

Appendix A

Fundamental Constants

Table A.1 Fundamental constants

Quantity & symbol		CGS	MKS (SI)
Speed of light in vacuum c	2.997925	10^{10} cm sec ⁻¹	10^8 m s ⁻¹
Magnetic constant $\mu_0 = 4\pi \times 10^{-7}$ (permeability of free space)	1.25664		10^{-6} H m ⁻¹
Electric constant $\epsilon_0 = 1/\mu_0 c^2$ (permittivity of free space)	8.8541853		10^{-12} F m ⁻¹
Electron charge e	1.60219		10^{-19} C
	4.80324	10^{-10} esu	
Electron volt eV	1.60219	10^{-12} erg eV ⁻¹	10^{-19} J eV ⁻¹
Electron rest mass m_0	9.10956	10^{-28} gm	10^{-31} kg
Planck's constant h	6.626196	10^{-27} erg sec	10^{-34} J s
Planck's constant $\hbar = h/2\pi$	1.05459	10^{-27} erg sec	10^{-34} J s
Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/m_0e^2$	0.529177	10^{-8} cm	10^{-10} m
Rydberg constant $R_y = \hbar^2/2m_0a_0^2$	13.6058	eV	eV
Fine structure constant $\alpha = e^2/2\epsilon_0hc$	7.297351	10^{-3}	10^{-3}
Avogadro's constant L, N_A	6.022169	10^{23} mol ⁻¹	10^{23} mol ⁻¹
Loschmidt's constant N_L	2.68719		10^{25} m ⁻³
Boltzmann's constant $k_B = R/L$	1.380622	10^{-16} erg K ⁻¹	10^{-23} J K ⁻¹
Faraday constant $F = Le$	9.64867		10^4 C mol ⁻¹
Universal gas constant $R = Lk_B$	8.31435	10^7 erg K ⁻¹ mol ⁻¹	J K ⁻¹ mol ⁻¹
Mechanical equivalent of heat	4.184	10^7 erg cal ⁻¹	J cal ⁻¹
Bohr magneton $\mu_B = e\hbar/2m_0c$	9.2741	10^{-21} erg G ⁻¹	10^{-24} J T ⁻¹
Proton rest mass m_p	1.67251	10^{-24} gm	10^{-27} kg
Nuclear magneton $\mu_N = e\hbar/2m_p c$	5.0508	10^{-24} erg G ⁻¹	10^{-27} J T ⁻¹
Neutron rest mass m_n	1.67492	10^{-24} gm	10^{-27} kg
Stefan-Boltzmann constant $\sigma = 2\pi^5 k_B^4/15h^3c^2$	5.6697		10^{-8} W m ⁻² K ⁻⁴

Table A.1 (Continued)

Quantity & symbol	CGS	MKS (SI)
Gravitational constant G	6.6732	$10^{-11} \text{ N m}^2 \text{ kg}^{-2}$
Acceleration of free fall g_n	9.80665	m s^{-2}

$1.0 \text{ [eV]} = 2.41796 \times 10^{14} \text{ [Hz]} = 8.0655 \times 10^3 \text{ wavenumber [cm}^{-1}] =$
 $1.1604 \times 10^4 \text{ [K]} = 1.239855 \text{ wavelength } [\mu\text{m}]$

W: watt, G: gauss, T: tesla, N: newton, C: coulomb

Appendix B

Quantum Physics

B.1 Black Body Radiation

Planck's law for the energy density distribution for the radiation from a black body at temperature T is

$$w(f, T) = \frac{8\pi hf^3}{c^3} \frac{1}{e^{hf/k_B T} - 1} \tag{B.1}$$

where h is the Planck's constant, and f is the frequency. Note that $\omega = 2\pi f$ is the angular frequency, and $\hbar = h/2\pi$. The low-frequency Rayleigh-Jens law

$$w(f, T) = \frac{8\pi f^2 k_B T}{c^3}$$

is obtained when $hf \ll k_B T$. Stefan-Boltzmann's law for the total radiation energy per unit volume can be derived

$$W(T) = \int_0^\infty w(f, T) df = \frac{8\pi^5 k_B^4}{15h^3 c^3} T^4 = \frac{4\sigma}{c} T^4 \tag{B.2}$$

where $\sigma = 2\pi^5 k_B^4 / 15h^3 c^2$ is the Stefan-Boltzmann constant. Wien's law for the wavelength λ_{\max} at which the energy density has its maximum value can be derived from Eq. (B.1)

$$\lambda_{\max} = \frac{b}{T} \tag{B.3}$$

where $b = 0.2898 \text{ cm}\cdot\text{K}$ is a universal constant. Note $\lambda = c/f$.

B.2 The Compton Effect

A photon with initial wavelength λ incident upon an electron at rest with a rest mass m_0 . After the collision, the photon has a wavelength of λ' scattered into a direction

at an angle θ with respect to its initial propagation direction, which is also referred to be the photon scattering angle.

$$\lambda' = \lambda + \frac{h}{m_0c}(1 - \cos\theta) = \lambda + \lambda_C(1 - \cos\theta) \quad (\text{B.4})$$

where $\lambda_C = h/m_0c$ is called the Compton wavelength of the electron.

B.3 Electron Diffraction

Diffraction pattern of electron from a crystal can be explained by the dual particle-wave nature of matter. A particle having a momentum p is associated the so-called de Broglie wavelength

$$\lambda = \frac{h}{p} \quad (\text{B.5})$$

B.4 Operators in Quantum Physics

In quantum mechanics, classical physical quantities are translated into quantum operators. The measurement of a physical quantity $\langle A \rangle$ is described quantum mechanically by

$$\langle A \rangle = \int \psi_1^* A \psi_2 d\mathbf{r} = \int (A \psi_1)^* \psi_2 d\mathbf{r} \quad (\text{B.6})$$

where ψ is the wave function that describes the quantum mechanical state of the system under measurement. The only possible values that can be obtained when measuring a physical quantity $\langle A \rangle$ are the eigen values of the quantum operator A . Thus, the operator is hermitian and its eigen values are real, i.e., $Au_n = a_n u_n$, where u_n is the eigen function, a_n is the eigen value which is real. Subscript n denotes the index of the eigen functions, i.e., operator A may have multiple eigen functions and eigen values.

B.5 The Schrödinger Equation

The momentum operator is given by $\mathbf{p} = -i\hbar\nabla$, and the position operator is $\mathbf{r} = i\hbar\nabla_p$. The energy operator is

$$E = i\hbar \frac{\partial}{\partial t}$$

The Hamiltonian of a particle with mass m and potential energy V is given by

$$H = \frac{p^2}{2m} + V$$

From the eigen equation $H\psi = E\psi$ follows the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}, t) + V\psi(\mathbf{r}, t) = i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} \quad (\text{B.7})$$

where $\psi(\mathbf{r}, t)$, which is a function of space \mathbf{r} and time t , is the wave function that describes the quantum mechanical state of the particle. The wave character of a particle is described by $\psi(\mathbf{r}, t)$, and can be interpreted as a measure for the probability $\rho(\mathbf{r}, t)$ to find the particle at \mathbf{r} and t

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \quad (\text{B.8})$$

The normalizing condition for the wave function is

$$\langle\psi|\psi\rangle = \int \psi^*\psi d\mathbf{r} = 1$$

At steady state,

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = E\psi(\mathbf{r}, t) \quad (\text{B.9})$$

so that

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-iEt/\hbar} \quad (\text{B.10})$$

we have the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V\psi(\mathbf{r}, t) = E\psi(\mathbf{r}) \quad (\text{B.11})$$

for $\psi(\mathbf{r})$.

The probability flux \mathbf{s} is given by

$$\mathbf{s}(\mathbf{r}, t) = \frac{\hbar}{2im}[\psi^*(\mathbf{r}, t)\nabla\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla\psi^*(\mathbf{r}, t)] \quad (\text{B.12})$$

which is related to the current density of the particle $\mathbf{j} = q\mathbf{s}$. Here q is the electric charge of the particle (for electron $q = -e$).

The following conservation law holds

$$\frac{\partial\rho(\mathbf{r}, t)}{\partial t} = -\nabla \cdot \mathbf{s}(\mathbf{r}, t) \quad (\text{B.13})$$

The time dependence of an operator A is given by (Heisenberg):

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{[A, H]}{i\hbar} \quad (\text{B.14})$$

where H is the Hamiltonian and $[A, B] \equiv AB - BA$ is the commutator of A and B . For hermitian operators the commutator is always complex. If $[A, B] = 0$, the operators A and B have a common set of eigen functions. By applying this to \mathbf{p} and \mathbf{r} it follows (Ehrenfest)

$$m \frac{d^2 \langle \mathbf{r} \rangle_t}{dt^2} = -\langle \nabla V \rangle \quad (\text{B.15})$$

which is the classical Newton's second law of motion.

A classical product AB becomes $\frac{1}{2}(AB + BA)$ in quantum mechanics.

B.6 The Uncertainty Principle

The uncertainty ΔA in A is defined as

$$(\Delta A)^2 = \langle \psi | A - \langle A \rangle |^2 \psi \rangle = \langle A^2 \rangle - \langle A \rangle^2$$

it follows

$$\Delta A \cdot \Delta B \geq \frac{1}{2} |\langle \psi | [A, B] | \psi \rangle| \quad (\text{B.16})$$

from which it follows:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}, \quad \Delta p_x \cdot \Delta x \geq \frac{\hbar}{2} \quad (\text{B.17})$$

B.7 Parity

The parity operator in one dimension is given by $\mathcal{P}\psi(x) = \psi(-x)$. If the wave function is split into even and odd functions, it can be expanded into eigen functions of \mathcal{P} :

$$\psi(x) = \underbrace{\frac{1}{2}[\psi(x) + \psi(-x)]}_{\text{even: } \psi^+} + \underbrace{\frac{1}{2}[\psi(x) - \psi(-x)]}_{\text{odd: } \psi^-} \quad (\text{B.18})$$

with

$$\psi^+ = \frac{1}{2}(1 + \mathcal{P})\psi(x), \quad \psi^- = \frac{1}{2}(1 - \mathcal{P})\psi(x)$$

both of which satisfy the Schrödinger equation. Hence, parity is a conserved quantity. Moreover, $[\mathcal{P}, H] = 0$.

B.8 The Tunneling Effect

The wave function of a particle in a one-dimensional infinitely high potential step from $x = 0$ to $x = a$ is given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \quad (\text{B.19})$$

where $k_n = n\pi/a$, n is an integer. The energy levels are given by

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2ma^2}$$

where m is the mass of the particle.

If the wave function with energy E meets a potential barrier of W , while $E < W$, the wave function will, unlike the classical case, be non-zero within the potential barrier. Consider a one-dimensional system along the x axis. Denote the potential barrier as

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ W & \text{for } 0 \leq x < a \\ 0 & \text{for } x \geq a \end{cases} \quad (\text{B.20})$$

For an wave Ae^{ikx} running into the potential barrier from $x = -\infty$, we express the total wave function as

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < 0 \\ Ce^{iqx} + De^{-iqx} & \text{for } 0 \leq x < a \\ A'e^{ikx} & \text{for } x \geq a \end{cases} \quad (\text{B.21})$$

with $q^2 = 2m(E - W)/\hbar^2$ and $k^2 = 2mE/\hbar^2$. Boundary conditions require that $\psi(x)$ and $\partial\psi(x)/\partial x$ continuous at $x = 0$ and $x = a$, which give B , C and D and A' in terms of A . The transmission coefficient T of the incident wave Ae^{ikx} through the potential barrier is defined by

$$T = \frac{|A'|^2}{|A|^2} = \left| \frac{(1 + k/q)^2 - (1 - k/q)^2}{(1 + k/q)^2 e^{-iqa} - (1 - k/q)^2 e^{iqa}} \right|^2 \quad (\text{B.22})$$

which is not zero even when $E < W$. The nonzero transmission coefficient is the tunneling effect. Moreover, $T = 1$ is not always true when the energy of the incident wave is higher than the potential barrier (i.e., $E \geq W$). $T = 1$ occurs only when $e^{2iqa} = 1$, i.e., $2qa = 2n\pi$, n is an integer.

B.9 Harmonic Oscillator

For the one-dimensional potential energy

$$V(x) = \frac{1}{2}bx^2 \quad (\text{B.23})$$

Let $\omega^2 = b/m$, the Hamiltonian H is then given by:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}\hbar\omega + \omega A^\dagger A \quad (\text{B.24})$$

with

$$A = \sqrt{\frac{m}{2\omega}}x + \frac{ip}{\sqrt{2m\omega}}, \quad A^\dagger = \sqrt{\frac{m}{2\omega}}x - \frac{ip}{\sqrt{2m\omega}} \quad (\text{B.25})$$

$A \neq A^\dagger$ is non hermitian. $[A, A^\dagger] = \hbar$ and $[A, H] = \hbar\omega A$. A is a so called creation operator, and A^\dagger an annihilation operator. $HAu_E = (E - \hbar\omega)Au_E$. There is a ground-state u_0 such $Au_0 = 0$. The energy in this ground state is $\frac{1}{2}\hbar\omega$, which is normally known as the zero-point energy. Let n be a positive integer, normalized eigen functions and corresponding eigen values are

$$u_n = \frac{1}{\sqrt{n!}} \left(\frac{A^\dagger}{\sqrt{\hbar}} \right)^n u_0, \quad u_0 = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right), \quad E_n = \left(\frac{1}{2} + n\right)\hbar\omega \quad (\text{B.26})$$

B.10 Angular Momentum and Spin

The orbital angular momentum operator is defined as

$$\mathbf{L} = -i\hbar\mathbf{r} \times \nabla \quad (\text{B.27})$$

$[L_z, L^2] = [L_z, H] = [L^2, H] = 0$, $[L_x, L_y] = i\hbar L_z$, $[L_y, L_z] = i\hbar L_x$, $[L_z, L_x] = i\hbar L_y$. Not all components of \mathbf{L} can be known at the same time with arbitrary accuracy

$$\Delta L_x \Delta L_y \geq \frac{\hbar}{2} L_z \quad (\text{B.28})$$

L_z in spherical polar and Cartesian coordinates is

$$L_z = x\mathbf{p}_y - y\mathbf{p}_x - i\hbar \frac{\partial}{\partial \varphi} = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \quad (\text{B.29})$$

The creation and annihilation operators L_\pm are defined by: $L_\pm = L_x \pm iL_y$. $L^2 = L_+L_- + L_z^2 - \hbar L_z$.

Eigen value relations of angular momentum \mathbf{L} with eigen function $Y_{\ell m}$

$$\begin{aligned} \mathbf{L}^2 Y_{\ell m} &= \ell(\ell + 1)\hbar^2 Y_{\ell m} \\ L_z Y_{\ell m} &= m\hbar Y_{\ell m} \end{aligned} \quad (\text{B.30})$$

where $\ell \geq 0$ and $2\ell + 1$ is an integer, $-\ell \leq m \leq \ell$ and can take on the values

$$m = -\ell, -\ell + 1, -\ell + 2, \dots, \ell - 1, \ell$$

$Y_{\ell m}$ is the spherical harmonics

$$Y_{\ell m}(\theta, \psi) = N_{\ell m} P_{\ell}^{|m|}(\cos \theta) e^{im\psi} \quad (\text{B.31})$$

where $P_{\ell}^{|m|}(\cos \theta)$ is the associated Legendre polynomials.

For integral values of ℓ , we discuss orbit angular momentum,

$$\begin{aligned} L_+ Y_{\ell m} &= \sqrt{\ell(\ell + 1) - m(m + 1)} \hbar Y_{\ell m+1} \\ L_- Y_{\ell m} &= \sqrt{\ell(\ell + 1) - m(m - 1)} \hbar Y_{\ell m-1} \end{aligned} \quad (\text{B.32})$$

Addition theorem for angular momentum:

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 \quad (\text{B.33})$$

\mathbf{L} has eigen functions $Y_{\ell m}$ with

$$\ell = |\ell_1 - \ell_2|, |\ell_1 - \ell_2| + 1, \dots, \ell_1 + \ell_2, \quad m = -\ell, -\ell + 1, \dots, \ell \quad (\text{B.34})$$

When ℓ takes on the values of half-odd integral, i.e., $\ell = 1/2, 3/2, \dots$, we discuss spin. Spin operators are defined by their commutation relations: $[S_x, S_y] = i\hbar S_z$, they do not act in the physical space (x, y, z) . Furthermore, $[\mathbf{L}, \mathbf{S}] = 0$ so that spin and angular momentum operators do not have a common set of eigen functions. The spin operators are given by $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$, where

$$\boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{B.35})$$

are Pauli spin matrices. Denote the eigen function of spin as χ ,

$$\mathbf{S}^2 \chi_{s, m_s} = s(s + 1)\hbar^2 \chi_{s, m_s}, \quad s = \frac{1}{2} \quad (\text{B.36})$$

We normally denote $\chi_{\frac{1}{2}, \frac{1}{2}} = \alpha$ and $\chi_{\frac{1}{2}, -\frac{1}{2}} = \beta$.

Addition of two spins $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$,

$$\left\{ \begin{array}{l} \text{triplet, parity} = 1 \\ \text{singlet, parity} = -1 \end{array} \right. \left\{ \begin{array}{l} \chi_{1,1} = \alpha_1 \alpha_2 \\ \chi_{1,0} = \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 + \beta_1 \alpha_2) \\ \chi_{1,-1} = \beta_1 \beta_2 \\ \chi_{0,0} = \frac{1}{\sqrt{2}}(\alpha_1 \beta_2 - \beta_1 \alpha_2) \end{array} \right. \quad (\text{B.37})$$

The electron has an intrinsic magnetic dipole moment \mathbf{M} due to its spin, $\mathbf{M} = -eg_s\mathbf{S}/2m$, with $g_s = 2(1 + \alpha/2\pi + \dots)$ is the gyromagnetic ratio. In the presence of an external magnetic field this gives a potential energy $V = -\mathbf{M} \cdot \mathbf{B}$. The Schrödinger equation then becomes (because $\partial\chi/\partial x_i \equiv 0$):

$$i\hbar \frac{\partial\chi(t)}{\partial t} = \frac{eg_s\hbar}{4m} \boldsymbol{\sigma} \cdot \mathbf{B}\chi(t) \quad (\text{B.38})$$

with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. If $\mathbf{B} = B\mathbf{e}_z$ there are two eigenvalues for this equation, $\pm eg_s\hbar B/4m = \pm\hbar\omega$, and the general solution is given by $\chi(t) = Ae^{-i\omega t} + Be^{i\omega t}$. From these,

$$\langle S_x \rangle = \frac{1}{2}\hbar \cos(2\omega t), \quad \langle S_y \rangle = \frac{1}{2}\hbar \sin(2\omega t) \quad (\text{B.39})$$

Thus the spin precesses about the z axis with frequency 2ω . This causes the Zeeman splitting of spectral lines.

B.11 Hydrogen Atom

The hydrogen atom contains one proton and one electron. The Schrödinger equation becomes a one-particle equation after the center-of-mass motion is separated out. In spherical coordinate, the potential energy is

$$V(r) = -\frac{e^2}{4\pi\epsilon r} \quad (\text{B.40})$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(\mathbf{r}) = \psi(\mathbf{r}) \quad (\text{B.41})$$

where m is the reduced mass which is approximately the same as the electron mass m_0 .

The solutions of the above Schrödinger equation in spherical coordinates if the potential energy is a function of r can be written as

$$\psi(r, \theta, \varphi) = R_{n\ell}(r) Y_{\ell m}(\theta, \varphi)$$

$Y_{\ell m}$ is the spherical harmonics in Eq. (B.31). Let $u_{n\ell}(r) = rR_{n\ell}(r)$, the equation that determines $u_{n\ell}(r)$ is

$$\frac{d^2 u_{n\ell}(r)}{dr^2} + \frac{2m}{\hbar^2} \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2mr^2} \right] u_{n\ell}(r) = 0 \quad (\text{B.42})$$

Solution of the above equation for $V(r)$ in Eq. (B.40) when $\epsilon = \epsilon_0$ and $m = m_0$

$$E_n = -\frac{R_y}{n^2} \quad (\text{B.43})$$

where $R_y = \hbar^2/2m_0a_0^2 = 13.6058$ eV is Rydberg, $a_0 = 4\pi\epsilon_0\hbar^2/m_0e^2 = 0.529$ Å is Bohr radius. The parity of these solutions is $(-1)^\ell$, and the functions are

$$2 \sum_{\ell=0}^{n-1} (2\ell + 1) = 2n^2$$

fold degenerated.

B.12 Interaction with Electromagnetic Fields

The Hamiltonian of an electron in an electromagnetic field is given by:

$$H = \frac{1}{2\mu}(\mathbf{p} + e\mathbf{A})^2 - e\phi = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{i\hbar e}{2\mu}(\mathbf{A} \cdot \nabla + \nabla \cdot \mathbf{A}) + \frac{e^2}{2\mu}A^2 - e\phi \quad (\text{B.44})$$

where μ is the reduced mass of the system, \mathbf{A} is the vector field and ϕ is the scalar field of the electromagnetic field. The term $\sim A^2$ can usually be neglected, except for very strong fields or macroscopic motions.

B.13 Time-Independent Perturbation Theory

Consider a time-independent perturbation V' so that the Schrödinger equation becomes $(H_0 + \lambda V')\Psi_n = E_n\Psi_n$. Let ψ_n be the complete set of eigen functions of the non-perturbed Hamiltonian H_0 , i.e., $H_0\psi_n = E_n^0\psi_n$. We write

$$\Psi_n = \psi_n + \sum_{k \neq n} c_{nk}(\lambda)\psi_k \quad (\text{B.45})$$

Expanding c_{nk} and E_n into λ

$$\begin{aligned} c_{nk} &= \lambda c_{nk}^{(1)} + \lambda^2 c_{nk}^{(2)} + \dots \\ E_n &= E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \end{aligned} \quad (\text{B.46})$$

inserting them into the Schrödinger equation result in the first-order correction

$$\begin{aligned} E_n^{(1)} &= \langle \phi_n | V' | \phi_n \rangle, & c_{nk, k \neq n}^{(1)} &= \frac{\langle \psi_k | V' | \psi_n \rangle}{E_n^0 - E_k^0} \\ \Psi_n &= \psi_n + \sum_{k \neq n} \frac{\langle \psi_k | V' | \psi_n \rangle}{E_n^0 - E_k^0} \psi_k \end{aligned} \quad (\text{B.47})$$

where $m \neq n$, and the second-order correction of the energy

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \psi_k | V' | \psi_n \rangle|^2}{E_n^0 - E_k^0} \quad (\text{B.48})$$

B.14 Time-Dependent Perturbation Theory

When the perturbation is time-dependent, i.e., $V'(t)$, the Schrödinger equation is

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = [H_0 + \lambda V'(t)] \Psi(t) \quad (\text{B.49})$$

and

$$\Psi(t) = \sum_n c_n(t) \exp\left(\frac{-iE_n^0 t}{\hbar}\right) \psi_n \quad (\text{B.50})$$

with $c_n(t) = \delta_{nk} + \lambda c_n^{(1)}(t) + \dots$. The first-order correction follows

$$c_n^{(1)}(t) = \frac{1}{i\hbar} \int_0^t \langle \psi_n | V'(\tau) | \psi_k \rangle \exp\left[\frac{i(E_n^0 - E_k^0)\tau}{\hbar}\right] d\tau \quad (\text{B.51})$$

B.15 N -Particle System

Identical particles are indistinguishable. For the total wave function of a system of identical particles,

1. Particles with a half-odd integer spin (Fermions): Ψ_{total} must be anti-symmetric with respect to interchanges of the coordinates (spatial and spin) of each pair of particles. The Pauli principle results from this: two Fermions cannot exist in an identical state because then $\Psi_{\text{total}} = 0$.
2. Particles with an integer spin (Bosons): Ψ_{total} must be symmetric with respect to interchange of the coordinates (spatial and spin) of each pair of particles.

For a system of two electrons there are 2 possibilities for the spatial wave function. When a and b are the quantum numbers of electron 1 and 2,

$$\begin{aligned} \psi_S(1, 2) &= \psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1) \\ \psi_A(1, 2) &= \psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1) \end{aligned} \quad (\text{B.52})$$

Following spin wave functions are possible:

$$\chi_A = \frac{1}{\sqrt{2}} [\chi_+(1)\chi_-(2) - \chi_+(2)\chi_-(1)] \quad (\text{B.53})$$

$$\chi_S = \begin{cases} \chi_+(1)\chi_+(2) \\ \frac{1}{\sqrt{2}}[\chi_+(1)\chi_-(2) + \chi_+(2)\chi_-(1)] \\ \chi_-(1)\chi_-(2) \end{cases}$$

Because the total wave function must be anti-symmetric, $\Psi_{\text{total}} = \psi_S \chi_A$, or $\Psi_{\text{total}} = \psi_A \chi_S$.

For N particles the symmetric spatial function is given by:

$$\psi_S(1, \dots, N) = \sum \psi(\text{all permutations of } 1, \dots, N) \quad (\text{B.54})$$

The anti-symmetric wave function is given by the Slater determinant

$$\psi_A(1, \dots, N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{E_1}(1) & \psi_{E_1}(2) & \cdots & \psi_{E_1}(N) \\ \psi_{E_2}(1) & \psi_{E_2}(2) & \cdots & \psi_{E_2}(N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{E_N}(1) & \psi_{E_N}(2) & \cdots & \psi_{E_N}(N) \end{vmatrix} \quad (\text{B.55})$$

B.16 Quantum Statistics

If a system exists in a state in which one has not the disposal of the maximal amount of information about the system, it can be described by a *density matrix* ρ . If the probability that the system is in state Ψ_i is given by c_i , one can write for the expectation value a of A

$$a = \langle A \rangle = \sum_i c_i \langle \Psi_i | A | \Psi_i \rangle \quad (\text{B.56})$$

If Ψ is expanded into an orthonormal basis $\{\psi_k\}$ as $\psi^{(i)} = \sum_k c_k^{(i)} \phi_k$,

$$\langle A \rangle = \sum_k (A\rho)_{kk} = \text{Tr}(A\rho) \quad (\text{B.57})$$

where $\rho_{\ell k} = c_k^* c_\ell$. ρ is hermitian, with $\text{Tr}(\rho) = 1$. Further holds

$$\rho = \sum r_i |\psi_i\rangle \langle \psi_i|$$

The probability to find eigenvalue a_n when measuring A is given by ρ_{nn} if one uses a basis of eigen vectors of A for $\{\phi_k\}$. For the time-dependence holds (in the Schrödinger image operators are not explicitly time-dependent):

$$i\hbar \frac{d\rho}{dt} = [H, \rho] \quad (\text{B.58})$$

For a macroscopic system in equilibrium holds $[H, \rho] = 0$. If all quantum states with the same energy are equally probable: $P_i = P(E_i)$, one can obtain the distribution:

$$P_n(E) = \rho_{nn} = \frac{e^{-E_n/k_B T}}{Z} \quad \text{with the state sum } Z = \sum_n e^{-E_n/k_B T} \quad (\text{B.59})$$

The thermodynamic quantities are related to these definitions as follows:

$$\begin{aligned} F &= -k_B T \ln(Z) \\ U = \langle H \rangle &= \sum_n p_n E_n = -\frac{\partial}{\partial k_B T} \ln(Z) \\ S &= -k_B \sum_n P_n \ln(P_n) \end{aligned} \quad (\text{B.60})$$

For a mixed state of M orthonormal quantum states with probability $1/M$ follows: $S = k_B \ln(M)$.

The distribution function for the internal states for a system in thermal equilibrium is the most probable function. This function can be found by taking the maximum of the function which gives the number of states with Stirling's equation:

$$\ln(n!) \approx n \ln(n) - n$$

and the conditions $\sum_k n_k = N$ and $\sum_k n_k W_k = W$. For identical particles which obey the Pauli exclusion principle the possible number of states is given by:

$$P = \prod_k \frac{g_k!}{n_k!(g_k - n_k)!} \quad (\text{B.61})$$

This results in the *Fermi-Dirac statistics*. For indistinguishable particles which *do not* obey the exclusion principle the possible number of states is given by:

$$P = N! \prod_k \frac{g_k^{n_k}}{n_k!} \quad (\text{B.62})$$

This results in the *Bose-Einstein statistics*.

The distribution functions which explain how particles are distributed over the different one-particle states k which are each g_k -fold degenerate depend on the spin of the particles. They are given by:

1. Fermi-Dirac statistics: $n_k = \frac{g_k}{\exp[(E_k - E_f)/k_B T] + 1}$
2. Bose-Einstein statistics: $n_k = \frac{g_k}{\exp[(E_k - E_f)/k_B T] - 1}$

where E_f is the Fermi-energy.

Appendix C

Electricity & Magnetism

C.1 The Maxwell Equations

The classical electromagnetic field is described by electric displacement \mathbf{D} , polarization \mathbf{P} , electric field strength \mathbf{E} , magnetic field strength \mathbf{H} , the magnetization \mathbf{M} and the magnetic flux density \mathbf{B} , via the Maxwell equations, in integral and differential forms:

$$\begin{aligned}
 \oiint_S \mathbf{D} \cdot d\mathbf{S} &= \iiint_{\Omega} \rho d\Omega & \nabla \cdot \mathbf{D} &= \rho \\
 \oiint_S \mathbf{B} \cdot d\mathbf{S} &= 0 & \nabla \cdot \mathbf{B} &= 0 \\
 \oint_{\ell} \mathbf{E} \cdot d\boldsymbol{\ell} &= -\frac{\partial}{\partial t} \iint_S \mathbf{B} \cdot d\mathbf{S} & \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
 \oint_{\ell} \mathbf{H} \cdot d\boldsymbol{\ell} &= \iint_S \left(\mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} \right) \cdot d\mathbf{S} & \nabla \times \mathbf{H} &= \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t}
 \end{aligned}
 \tag{C.1}$$

In the first two integral equations, Ω is the volume totally enclosed by surface S ; In the last two integral equations, S is the surface totally enclosed by line ℓ . In the above equations, ρ is the density of free electric charge and \mathbf{j} is the electric current density. \mathbf{D} , \mathbf{P} and \mathbf{E} depend on each other according to $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon \mathbf{E}$, while \mathbf{H} , \mathbf{M} and \mathbf{B} depend on each other according to $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}) = \mu \mathbf{H}$.

There is the law of charge conservation which is implicit in the above Maxwell equations (also in its integral and differential forms)

$$\oiint_S \mathbf{j} \cdot d\mathbf{S} + \frac{\partial}{\partial t} \oiint_S \mathbf{D} \cdot d\mathbf{S} = 0, \quad \nabla \cdot \mathbf{j} + \frac{\partial \rho}{\partial t} = 0
 \tag{C.2}$$

C.2 Force and Potential

The vector fields from a particle of charge Q_1 and velocity \mathbf{v} are

$$\mathbf{E}_1 = \frac{Q_1}{4\pi\epsilon_0} \frac{\mathbf{r}}{r^3} \left(1 - \frac{v^2}{c_0^2}\right), \quad \mathbf{B}_1 = \frac{\mu_0 Q_1}{4\pi} \frac{\mathbf{v} \times \mathbf{r}}{r^3} \left(1 - \frac{v^2}{c_0^2}\right) \quad (\text{C.3})$$

The force between two stationary (or quasi stationary, i.e., their velocities are far less than the speed of light) point charges Q_1 and Q_2 in a homogeneous space with a dielectric constant ϵ are given by:

$$\mathbf{F} = Q_2 \mathbf{E}_1 = \frac{Q_1 Q_2}{4\pi\epsilon_0} \frac{\mathbf{r}}{r^3} \quad (\text{C.4})$$

A particle with charge Q_1 experiences the so-called Lorentz force when moving at an instantaneous velocity \mathbf{v} in a \mathbf{B} field

$$\mathbf{F} = Q_1 \mathbf{v} \times \mathbf{B} \quad (\text{C.5})$$

The electromagnetic field can be described by a vector potential \mathbf{A} and a scalar potential ϕ

$$\mathbf{E} = -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A} \quad (\text{C.6})$$

The magnetic field, resulting from an electric current $\mathbf{j} = j d\boldsymbol{\ell}$ is given by the law of Biot-Savart, also known as the law of Laplace.

$$\mathbf{B} = \int \frac{\mu_0 j}{4\pi} \frac{d\boldsymbol{\ell} \times \mathbf{r}}{r^3} \quad (\text{C.7})$$

where \mathbf{r} is the spatial vector from the current $j d\boldsymbol{\ell}$ to the location at which \mathbf{B} is being calculated. If the current is time-dependent one has to take retardation into account that the substitution $j(t) \rightarrow j(t - r/c)$ has to be applied.

C.3 Electromagnetic Waves

By introducing a vector potential, \mathbf{A} , and a scalar potential, ϕ , the electric and magnetic fields can be obtained from the relations of

$$\begin{aligned} \mathbf{E} &= -\nabla\phi - \frac{\partial\mathbf{A}}{\partial t} \\ \mathbf{B} &= \nabla \times \mathbf{A} \end{aligned} \quad (\text{C.8})$$

The first and last Maxwell equations are automatically satisfied by the definitions. By the relation of

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$$

and in the Lorentz gauge of

$$\frac{1}{\mu} \nabla \cdot \mathbf{A} + \epsilon \frac{\partial \phi}{\partial t} = 0 \quad (\text{C.9})$$

we have the following equations for the vector and scalar potentials

$$\nabla^2 \mathbf{A} - \epsilon \mu \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu \mathbf{J} \quad (\text{C.10})$$

$$\nabla^2 \phi - \epsilon \mu \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\epsilon} \quad (\text{C.11})$$

The wave equation $\square \Psi(\mathbf{r}, t) = -f(\mathbf{r}, t)$ has the following general solution

$$\Psi(\mathbf{r}, t) = \int \frac{f(\mathbf{r}', t - |\mathbf{r} - \mathbf{r}'|/c)}{4\pi |\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \quad (\text{C.12})$$

where $c = 1/\sqrt{\epsilon\mu}$. When $\mathbf{J}(\mathbf{r}, t)$ and $\rho(\mathbf{r}, t)$ can be expressed as $\mathbf{J}(\mathbf{r}) \exp(-i\omega t)$ and $\rho(\mathbf{r}) \exp(-i\omega t)$, respectively, $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ have the similar forms of $\mathbf{A}(\mathbf{r}) \exp(-i\omega t)$ and $\phi(\mathbf{r}) \exp(-i\omega t)$ with:

$$\begin{aligned} \mathbf{A}(\mathbf{r}) &= \frac{\mu}{4\pi} \int \mathbf{J}(\mathbf{r}') \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] }{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \\ \phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon} \int \rho(\mathbf{r}') \frac{\exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] }{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \end{aligned} \quad (\text{C.13})$$

An ideal dipole that oscillates in time

$$\mathbf{p}(t) = \mathbf{p}_0 \cos(\omega t) \quad (\text{C.14})$$

The electric and magnetic fields, the Poynting flux, and angular distribution of this oscillating dipole are

$$\begin{aligned} \mathbf{E} &= -\theta_0 \frac{p_0}{4\pi\epsilon_0 r} \frac{\omega^2}{c_0^2} \sin\theta \cos(\omega t - \mathbf{k} \cdot \mathbf{r}) \\ \mathbf{B} &= -\phi_0 \frac{\mu_0 p_0}{4\pi r} \frac{\omega^2}{c_0} \sin\theta \cos(\omega t - \mathbf{k} \cdot \mathbf{r}) \\ \mathbf{S} &= \mathbf{r}_0 \frac{p_0^2}{16\pi^2 \epsilon_0 r^2} \frac{\omega^4}{c^3} \sin^2\theta \cos^2(\omega t - \mathbf{k} \cdot \mathbf{r}) \\ \langle \mathbf{S} \rangle_t &= \mathbf{r}_0 \frac{p_0^2 \sin^2\theta}{32\pi^2 \epsilon_0 r^2} \frac{\omega^4}{c^3} \\ \frac{dP}{d\Omega} &= r^2 \mathbf{r}_0 \cdot \langle \mathbf{S} \rangle_t = \frac{p_0^2 \sin^2\theta}{32\pi^2 \epsilon_0 r^2} \frac{\omega^4}{c^3} \end{aligned} \quad (\text{C.15})$$

in spherical coordinate, where \mathbf{r}_0 , $\boldsymbol{\theta}_0$ and $\boldsymbol{\phi}_0$ are the three unit vectors. Note that the above expressions are valid for the following conditions: the dipole dimension is much less than the distance to the dipole, it is also very small compared with the wavelength of radiation. The distance to the dipole is much longer than the wavelength.

The wave equations in matter, with $c_{\text{mat}} = (\varepsilon\mu)^{-1/2}$ the light speed in matter, are:

$$\begin{aligned} \left(\nabla^2 - \varepsilon\mu \frac{\partial^2}{\partial t^2} - \frac{\mu}{\rho} \frac{\partial}{\partial t} \right) \mathbf{E} &= 0 \\ \left(\nabla^2 - \varepsilon\mu \frac{\partial^2}{\partial t^2} - \frac{\mu}{\rho} \frac{\partial}{\partial t} \right) \mathbf{B} &= 0 \end{aligned} \quad (\text{C.16})$$

give, after substitution of monochromatic plane waves:

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)] \quad \text{and} \quad \mathbf{B} = \mathbf{B}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$$

the dispersion relation:

$$k^2 = \varepsilon\mu\omega^2 + \frac{i\mu\omega}{\rho} \quad (\text{C.17})$$

The first term arises from the displacement current, the second from the conductance current. If k is written in the form $k = k' + ik''$ it follows that:

$$k' = \omega \sqrt{\frac{1}{2}\varepsilon\mu} \sqrt{1 + \sqrt{1 + \frac{1}{(\rho\varepsilon\omega)^2}}} \quad \text{and} \quad k'' = \omega \sqrt{\frac{1}{2}\varepsilon\mu} \sqrt{-1 + \sqrt{1 + \frac{1}{(\rho\varepsilon\omega)^2}}} \quad (\text{C.18})$$

This results in a damped wave:

$$\mathbf{E} = \mathbf{E}_0 \exp(-k'' \mathbf{n} \cdot \mathbf{r}) \exp[i(k' \mathbf{n} \cdot \mathbf{r} - \omega t)] \quad (\text{C.19})$$

Appendix D

Solid State Physics

D.1 Crystal Structure

A lattice is defined by the 3 translation vectors \mathbf{a}_i , so that the atomic composition looks the same from each point \mathbf{r} and $\mathbf{r}' = \mathbf{r} + \mathbf{R}$, where \mathbf{R} is a translation vector given by: $\mathbf{R} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$ with u_i are integers. A lattice can be constructed from primitive cells. As a primitive cell one can take a parallelepiped, with volume

$$\Omega_{\text{cell}} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) \tag{D.1}$$

Because a lattice has a periodical structure the physical properties n which are connected with the lattice have the same periodicity (neglecting boundary effects):

$$n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r}) \tag{D.2}$$

This periodicity is suitable to use Fourier analysis: $n(\mathbf{r})$ is expanded as:

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G} \cdot \mathbf{r}) \tag{D.3}$$

with

$$n_{\mathbf{G}} = \frac{1}{\Omega_{\text{cell}}} \int_{\text{cell}} n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) d\mathbf{r} \tag{D.4}$$

\mathbf{G} is the *reciprocal lattice vector*. If \mathbf{G} is written as $\mathbf{G} = v_1\mathbf{b}_1 + v_2\mathbf{b}_2 + v_3\mathbf{b}_3$ with v_i as integers, it follows for the vectors \mathbf{b}_i , cyclically:

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_{i+1} \times \mathbf{a}_{i+2}}{\mathbf{a}_i \cdot (\mathbf{a}_{i+1} \times \mathbf{a}_{i+2})} \tag{D.5}$$

The set of \mathbf{G} -vectors determines the Röntgen diffractions: a maximum in the reflected radiation occurs if: $\Delta\mathbf{k} = \mathbf{G}$ with $\Delta\mathbf{k} = \mathbf{k} - \mathbf{k}'$. So: $2\mathbf{k} \cdot \mathbf{G} = G^2$. From this follows for parallel lattice planes (Bragg reflection) that for the maxima holds: $2d \sin(\theta) = n\lambda$.

The Brillouin zone is defined as a Wigner-Seitz cell in the reciprocal lattice.

D.2 Crystal Binding

A distinction can be made between 4 binding types:

1. van der Waals bond
2. Ion bond
3. Covalent or homopolar bond
4. Metallic bond

The interaction in a covalent bond depends on the relative spin orientations of the electrons constituting the bond. The potential energy for two parallel spins is higher than the potential energy for two antiparallel spins. Furthermore the potential energy for two parallel spins has sometimes no minimum. In that case binding is not possible.

D.3 Crystal Vibrations

For a lattice with one type of atoms and only nearest-neighbor interactions are taken into account, the force on atom s with mass M can then be written as:

$$F_s = M \frac{d^2 u_s}{dt^2} = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \quad (\text{D.6})$$

Assuming that all solutions have the same time-dependence $\exp(-i\omega t)$ this results in:

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \quad (\text{D.7})$$

Further it is postulated that: $u_{s\pm 1} = u \exp(isKa) \exp(\pm iKa)$. This gives: $u_s = \exp(iKsa)$. Substituting the latter two equations in the first results in a system of linear equations, which has only one solution if their determinant is 0. This gives:

$$\omega^2 = \frac{4C}{M} \sin^2\left(\frac{1}{2}Ka\right) \quad (\text{D.8})$$

Only vibrations with a wavelength within the first Brillouin Zone have a physical significance. This requires that $-\pi < Ka \leq \pi$. The group velocity of these vibrations is given by:

$$v_g = \frac{d\omega}{dK} = \sqrt{\frac{Ca^2}{M}} \cos\left(\frac{1}{2}Ka\right) \quad (\text{D.9})$$

and is 0 on the edge of a Brillouin Zone. Here, there is a standing wave.

For a lattice with two types of atoms, the solutions are:

$$\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2(Ka)}{M_1 M_2}} \quad (\text{D.10})$$

Connected with each value of K are two values of ω . The larger value describes the optical vibrational mode, the lower value the acoustical mode. In the optical mode, both types of ions oscillate in opposite phases, in the acoustical mode they oscillate in the same phase. This results in a much larger induced dipole moment for optical oscillations, and also a stronger emission and absorption of radiation. Furthermore each vibrational mode has three polarization directions, one longitudinal and two transversal.

D.4 Free Electron Fermi Gas

D.4.1 Thermal Heat Capacity

The solution with period L of the one-dimensional Schrödinger equation is:

$$\psi_n(x) = A \sin\left(\frac{2\pi x}{\lambda_n}\right)$$

with $n\lambda_n = 2L$. From this follows

$$E = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 \quad (\text{D.11})$$

In a linear lattice the only important quantum numbers are n and m . The *Fermi level* is the uppermost filled level, which has the *Fermi-energy* E_f . If n_f is the quantum number of the Fermi level, it can be expressed as: $2n_f = N$ so $E_f = \hbar^2\pi^2 N^2/8mL$. Here N is the total number of electrons. In three dimensions holds:

$$k_f = \left(\frac{3\pi^2 N}{\Omega}\right)^{1/3}, \quad E_f = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{\Omega}\right)^{2/3} \quad (\text{D.12})$$

The number of states with energy $\leq E$ is then: $N = \frac{\Omega}{3\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{3/2}$, and the density of states becomes

$$D(E) = \frac{dN}{dE} = \frac{\Omega}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} = \frac{3N}{2E} \quad (\text{D.13})$$

The heat capacity of the electrons is approximately 0.01 times the classical expected value $\frac{3}{2}Nk_B$. This is caused by the Pauli exclusion principle and the Fermi-Dirac distribution: only electrons within an energy range $\sim k_B T$ of the Fermi level are excited thermally. There is a fraction $\approx T/T_f$ excited thermally. The internal energy then becomes:

$$U \approx Nk_B T \frac{T}{T_f}, \quad C = \frac{\partial U}{\partial T} \approx Nk_B \frac{T}{T_f} \quad (\text{D.14})$$

A more accurate analysis gives:

$$C_{\text{electrons}} = \frac{1}{2} \pi^2 N k_B T / T_f \sim T$$

Together with the T^3 dependence of the thermal heat capacity of the phonons the total thermal heat capacity of metals is described by

$$C = \gamma T + AT^3$$

D.4.2 Electric Conductance

The equation of motion for the charge carriers is:

$$F = m \frac{d\mathbf{v}}{dt} = \hbar \frac{d\mathbf{k}}{dt} \quad (\text{D.15})$$

The variation of \mathbf{k} is given by

$$\delta\mathbf{k} = \mathbf{k}(t) - \mathbf{k}(0) = \frac{-e\mathbf{E}t}{\hbar}$$

If τ is the characteristic collision time of the electrons, $\delta\mathbf{k}$ remains stable if $t = \tau$.

$$\langle \mathbf{v} \rangle = \mu \mathbf{E} \quad (\text{D.16})$$

with $\mu = e\tau/m$ the mobility of the electrons. The current in a conductor is given by:

$$\mathbf{J} = nq\mathbf{v} = \sigma \mathbf{E} = \frac{\mathbf{E}}{\rho} = ne\mu \mathbf{E} \quad (\text{D.17})$$

D.5 Energy Bands

In the tight-bond approximation it is assumed that

$$\psi = e^{ikna} \phi(x - na)$$

from this follows for the energy:

$$\langle E \rangle = \langle \psi | H | \psi \rangle = E_{\text{at}} - \alpha - 2\beta \cos(ka)$$

This gives a cosine superimposed on the atomic energy, which can often be approximated by a harmonic oscillator. If it is assumed that the electron is nearly free one can postulate

$$\psi = e^{i\mathbf{k}\cdot\mathbf{r}}$$

i.e., a traveling wave. This wave can be decomposed into two standing waves:

$$\psi(+) = \exp(i\pi x/a) + \exp(-i\pi x/a) = 2 \cos(\pi x/a)$$

$$\psi(-) = \exp(i\pi x/a) - \exp(-i\pi x/a) = 2i \sin(\pi x/a)$$

The probability density $|\psi(+)|^2$ is high near the atoms of the lattice and low in between. The probability density $|\psi(-)|^2$ is low near the atoms of the lattice and high in between. Hence the energy of $\psi(+)$ is also lower than the energy of $\psi(-)$. Suppose that $V(x) = V \cos(2\pi x/a)$, then the bandgap is given by:

$$E_g = \int_0^1 V(x)[|\psi(+)|^2 - |\psi(-)|^2]dx = V \quad (\text{D.18})$$

Index

A

Acceleration effective mass, 31
Angular momentum, 4–5, 7, 142, 149,
388–389

B

Biaxially strain, 42
Bloch theorem, 1, 19–21, 50, 59, 75, 84, 130,
226, 353
Bloch wave function, 69, 363
Body-centered cubic lattices, 11
Bohr radius, 4, 6, 96–97, 141, 143–144, 160,
178, 324, 330, 348, 391
Boltzmann (electron wave) transport, 97, 100,
239
Bose-Einstein distribution, 394
Bowling parameter, 38
Bravais crystal, 10, 13, 44, 90, 137
Bravais lattice, 10, 13
Brillouin zone, 14, 32, 130, 135, 138, 288,
353, 399–400

C

Carrier-concentration effective mass, 32,
315–316
Cauchy stress tensor, 42
Cauchy's infinitesimal strain tensor, 42
Cayley form, 71, 377
Cladding layer, 347
Complementary metal-oxide-semiconductor,
CMOS, 190–191, 233, 253, 257–258
Complex conjugate, c.c., 114–116, 158, 211,
358
Compound semiconductor, 103
Conduction channel, 190, 237, 239–242,
244–247, 249–250, 252–254, 258
Conductivity effective mass, 31, 33

Core electron, 9–10, 302, 345–346
Coulomb blockade, 245, 258, 261
Crystal lattice and lattice basis, 10, 14, 17, 44,
89–91, 137
Crystal momentum, 118
Czochralski (CZ) technique, 15

D

Deformation potential, 34–35, 103, 170
 δ doping, 230–231, 233, 302, 345–346
Density of states, 32–33, 59–62, 82, 93, 98,
170, 180, 187, 200, 216, 233–236,
285–286, 338–339, 369, 373
Density-of-states effective mass, 32
Depletion layer, 219
Diamond crystal structure, 10
Dielectric coefficient, 323
Dielectric polarization, 158, 160, 162, 165,
324, 329
Diffusion coefficient, 90, 100–101, 192, 346
Diffusion length, 56
Distributed Bragg reflector, DBR, 399
Dynamic random access memory, DRAM, 2

E

Edge emission, 222
Effective mass, 29–33, 38, 53–54, 56–57, 93,
118, 136–137, 142–143, 147–148,
249–250, 276–280, 282–286, 306–307,
314–316, 353–355
Effective mass approximation, 53–54, 118,
137, 142, 147–148, 177, 307
Effective medium approximation, 25–26, 48
Einstein ratio, 101, 191
Einstein relation, 101, 191
Electron affinity, 24, 147, 188, 190
Electron-beam direct-writing technique, 3,
257–258

Electron-phonon interaction, 104–105,
107–108, 207, 209–213
Electron wavelength, 2
Elemental semiconductor, 103
Ellipsoidal band, 31
Energy band offset, 24
Energy dispersion relation, 85, 114
Envelope function, 1, 27–28, 52–53, 56–59,
92, 134, 140, 143–144, 160, 226, 275,
277, 311, 340, 353
Evanescent states, 108, 195, 209, 211–212
Exciton, x , 79, 111, 117, 134–135, 137–146,
157–163, 165–168, 172–173, 176, 298,
317, 323–325, 327–335, 348–349
Exciton binding energy, 141, 144, 146
Exciton Bohr radius, 141, 143, 324, 330, 348
Exciton polariton, 117, 162, 298, 323, 332

F

Fabry-Perot microcavity, 342
Face-centered cubic lattice, 11–12
Fermi level, 23, 89, 95–96, 102–103, 106–107,
187–188, 190, 208, 219, 228, 230–231,
315–316, 336–337, 353–355, 401
Field-effect transistor, v , 2, 185, 188, 230–231,
233, 239, 245, 248–249, 253, 255, 368
First-order perturbations, 28, 74, 78–79, 83,
85, 157–158, 167, 204
Fourier transform, 53, 138–139, 332
Frequency multiplier, 213–214

G

Gate length, 2, 236, 252
Gaussian wave packet, 71–72, 378
Gunn effect, 213

H

Harmonics, 5, 153, 179, 213, 295, 326,
389–390
Heterostructure, vi , 1, 3, 17–18, 39, 50, 53–56,
104, 185, 213–216, 218, 224, 249,
313–314, 343–344
Heterostructure barrier varactor, HBV, 185,
213–214, 216, 249
Heterostructure barrier varactor diode, HBV,
213
High-electron-mobility transistor, HEMT, 185,
224–226, 229–230, 243–245, 247, 263

I

Impurity state, 93–94, 96
Index guiding, 343
Infinitely deep quantum well, 62, 144–145,
272–274, 278, 305, 373
Interface diffusion, 18, 51
Inverse effective mass, 276–277, 279–280,
282–283

K

Kane parameter, 36
Kramers' theorem, 21

L

Large scale integration, LSI, 112, 262
Localized state, 107, 223, 366
Longitudinal effective mass, 31, 38, 276, 355
Luttinger parameters, 36

M

Maxwell equations, 113–114, 324, 395–396
Metal-organic chemical vapor deposition,
MOCVD, 3, 15, 18–19, 43, 310
Metal-oxide-semiconductor, MOSFET, v , 2,
188–191, 230–231, 252–255, 257, 262,
368
Misfit dislocation, 24, 40
Mobility, vi , 33, 67, 100–101, 185, 192,
224–226, 228–230, 233, 238, 243, 247,
263, 287, 320
Mole fraction, 26–27, 36, 47–48, 55
Molecular beam epitaxy, MBE, 3, 15, 17–19,
40, 200, 224, 230, 246, 310
Momentum operator, 27–28, 118, 141, 159,
384, 388
Monte Carlo scheme, 45, 170–172
Mott phase transition, 94, 354–355

N

Nanofabrication technique, 3

O

Optical absorption coefficient, 279, 302,
306–307
Optical grating, 271, 289, 294, 298, 307–308,
310, 312
Optical transition matrix, 35, 128, 131, 142,
163, 275–276, 302, 306, 322
Orbital angular momentum, 7, 388
Oscillator strength, 402

P

Pauli exclusion principle, 8, 68, 89, 93, 98,
117, 127, 193, 227, 296, 317, 394, 401

Photocurrent, 302, 305, 307–308, 310,
312–313, 316, 319–323
Photonic bandgap, 328
Photonic bandgap crystal, PBC, 323
Photonic crystal, 309, 323
Poisson effect, 234, 315, 368
Population inversion, 128, 133, 167, 336–337,
342–343, 345
Poynting vector, 114, 116–117, 165–166
Primitive vector, 10–13, 20

Q

Quantum cascade laser, 345
Quantum confinement, 57–58, 61, 133, 146,
160, 178, 243, 348
Quantum dot, QD, 43, 45–47, 61–62,
133–134, 146–148, 150, 160–163,
167–174, 257–261, 312, 318, 322–324,
328–330, 332–333, 348–350
Quantum dot cellular automata, QCA,
258–259, 261
Quantum effect device, 3
Quantum efficiency, 317
Quantum number, 4, 7, 20, 57, 138, 142, 401
Quantum well, QW, 46–48, 53–55, 59,
130–131, 133–134, 144–146, 223,
229–230, 271–279, 281–291, 299–308,
341, 346–347, 367–369, 373
Quantum well infrared photodetector, QWIP,
290–291, 294, 299–300, 302–303,
305–308
Quantum wire, QWR, 57, 59, 61–62, 71–73,
108, 132–134, 154–155, 238–239, 253,
255–257, 262–263, 307–308, 310–311,
368–369, 375–377

R

Radial Schrödinger equation, 6, 149
Random walking, 45
Reciprocal lattice vector, 13, 130, 399
Reciprocal space, 12–14
Recursion method, 234, 368
Reflection high energy electron diffraction,
RHEED, 18
Resonant cavity, 342
Resonant tunneling diode, RTD, 106, 185,
195–196, 198, 200, 208, 218, 339–340,
359
Resonant-tunneling light-emitting diode,
RTLED, 339
Rydberg constant, 4, 381

S

Schottky barrier, 213, 313
Schottky diode, 213
Schrödinger equation, 5–6, 19–20, 27–28,
68–71, 77, 92–93, 143, 168–169, 198,
234, 239–240, 259–260, 368, 385–386,
390–392
Second-order perturbations, 28
Secular determinant, 22
Secular equation, 22
Selection rule, 153, 276, 282, 307–308
Semiclassical picture (theory), 192
Semiconductor microelectronics, 2
Semiconductor optoelectronics, 2
Sequential tunneling, 199, 202
Shockley matrix, 35
Si-on-insulator, 253, 257
Silicon on insulator, SOI, 253, 257
Simple cubic lattice, 11, 14
Single electron transistor, SET, 257–258,
261–263
Slater determinant, 135, 177, 393
Soft lithography, 3
Spherical band, 31, 276
Spherical harmonics, 5, 153, 179, 389–390
Spherical symmetry, 5
Spin angular momentum, 7
Spin split off, 30, 33
Stark effect, 347, 367–368
Stranski-Krastanov growth, 40, 42–43
Superlattice, 18, 51, 195, 271, 287–289, 345,
362–363, 365
Surface emission, 51

T

Tight-binding model, 21–23, 55, 136, 148
Transfer-matrix method, 288, 363
Transition matrix, 35, 76, 87, 109, 121, 128,
131, 142, 163–164, 275–276, 302, 306,
321–322, 340
Transverse effective mass, 31, 38, 276, 355
Tunneling probability, 200–201, 206, 209–211,
314
Two-dimensional electron gas, 2DEG,
225–226, 228–230

U

Uniaxially strain, 43
Unit cells, 20–25, 44, 50–51, 57, 70, 86–87,
89–90, 104, 129–131, 137, 211

V

Valence-band offset, VBO, 36, 362
Valence electron, 9–10, 21–23, 91–92, 185

Valence-force-field (VFF) approach, 43
Varactor, 185, 213–218, 221, 223–224, 249
Varshni approximation, 36
Varshni parameters, 36
Vertical cavity surface emitting laser, VCSEL,
345
Virtual crystal approximation, 37, 56

W

Wannier function, 50–52, 92
Wave vector space, 12
Wavelength division multiplexing, 116, 165
Work function, 188, 190

Z

Zincblende crystal structure, 12, 22, 44