Let $k>0$, $\omega>0$ and $\alpha>0$.

Traveling waves: (a), (b), (d)

Standing waves: (c), (e), (f)



P161.2 The electron affinity to an isolated neutral Si atom is 1.39eV while to a neutral Si crystal it is 4.02eV. Why is it larger in Si crystal? Give a simple explanation based on electrostatic or Coulomb force.

The electron affinity is the energy required to remove an electron from the subject. It is smaller in an isolated neutral Si atom because the to-be-removed electron is bound to the Si^{+4} atomic core which is screened by the other three nearby valence electrons so the net positive charge is much less than +4 and the attractive force is hence much less than that due to a +4q charge. In addition, the electron-electron repulsion energy between this and other three valence electrons reduces the binding. In the Si crystal the electron affinity is larger, almost by a factor of three, because all the four valence electrons of each Si atom are spread out over the entire crystal owing to the small interatomic distance or the presence and the proximity of the neighboring Si^{+4} ions so that the +4q charges and their Coulomb attraction force on the to-be-removed electron is not as much reduced as in an isolated neutral Si atom.

P172.1 Why are the valence electrons the most important on influencing the electrical properties of silicon? Why are the core electrons not as important? Why are the core electrons important to distinguish Si, Ge, GaAs and others?

The valence electron radii are comparable to the interatomic spacing and hence are spread out over the entire crystal. Thus, they are more responsive to the applied electric field to conduct electricity. The core electrons are tightly bound to each atomic core and hence are not responsive to the applied forces. Thus the electrical properties are mainly determined by the responses of the valence electrons of the atoms composing the solid to the applied forces.

Although the core electrons are not directly responsible for electrical conduction, their spatial distribution around the positively charged nucleus determine the net positive charge seen by the valence electrons. This core-electron-screened attractive force from the protons in the nucleus influence the mobility of the valence electrons moving in an electric field which is represented by an effective mass. The nuclear charge and the spatial distribution of its core electrons are different for Ga, As and Si cores and this difference is responsible for the different electrical and electro-optical properties exhibited by these semiconductors.

P172.4 If all the valence electrons in silicon are in the valence band, what is the minimum photon energy that is just enough to release an electron from silicon into vacuum?

From Figure 172.2, this is

$$\begin{aligned} h\nu_{\text{minimum}} &= \text{electron affinity} + \text{energy gap} \\ &= \chi_{\text{Si}} + E_G \\ &= 4.02 \text{ eV} + 1.18 \text{ eV} = 5.2 \text{ eV} \end{aligned}$$

P172.8 Draw an energy band diagram, especially near the semiconductor-vacuum interface or the semiconductor surface, in the presence of an electric field.

The effect of an electric field on the energy band diagram may be obtained from the relations between electric field, electric potential and electron energy: Electric field(V/cm) = $-dV/dx$;

Electron energy(eV) = $-qV$; and

$V = [\text{Electron energy(eV)}]/(-q)$.

These give:

$$\begin{aligned} \text{Electric field(V/cm)} &= \\ &= -(d/dx)(\text{Electron energy}/(-q)) \\ &= (1/q)(d/dx)(\text{Electron energy}). \end{aligned}$$

Thus, an applied electric field tilts the energy band by a slope given above.

