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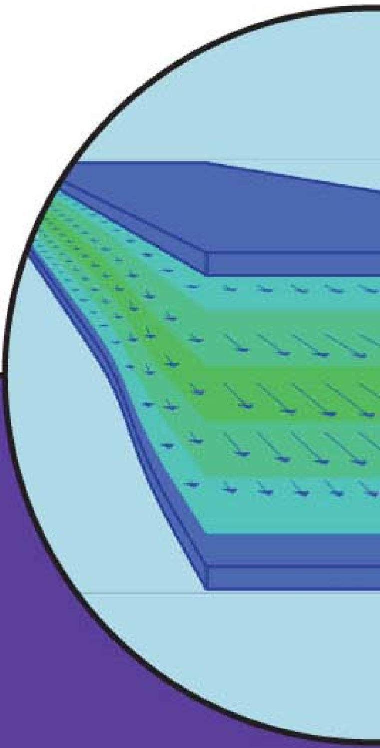
Theoretical Microfluidics



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Preface

This book on theoretical microfluidics has grown out from a set of lecture notes that I began writing in the summer of 2004. Much of the material has been tested in my teaching at the Technical University of Denmark at BSc-, MSc- and PhD-level lecture courses. The courses have been followed by students of both experimental and of theoretical inclination, and it is my experience that both groups of students have benefitted from the lecture notes. The more than 200 students I have been in contact with during the past three years have helped me shape the presentation of the material in a way that appears useful for them in their studies.

Microfluidics is a vast and rapidly evolving research field, and this textbook is in no way meant to be an exhaustive review. Instead, my ambition has been to write a final-year undergraduate textbook, which in a self-contained manner presents the basic theoretical concepts and methods used in the cross-disciplinary field of microfluidics, thus closing the gap between a number of basic physics textbooks and contemporary research in microfluidics. It is my hope that the presentation of basic theory, many worked-through examples and exercises with solutions, will get the advanced undergraduate students or first-year graduate students to understand the foundation of the theory, to be able to use the theory as a practical tool, and to be able to read research papers about microfluidics and lab-on-a-chip systems. Moreover, I have tried to write the text so that the students in principle can read the book as a self-study. The gaps in the logical and mathematical progression are deliberately made relatively small, thus making it possible for a student to fill them in by herself.

To write a textbook is hard work, but I have been so fortunate that many students and colleagues have helped me on the way with inspiring discussions and in many cases direct comments on the book as it evolved. In particular, I would like to thank my talented PhD students for many interesting joint research projects: Goran Goranović, Christian Mikkelsen, Anders Brask, Mads Jakob Jensen, Lennart Bitsch, Laurits Højgaard Olesen, Martin Heller and Misha Gregersen, as well as PhD students S. Melker Hagsäter and Kristian Smistrup, whom I have co-supervised. Also, my latest MSc students, Thomas Eilkær Hansen, Thomas Glasdam Jensen and Peder Skafte-Pedersen, have been very helpful. Among my local theory colleagues I have in particular enjoyed the feedback from Niels Asger Mortensen and Fridolin Okkels in connection with the courses on microfluidics that we have taught together. Several of my experimental colleagues have contributed with pictures and measurement results, and they have been thanked at each individual instance throughout the book.

In a broader context, I have received much inspiration from my colleagues at the Center for Fluid Dynamics at the Technical University of Denmark (Fluid•DTU) Hassan Aref, Tomas Bohr, Morten Brøns, Ole Hassager, Jens Nørkær Sørensen and Jens H. Walther, and the same can be said about my international colleagues Armand Ajdari, Daniel Attinger, Martin Bazant, Steffen Hardt, Ralph Lindken, Howard Stone and Patrick Tabeling.

Finally, I am grateful to Pernille and Christian for letting me use their beach house at Kandestederne as an author's refuge in two absolutely critical phases during my writing of this book: a couple of weeks in August 2004, when I wrote what is now the first couple of chapters in the book, and again several weeks in March, April and May 2007, when I wrote the last chapters and finished the book.

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Contents

List of symbols

Symbol	**Meaning**	**Definition**
$\equiv$	Equal to by definition	Eq. (1.4a)
$\approx$	Approximately equal to	Eq. (1.1)
$\propto$	Proportional to	Eq. (1.1)
$\ll, \gg$	Much smaller than, much bigger than	Section 1.5
$\cdot$	Scalar product	Eq. (1.11)
$:$	Tensor contraction, trace	Eq. (1.14)
$\times$	Cross-product or multiplication sign	Eqs. (1.24) and (1.7)
$\partial_j = \frac{\partial}{\partial x_j}$	Partial derivative after jth co-ordinate	Eq. (1.15)
$\boldsymbol{\nabla}$	Nabla or gradient operator	Eq. (1.17)
$\boldsymbol{\nabla}\cdot$	Divergence operator	Eq. (1.20)
$\boldsymbol{\nabla}\times$	Rotation operator	Eq. (1.25)
∇^2	Laplace operator	Eq. (1.18)
$\langle\bullet\|$, $\|\bullet\rangle$, $\langle\bullet\|\bullet\rangle$	Dirac bra-ket notion for functions	Eq. (1.42)
$\mathcal{A}, \mathcal{A}_n$	Area and effective area	Eqs. (3.25) and (4.15a)
$\mathcal{A}$	Absorbance	Eq. (16.22)
a	Radius of a cylinder or a sphere	Figs. 3.7 and 3.12
$\mathbf{B}$	Magnetic induction	Eqs. (11.1) and (16.1)
b	Stokes mobility	Eq. (11.15b)
Bo	Bond number	Eq. (7.30)
C_α	Dimensionless concentration, mass fraction	Eq. (5.16)
Ca	Capillary number	Eq. (7.31)
C_hyd	Compliance	Section 4.6
$\mathcal{C}$	Compactness	Eq. (4.19)
c, c_α	Concentration, molecules per volume	Eq. (5.24)
c_0	Speed of light in vacuum	Eq. (16.7)
c_a	Speed of sound	Eq. (15.12)
c_p	Specific heat, constant pressure	Eq. (2.65)
$\mathcal{D}$	Arbitrary differential operator	Eq. (15.12)
$\mathbf{D}$	Electric displacement	Eqs. (8.2) and (8.12)
D	Molecular diffusivity	Eqs. (5.9) and (5.21)
D_t	Material time derivative	Eq. (2.34)
D_th	Thermal diffusivity	Eq. (2.67)
$\mathrm{d}_t = \frac{\mathrm{d}}{\mathrm{d}t}$	Total time derivative	Eq. (1.16)

Symbol	**Meaning**	**Definition**
$\mathbf{E}$	Electric field	Eq. (8.2)
e	The exponential constant exp(1)	Eq. (1.29)
e	The elementary charge	Eq. (8.13)
F, F_1	Helmholtz free energy	Eqs. (D.2) and (D.4)
$\mathbf{F}_{\mathrm{DEP}}$	Dielectrophoretic force	Eqs. (10.23) and (10.43)
$\mathbf{F}_{\mathrm{drag}}$	Stokes' drag force	Section 3.7
$\mathbf{F}_{\mathrm{el}}$	Electric force	Eqs. (8.4) and (8.13)
f	Frequency	Eqs. (16.8b) and (E.5b)
$\mathbf{f}$	Force density	Section 2.2.6
G	Gibbs free energy	Eqs. (7.1) and (D.5)
$\mathbf{g}$, g	Gravitational acceleration	Section 3.1
$\mathbf{H}$	Magnetic field	Eqs. (11.5) and (16.1)
h	Channel height	Fig. 3.6
h	Planck's constant	Eq. (16.21)
i	The imaginary unit $\sqrt{-1}$	Eq. (1.29)
I_{eo}	Electro-osmotic current	Eq. (9.18)
I_{th}	Heat current	Eq. (12.58)
$\mathbf{J}$	Flux density, current density	Eq. (2.3)
$\mathbf{J}_{\mathrm{heat}}$	Heat-flux density	Eq. (2.55)
$K(\epsilon_1,\epsilon_2)$	Clausius–Mossotti factor	Eq. (10.19)
k_{B}	Boltzmann's constant	Eq. (6.50)
L	Length of a channel	Fig. 3.5
$\mathbf{M}$	Magnetization	Eq. (11.3)
N_{St}	Stokes number	Eq. (7.32)
$\mathcal{O}(x^n)$	Terms of order x^n and higher powers	Eq. (1.36)
$P(s)$	Normal distribution	Eq. (5.30)
$\mathbf{P}$	Polarization	Eqs. (8.8) and (10.1)
$\mathbf{p}$	Electric dipole moment	Eqs. (8.5b) and (10.18)
$\mathcal{P}$	Perimeter	Eq. (4.15b)
p^*	Standard pressure	Eq. (3.3)
$p(\mathbf{r},t)$	Pressure field	Sections 1.3.3 and 2.2.2
p_{eo}	Electro-osmotic pressure	Eq. (9.35b)
$P\acute{e}$	Péclet number	Eq. (5.53)
$P\acute{e}_{\mathrm{th}}$	Thermal Péclet number	Eq. (12.45)
Q, Q_{mass}	Volumetric and mass flow rates	Eqs. (3.21a) and (3.21b)
$\mathbf{q}$	2D mass flux vector	Eq. (14.34)
Q_{eo}	Electro-osmotic flow rate	Eqs. (9.15) and (9.35a)
$\mathcal{R}$	Half the hydraulic diameter	Eq. (3.26)
R_{hyd}	Hydraulic resistance	Chapter 4
$\mathbf{r}$	Position vector	Eq. (1.9)
Re	Reynolds number	Section 2.2.7
s	Entropy per unit mass	Section 2.3
T	Temperature	Eqs. (2.50) and (12.2)
$\mathcal{T}$	Transmittance	Eq. (16.22)
Tr	Trace of a tensor	Eq. (1.14)
$\mathcal{V}$, $\Delta\mathcal{V}$	Volume	Eq. (1.4a)
$\mathbf{v}(\mathbf{r},t)$	Eulerian velocity field	Section 1.3.3
$\mathbf{v}(\mathbf{r}(t),t)$	Lagrangian velocity field	Section 1.3.3

Symbol	**Meaning**	**Definition**
$V_{\mathrm{LJ}}(\mathbf{r})$	Lennard-Jones potential	Eqs. (1.54) and (17.36)
v_{eo}	Electro-osmotic velocity	Eq. (9.11)
Z	Integer valence number	Eq. (8.13)
Z	Acoustic impedance	Eq. (15.61)
Z_1, Z_N	Single- and N-particle partition function	Section D.1
α	Perturbation parameter	Section 1.5
α_{p}	Permeability of a porous medium	Eq. (14.39)
β	Dimensionless viscosity ratio	Eq. (2.19c)
Γ	Radius ratio	Eq. (10.30)
γ	Surface tension	Eq. (7.2)
γ	Dimensionless damping coefficient	Eqs. (15.38) and (16.14)
$\dot{\gamma}_{ij}$	Shear rate tensor	Eq. (2.46a)
δ	Dimensionless extinction coefficient	Eq. (6.42a)
δ_{ij}	Kronecker delta	Eq. (1.22)
ε	Energy per unit mass	Section 2.3.1
ϵ,ϵ_0	Electric permittivity	Eq. (8.12)MDeD
$\epsilon(\omega)$	Complex dielectric function	Eq. (10.42)
ϵ_{ijk}	Levi–Civita symbol	Eq. (1.23)
ζ	Dimensionless z co-ordinate	Eq. (3.60)
ζ	Second viscosity	Eq. (2.19b)
ζ	Zeta-potential	Eq. (8.21)
η	Dimensionless y co-ordinate	Eq. (3.60)
η	Dynamic viscosity	Eq. (2.19a)
η^*	Standard dynamic viscosity	Eq. (3.61)
Θ	Dimensionless temperature difference	Eq. (12.2)
θ	Polar angle	Section C.3
κ	Thermal conductivity	Eq. (2.55)
$\kappa(\mathbf{r})$, $\kappa(s)$	Curvature of surfaces and curves	Eqs. (7.10) and (7.11)
λ	Wavelength	Appendix E
λ^*	Size of a fluid particle	Eq. (1.2)
$\lambda(\xi)$	Shape perturbation function	Eqs. (3.69) and (14.4)
λ_{D}	Debye length	Eq. (8.26)
λ_{s}	Navier slip length	Eq. (17.1)
μ, μ_{r}	Magnetic and relative magnetic permeability	Eqs. (11.8b) and (16.2b)
μ_0	Magnetic permeability of vacuum	Eq. (16.9)
μ_{eo}	Electro-osmotic mobility	Eq. (9.12)
μ_{ion}	Ionic mobility	Eq. (8.15)
ν	Kinematic viscosity	Eq. (5.44)
ξ	Dimensionless x co-ordinate	Eqs. (3.60) and (14.4)
Π_{ij}	Momentum flux density tensor	Eq. (2.15)
$\rho(\mathbf{r},t)$	Density field	Sections 1.3.3 and 2.1
ρ^*	Standard density	Eq. (3.6)
ρ_{el}	Electric charge density	Eqs. (8.3b) and (8.23)
σ_{ij}	Full stress tensor	Eq. (2.26)
σ'_{ij}	Viscous stress tensor	Eq. (2.18)
σ_{el}	Electric conductivity	Eqs. (8.2d) and (16.4)
σ_{ion}	Ionic conductivity	Eq. (8.18)

Symbol	**Meaning**	**Definition**
τ	Characteristic time scale	Eq. (6.11), (7.35),(12.16b)
τ_{th}	Thermal diffusion time	Eq. (12.16a)
ϕ	Azimuthal angle	Sections C.2 and C.3
ϕ, ϕ_i	Velocity potential	Eq. (13.6), (15.3), (15.15)
ϕ_{eq}, ϕ_{ext}	Equilibrium and external electric potential	Eq. (9.2)
ϕ_{dip}	Potential from a point dipole	Eq. (10.6)
χ	Electric susceptibility	Eqs. (8.12) and (10.1)
χ	Magnetic susceptibility	Eq. (11.7)
ψ	Stream function	Eq. (6.32)
Ω	Region of interest in 2D or 3D	Eq. (2.1)
$\partial\Omega$	Surface of region Ω	Eq. (2.1)
$\boldsymbol{\omega}$	Vorticity	Eq. (2.43)
ω	Angular frequency	Eq. (E.5b)
ω_{c}	Critical dielectric frequency	Eq. (10.45)
ω_{D}	Debye frequency	Eqs. (8.45) and (14.52c)
ᚠ	Imprint speed ratio	Exercise 17.6

1

Basic concepts in microfluidics

Theoretical microfluidics deals with the theory of flow of fluids and of suspensions in submillimeter-sized systems influenced by external forces. Although an old discipline in hydrodynamics, the scientific and technological interest in and development of microfluidics has been particularly significant during the past decade and a half following the emerging and rapidly evolving field of lab-on-a-chip systems. This field is mainly driven by technological applications, the vision being to develop entire bio/chemical laboratories on the surface of silicon or polymer chips. Many of the amazing techniques developed over the past fifty years in connection with the silicon-based microelectronics industry are now used to fabricate lab-on-chip systems. In recent years, also polymer-based lab-on-a-chip systems have emerged, and these systems promise cheaper and faster production cycles. As microfluidic technology advances the demand for better theoretical insight grows, and this has been one of the motivating factors behind this book.

1.1 Lab-on-a-chip technology

There are several advantages of scaling down standard laboratory setups by a factor of 1000 or more from the decimeter scale to the 100 µm scale. One obvious advantage is the dramatic reduction in the amount of required sample. A linear reduction by a factor of 10^3 amounts to a volume reduction by a factor of 10^9, so instead of handling 1 L or 1 mL a lab-on-a-chip system could easily deal with as little as 1 nL or 1 pL. Such small volumes allow for very fast analysis, efficient detection schemes, and analysis, even when large amounts of sample are unavailable. Moreover, the small volumes makes it possible to develop compact and portable systems that might ease the use of bio/chemical handling and analysis systems tremendously. Finally, as has been the case with microelectronics, it is the hope by mass production to manufacture very cheap lab-on-a-chip systems.

Lab-on-a-chip (LOC) systems can be thought of as the natural generalization of the existing electronic integrated circuits and microelectromechanical systems (MEMS). Why confine the systems to contain only electric and mechanical parts? Indeed, a lab-on-chip system can really be thought of as the shrinking of an entire laboratory to a chip. Two examples of a systems evolving in that direction are shown in Fig. 1.1: In panel (a) is shown the CalTech microfluidics large-scale integration chip containing 256 subnanoliter reaction chambers controlled by 2056 on-chip microvalves, while in panel (b) is shown the MIC-DTU integrated optochemical lab-on-a-chip system containing optical (lasers and waveguides), chemical (channels and mixers), and electronic (photodiodes) components. Perhaps, only our imagination sets the limits of what could be in a lab-on-a-chip system. It is expected

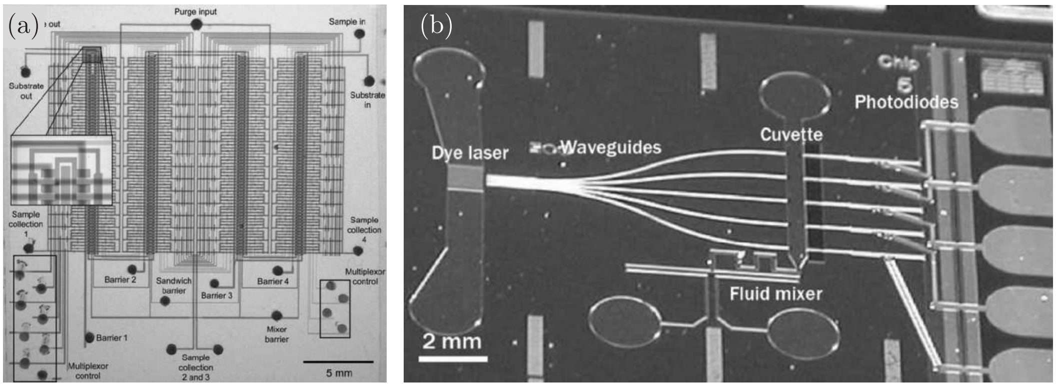

Fig. 1.1 (a) An optical micrograph of a 27 mm by 27 mm polydimethylsiloxane-based (PDMS) large-scale integrated microfluidic comparator containing 256 subnanoliter reaction chambers and 2056 microvalves fabricated at CalTech by Thorsen *et al.*, Science **298**, 580-584 (2002), reprinted with permission from AAAS. (b) An optical micrograph of a 15 mm by 20 mm integrated opto-chemical lab-on-a-chip system for optical analysis of chemical reactions fabricated at MIC-DTU by Balslev *et al.*, Lab Chip **6**, 213-217 (2006), reproduced by permission of The Royal Society of Chemistry. The system is a hybrid polymer/silicon device made on a silicon substrate containing the integrated photodiodes, while the laser, waveguides, mixer and cuvette are made in a SU-8 polymer film on top of the substrate.

that lab-on-a-chip systems will have great impact in biotechnology, pharmacology, medical diagnostics, forensics, environmental monitoring and basic research.

The fundamental laws of Nature underlying our understanding of the operation of lab-on-a-chip systems are all well known. Throughout the book we shall draw on our knowledge from mechanics, fluid dynamics, acoustics, electromagnetism, thermodynamics and physical chemistry. What is new, however, is the interplay between many different forces and the change of the relative importance of these forces as we pass from the m- and mm-sized macrosystems to µm- and nm-sized micro- and nanosystems.

1.2 Scaling laws in microfluidics

When analyzing the physical properties of microsystems, it is helpful to introduce the concept of scaling laws. A scaling law expresses the variation of physical quantities with the size ℓ of the given system or object, while keeping other quantities such as time, pressure, temperature, *etc.* constant. As an example, consider volume forces, such as gravity and inertia, and surface forces, such as surface tension and viscosity. The basic scaling law for the ratio of these two classes of forces can generally be expressed by

$$\frac{\text{surface forces}}{\text{volume forces}} \propto \frac{\ell^2}{\ell^3} = \ell^{-1} \underset{\ell\to 0}{\longrightarrow} \infty. \tag{1.1}$$

This scaling law implies that when scaling down to the microscale in lab-on-a-chip systems, the volume forces, which are very prominent in our daily life, become largely unimportant. Instead, the surface forces become dominant, and as a consequence, we must rebuild our intuition and be prepared for some surprises on the way.

Table 1.1 The scaling laws as a function of a typical length scale, object size or distance ℓ for a number of physical quantities studied in this book.

Area	ℓ^2	Eq. (1.1)	Time	ℓ^0	Section 1.2
Volume	ℓ^3	Eq. (1.1)	Velocity	ℓ^1	Section 1.2
Rel. fluctuations	$\ell^{-\frac{1}{2}}$	Exercise 1.3	Hydrostatic pressure	ℓ^1	Eq. (3.3)
Reynolds number Re	ℓ^2	Eq. (2.39)	Hydraulic resistance	ℓ^{-4}	Table 4.1
Péclet number	ℓ^2	Eq. (5.53)	Stokes drag	ℓ^1	Eq. (3.128)
Diffusion time	ℓ^2	Eq. (5.10)	Particle diffusion const.	ℓ^{-1}	Eq. (6.49)
Fluid acceleration time	ℓ^2	Eq. (6.25)	Taylor dispersion time	ℓ^{-2}	Eq. (5.71)
Young–Laplace pressure	ℓ^{-1}	Eq. (7.8)	Contact angle	ℓ^0	Eq. (7.14)
Bond number Bo	ℓ^2	Eq. (7.30)	Capillary rise height	ℓ^{-1}	Eq. (7.21)
Marangoni force	ℓ^{-1}	Eq. (7.39)	Capillary speed	ℓ^1	Eq. (7.36)
Electric field	ℓ^{-1}	Eq. (8.3a)	EO velocity	ℓ^{-1}	Eq. (9.11)
Ionic mobility	ℓ^{-1}	Eq. (8.15)	EO mobility	ℓ^0	Eq. (9.12)
Debye length	ℓ^0	Eq. (8.26)	EO flow rate	ℓ^1	Eq. (9.35a)
Debye frequency	ℓ^{-1}	Eq. (8.45)	EO pressure	ℓ^{-2}	Eq. (9.35b)
DEP force, particle	ℓ^3	Eq. (10.23)	MAP force, particle	ℓ^3	Eq. (11.13)
DEP force, system	ℓ	Eq. (10.31)	MAP force, system	ℓ	Eq. (11.13)
Thermal diffusion time	ℓ^2	Eq. (12.16a)	Acoustic impedance	ℓ^0	Eq. (15.61)
Thermal resistance	ℓ^{-1}	Eq. (12.59)	Acoustic radiation force	ℓ^3	Eq. (15.81)
Thermal capacitance	ℓ^3	Eq. (12.61)	Optical absorbance	ℓ^1	Eq. (16.25b)
Thermal RC-time	ℓ^2	Eq. (12.63)	Optical damping coeff.	ℓ^0	Eq. (16.14)

In Table 1.1 are listed the scaling laws for a number of physical quantities studied in this book. Depending on the context the length scale ℓ is either controlling all lengths in the system while maintaining constant aspect ratios or it represents a single object-size or -distance, which is being downscaled while maintaining all other lengths of the system. The table gives a first impression of the intricate interplay between the many physical forces present in microfluidic systems.

1.3 Fluids and fields

The main purpose of a lab-on-a-chip system is to handle fluids. A fluid, i.e. either a liquid or a gas, is characterized by the property that it will deform continuously and with ease under the action of external forces. The shape of a fluid is determined by the vessel containing it, and different parts of the fluid may be rearranged freely without affecting the macroscopic properties of it. In a fluid the presence of shear forces, however small in magnitude, will result in large changes in the relative positions of the fluid elements. In contrast, the changes in the relative positions of the atoms in a solid remain small under the action of any small external force. When applied external forces cease to act on a fluid, it will not necessarily retract to its initial shape. This property is also in contrast to a solid, which relaxes to its initial shape when no longer influenced by (small) external forces.

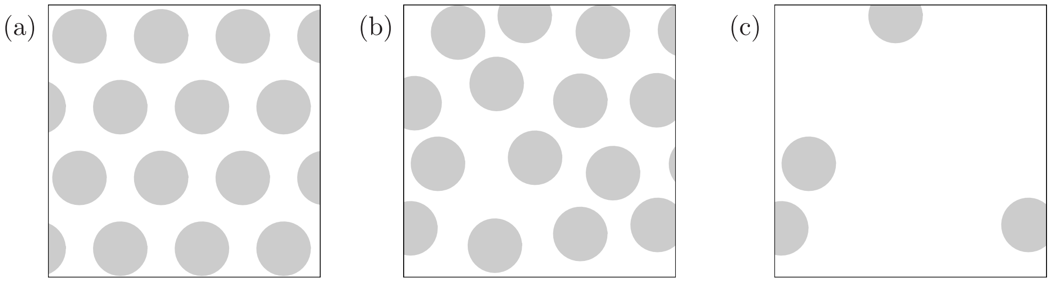

Fig. 1.2 (a) A sketch of a typical solid with 0.1 nm wide molecules (atoms) and a lattice constant of 0.3 nm. The atoms oscillate around the indicated equilibrium points forming a regular lattice. (b) A sketch of a liquid with the same molecules and same average intermolecular distance 0.3 nm as in panel (a). The atoms move around in a thermally induced irregular pattern. (c) A sketch of a gas with the same atoms as in panel (a). The average interatomic distance is 3 nm, and the motion is free between the frequent interatomic collisions.

1.3.1 Fluids: liquids and gases

The two main classes of fluids, the liquids and the gases, differ primarily by the densities and by the degree of interaction between the constituent molecules as sketched in Fig. 1.2. The density $\rho_{\mathrm{gas}} \approx 1\ \mathrm{kg\,m^{-3}}$ of an ideal gas is so low, at least a factor of 10^3 smaller than that of a solid, that the molecules move largely as free particles that only interact by direct collisions at atomic distances, ≈ 0.1 nm. The relatively large distance between the gas molecules, ≈ 3 nm, makes the gas compressible. The density $\rho_{\mathrm{liq}} \approx 10^3\ \mathrm{kg\,m^{-3}}$ of a liquid is comparable to that of a solid, i.e. the molecules are packed as densely as possible with a typical average intermolecular distance of 0.3 nm, and a liquid can, for many practical purposes, be considered incompressible.

The intermolecular forces in a liquid are of quite an intricate quantum and electric nature since each molecule is always surrounded by a number of molecules within atomic distances. In model calculations of simple liquids many features can be reproduced by assuming the basic Lennard-Jones pair-interaction potential, $V_{\mathrm{LJ}}(r) = 4\varepsilon\big[(\sigma/r)^{12} - (\sigma/r)^{6}\big]$, between any pair of molecules. Here, r is the distance between the molecules, while the maximal energy of attraction ε and the collision diameter σ are material parameters typically of the order $100\ \mathrm{K}\times k_{\mathrm{B}}$ and 0.3 nm, respectively. The corresponding intermolecular force is given by the derivative $F_{\mathrm{LJ}}(r) = -\mathrm{d}V_{\mathrm{LJ}}/\mathrm{d}r$. The Lennard-Jones potential is shown in Fig. 1.3(a) and discussed further in Exercise 1.2.

At short time intervals and up to a few molecular diameters the molecules in a liquid are ordered almost as in a solid. However, whereas the ordering in solids remains fixed in time and space,[1] the ordering in liquids fluctuates. In some sense the thermal fluctuations are strong enough to overcome the tendency to order, and this is the origin of the ability of liquids to flow.

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[1] The molecules in a solid execute only small, thermal oscillations around equilibrium points well described by a regular lattice.

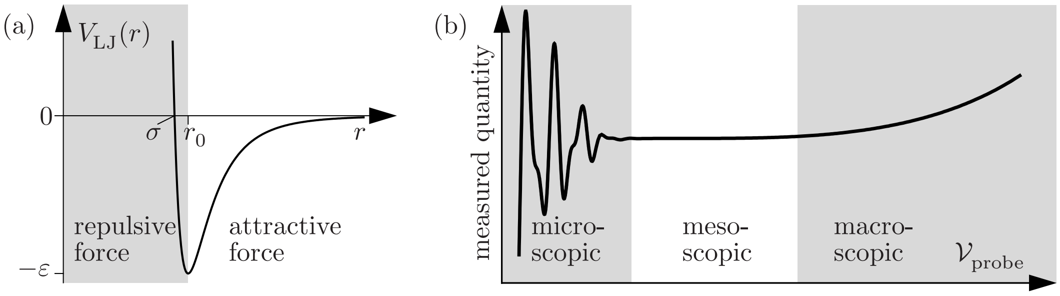

Fig. 1.3 (a) The Lennard-Jones pair-potential $V_{\mathrm{LJ}}(r)$ often used to describe the interaction potential between two molecules at distance r, see also Exercise 1.2. For small distances, $r < r_0 \approx 0.3$ nm the interaction forces are strongly repulsive (gray region), while for large distances, $r > r_0$, they are weakly attractive. (b) A sketch adopted from Batchelor (2000) of some measured physical quantity of a liquid as a function of the volume $\mathcal{V}_{\mathrm{probe}}$ probed by some instrument. For microscopic probe volumes (left gray region) large molecular fluctuations will be observed. For mesoscopic probe volumes (white region) a well-defined local value of the property can be measured. For macroscopic probe volumes (right gray region) gentle variations in the fluid due to external forces can be observed.

1.3.2 The continuum hypothesis and fluid particles

Although fluids are quantized on the length scale of intermolecular distances (of the order 0.3 nm for liquids and 3 nm for gases), they appear continuous in most lab-on-a-chip applications, since these typically are defined on macroscopic length scales of the order 10 µm or more. In this book we shall therefore assume the validity of the continuum hypothesis, which states that the macroscopic properties of a fluid is the same if the fluid were perfectly continuous in structure instead of, as in reality, consisting of molecules. Physical quantities such as the mass, momentum and energy associated with a small volume of fluid containing a sufficiently large number of molecules are to be taken as the sum of the corresponding quantities for the molecules in the volume.

The continuum hypothesis leads to the concept of fluid particles, the basic constituents in the theory of fluids. In contrast to an ideal point particle in ordinary mechanics, a fluid particle in fluid mechanics has a finite size. But how big is it? Well, the answer to this question is not straightforward. Imagine, as illustrated in Fig. 1.3(b), that we probe a given physical quantity of a fluid with some probe sampling a volume $\mathcal{V}_{\mathrm{probe}}$ of the fluid at each measurement. Let $\mathcal{V}_{\mathrm{probe}}$ change from (sub-)atomic to macroscopic dimensions. At the atomic scale (using, say, a modern AFM or STM tool) we would encounter large fluctuations due to the molecular structure of the fluid, but as the probe volume increases we soon enter a size where steady and reproducible measurements are obtained. This happens once the probe volume is big enough to contain a sufficiently large number of molecules, such that well-defined average values with small statistical fluctuations are obtained. As studied in Exercise 1.3 a typical possible side length λ^* in a cubic fluid particle in a liquid is

$$\lambda^* \approx 10 \text{ nm}, \ \text{(for a liquid)}. \tag{1.2}$$

Such a liquid particle contains approximately 4×10^4 molecules and exhibits number fluctuations of the order 0.5%. For a fluid particle in a gas λ^* is roughly ten time larger. If the size of the fluid particle is taken too big the probe volume could begin to sample regions of the fluid with variations in the physical properties due to external forces. In that case we are beyond the concept of a constituent particle and enter the regime we actually would like to study, namely, how do the fluid particles behave in the presence of external forces.

A fluid particle must thus be ascribed a size λ^* in the mesoscopic range. It must be larger than microscopic lengths ($\simeq 0.3$ nm) to contain a sufficiently large number of molecules, and it must be smaller than macroscopic lengths ($\simeq 10$ µm) over which external forces change the property of the fluid. Of course, this does not define an exact size, and in fluid mechanics it is therefore natural to work with physical properties per volume, such as mass density, energy density, force density and momentum density. In such considerations the volume is taken to the limit of a small, but finite, fluid-particle volume, and not to the limit of an infinitesimal volume.

The continuum hypothesis breaks down when the system under consideration approaches the molecular scale. This happens in nanofluidics, e.g. in liquid transport through nanopores in cell membranes or in artificially made nanochannels.

1.3.3 The velocity, pressure and density field

Once the concept of fluid particles in a continuous fluid has been established we can move on and describe the physical properties of the fluid in terms of fields. This can basically be done in two ways, as illustrated in Fig. 1.4 for the case of the velocity field. In these notes we shall use the Eulerian description, Fig. 1.4(a), where one focuses on fixed points $\mathbf{r}$ in space and observes how the fields evolve in time at these points, i.e. the position $\mathbf{r}$ and the time t are independent variables. The alternative is the Lagrangian description, Fig. 1.4(b), where one follows the history of individual fluid particles as they move through the system, i.e. the co-ordinate $\mathbf{r}_a(t)$ of particle a depends on time.

In the Eulerian description the value of any field variable $F(\mathbf{r},t)$ is defined as the average value of the corresponding molecular quantity $F_\mathrm{mol}(\mathbf{r}',t)$ for all the molecules contained in some liquid particle of volume $\Delta\mathcal{V}(\mathbf{r})$ positioned at $\mathbf{r}$ at time t,

$$F(\mathbf{r},t) = \big\langle F_\mathrm{mol}(\mathbf{r}',t)\big\rangle_{\mathbf{r}'\in\Delta\mathcal{V}(\mathbf{r})}. \tag{1.3}$$

If we for brevity let m_i and $\mathbf{v}_i$ be the mass and the velocity of molecule i, respectively, and

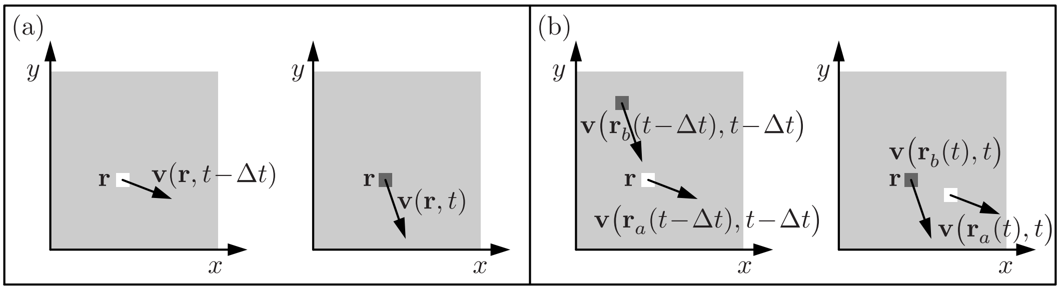

Fig. 1.4 (a) The velocity field $\mathbf{v}(\mathbf{r},t)$ in the Eulerian description at the point $\mathbf{r}$ at the two times $t-\Delta t$ and t. The spatial co-ordinates $\mathbf{r}$ are independent of the temporal co-ordinate t. (b) The Lagrangian velocity fields $\mathbf{v}\big(\mathbf{r}_a(t),t\big)$ and $\mathbf{v}\big(\mathbf{r}_b(t),t\big)$ of fluid particles a (white) and b (dark gray). The particles pass the point $\mathbf{r}$ at time $t-\Delta t$ and t, respectively. The particle co-ordinates $\mathbf{r}_{a,b}(t)$ depend on t. Note that $\mathbf{r}_a(t-\Delta t) = \mathbf{r}$ and $\mathbf{r}_b(t) = \mathbf{r}$.

furthermore let $i \in \Delta\mathcal{V}$ stand for all molecules i present inside the volume $\Delta\mathcal{V}(\mathbf{r})$ at time t, then the definition of the density $\rho(\mathbf{r},t)$ and the velocity field $\mathbf{v}(\mathbf{r},t)$ can be written as

$$\rho(\mathbf{r},t) \equiv \frac{1}{\Delta\mathcal{V}} \sum_{i\in\Delta\mathcal{V}} m_i, \tag{1.4a}$$

$$\mathbf{v}(\mathbf{r},t) \equiv \frac{1}{\rho(\mathbf{r},t)\Delta\mathcal{V}} \sum_{i\in\Delta\mathcal{V}} m_i\mathbf{v}_i. \tag{1.4b}$$

Here, we have introduced the "equal-to-by-definition sign" $\equiv$. Notice how the velocity is defined through the more fundamental concept of momentum. Through the technique of micro particle-image velocity, micro-PIV, see Santiago *et al.* (1998), it is possible to measure the velocity field in a transparent microfluidic device. Microparticles with diameters of the order 1 µm are suspended in the flow to be measured. Their positions are recorded as gray-scale values in a CCD camera through an optical microscope using either either transmitted or reflected light. Two pictures are recorded by sending two light pulses in quick succession of the order milliseconds apart at time t_1 and t_1, and the corresponding light intensities in each CCD camera pixel positioned at $\mathbf{r}$ are denoted $I_1(\mathbf{r})$ and $I_2(\mathbf{r})$. The CCD pixel array is divided into a number of interrogartion areas n, and for each of those a cross-correlation function $R_n(\Delta\mathbf{r})$ is defined as the average over all pixel co-ordinates in the given interrogation area n as $R_n(\Delta\mathbf{r}) \equiv \langle I_1(\mathbf{r})I_2(\mathbf{r}+\Delta\mathbf{r})\rangle_n$, where $\Delta\mathbf{r}$ is some pixel displacement vector. The value $\Delta\mathbf{r}_n$ of $\Delta\mathbf{r}$ that maximizes $R_n(\Delta\mathbf{r})$ is a statistical measure of the overall displacement of the fluid inside the given interrogation area n. Thus the average flow velocity $\mathbf{v}_n$ of that area is given by

$$\mathbf{v}_n \equiv \frac{\Delta\mathbf{r}_n}{t_2 - t_1}. \tag{1.5}$$

Examples of micro-PIV measurements of velocity fields can be seen in Figs. 15.4 and 15.5.

In general, the field variables in microfluidics can be scalars (such as density ρ, viscosity η, pressure p, temperature T, and free energy $\mathcal{F}$), vectors (such as velocity $\mathbf{v}$, current density $\mathbf{J}$, pressure gradient $\boldsymbol{\nabla}p$, force densities $\mathbf{f}$, and electric fields $\mathbf{E}$) and tensors (such as stress tensor σ and velocity gradient $\boldsymbol{\nabla}\mathbf{v}$).

To obtain a complete description of the state of a moving fluid it is necessary to know the three components of the velocity field $\mathbf{v}(\mathbf{r},t)$ and any two of the thermodynamical variables of the fluid, e.g. the pressure field $p(\mathbf{r},t)$ and the density field $\rho(\mathbf{r},t)$. All other thermodynamical quantities can be derived from these fields together with the equation of state of the fluid.

1.4 SI units and mathematical notation

Notation is an important part in communicating scientific and technical material. Especially in fluid mechanics the mathematical notation is important due to the involved many-variable differential calculus on the scalar, vector and tensor fields mentioned in the previous section. Instead of regarding units and notation as an annoying burden the student should instead regard it as part of the trade that needs to be mastered by the true professional. Learn the basic rules, and stick to them thereafter.

1.4.1 SI units

Throughout these notes we shall use the SI units. If not truly familiar with this system, the name and spelling of the units, or the current best values of the fundamental physical constants of Nature, the reader is urged to consult the websites of the Bureau International des Poids et Mesures (BIPM) or the National Institute of Standards and Technology (NIST) for constants, units, and uncertainty at

$$\text{http://www.bipm.fr/en/si/}\,, \tag{1.6a}$$

$$\text{http://physics.nist.gov/cuu/}\,. \tag{1.6b}$$

A scalar physical variable is given by a number of significant digits, a power of ten and a proper SI unit. The power of ten can be moved to the unit using prefixes such as giga, kilo, micro, atto, *etc.* The SI unit can be written in terms of the seven fundamental units or suitable derived units. As an example the viscosity η of water at 20 ℃ is written as

$$\eta = 1.002 \times 10^{-3}\ \mathrm{kg\,m^{-1}s^{-1}} = 1.002\ \mathrm{mPa\,s}. \tag{1.7}$$

Note the multiplication sign before the power of ten and the space after it, and note that the SI units are written in roman and *not in italics.* Unfortunately, most typesetting systems will automatically use italics for letters written in equations. Note also the space inserted between the units. Be aware that even though many units are capitalized, as are the names of the physicists that gave rise to them, e.g. Pa and Pascal, the unit itself is never capitalized when written in full, e.g. pascal. Also, the unit is written pascal without plural form whether there is one, five or 3.14 of them.

There will be two exceptions from the strict use of SI units. Sometimes, just as above, temperatures will be given in °C, so be careful when inserting values for temperature in formulae. Normally, a temperature T in an expression calls for values in kelvin. The other exception from SI units is the atomic unit of energy, electronvolt (eV),

$$1\ \mathrm{eV} = 1.602 \times 10^{-19}\ \mathrm{J} = 0.1602\ \mathrm{aJ}. \tag{1.8}$$

Note that it would be possible to use attojoule instead of electronvolt, but this is rarely done.

1.4.2 Vectors, derivatives and the index notation

The mathematical treatment of microfluidic problems is complicated due to the presence of several scalar, vector and tensor fields and the non-linear partial differential equations that govern them. To facilitate the treatment some simplifying notation is called for.

First, a suitable co-ordinate system must be chosen. We shall encounter three, as summarized in Appendix C: Cartesian co-ordinates (x, y, z) with corresponding basis vectors $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$; cylindrical co-ordinates (r, ϕ, z) with corresponding basis vectors $\mathbf{e}_r$, $\mathbf{e}_\phi$, and $\mathbf{e}_z$; and spherical co-ordinates (r, θ, ϕ) with corresponding basis vectors $\mathbf{e}_r$, $\mathbf{e}_\theta$, and $\mathbf{e}_\phi$. All sets of basis vectors are orhtonormal, which means that the involved vectors have unity length and are mutually orthogonal, but the Cartesian basis vectors are special since they are constant in space, whereas all other sets of basis vectors depend on position in space. For simplicity, we postpone the usage of the curvilinear co-ordinates to later chapters and use only Cartesian co-ordinates in the following.

The position vector $\mathbf{r} = (r_x, r_y, r_z) = (x, y, z)$ can be written as

$$\mathbf{r} = r_x\,\mathbf{e}_x + r_y\,\mathbf{e}_y + r_z\,\mathbf{e}_z = x\,\mathbf{e}_x + y\,\mathbf{e}_y + z\,\mathbf{e}_z. \tag{1.9}$$

In fact, any vector $\mathbf{v}$ can be written in terms of its components v_i (where for Cartesian co-ordinates $i = x, y, z$) as

$$\mathbf{v} = \sum_{i=x,y,z} v_i\,\mathbf{e}_i \equiv v_i\,\mathbf{e}_i. \tag{1.10}$$

In the last equality we have introduced the Einstein summation convention: by definition a repeated index always implies a summation over that index. Other examples of this handy notation, the so-called index notation, is the scalar product,

$$\mathbf{v}\cdot\mathbf{u} = v_i u_i, \tag{1.11}$$

the length v of a vector $\mathbf{v}$,

$$v = |\mathbf{v}| = \sqrt{\mathbf{v}^2} = \sqrt{\mathbf{v}\cdot\mathbf{v}} = \sqrt{v_i v_i}, \tag{1.12}$$

and the ith component of the vector-matrix equation $\mathbf{u} = M\mathbf{v}$,

$$u_i = M_{ij}\,v_j. \tag{1.13}$$

Likewise, the full contraction or double-dot product of two tensors T and S, which in fact is the trace $\mathrm{Tr}\,(TS)$, can be written as

$$T\!:\!S \equiv \sum_{i,j} T_{ij}S_{ji} = T_{ij}S_{ji} = \mathrm{Tr}\,(TS). \tag{1.14}$$

Further studies of the index notation can be found in Exercise 1.4.

For the partial derivatives of some function $F(\mathbf{r}, t)$ we use the symbols ∂_i, with $i = x, y, z$, and ∂_t,

$$\partial_x F \equiv \frac{\partial F}{\partial x}, \quad \text{and} \quad \partial_t F \equiv \frac{\partial F}{\partial t}, \tag{1.15}$$

while for the total time derivative, as, e.g. in the case of the Lagrangian description of some variable $F\big(\mathbf{r}(t), t\big)$ following the fluid particles, see Fig. 1.4(b), we use the symbol d_t,

$$\mathrm{d}_t F \equiv \frac{\mathrm{d}F}{\mathrm{d}t} = \partial_t F + \big(\partial_t r_i\big)\partial_i F = \partial_t F + v_i \partial_i F. \tag{1.16}$$

The nabla operator $\boldsymbol{\nabla}$ containing the spatial derivatives plays an important role in differential calculus. In Cartesian co-ordinates it is given by

$$\boldsymbol{\nabla} \equiv \mathbf{e}_x\partial_x + \mathbf{e}_y\partial_y + \mathbf{e}_z\partial_z = \mathbf{e}_i\partial_i. \tag{1.17}$$

Note that we have written the differential operators to the right of the unit vectors. While not important for Cartesian co-ordinates it is crucial when working with curvilinear co-ordinates. The Laplace operator, which appears in numerous partial differential equations in theoretical physics, is just the square of the nabla operator,

$$\boldsymbol{\nabla}^2 \equiv \nabla^2 \equiv \partial_i \partial_i. \tag{1.18}$$

In terms of the nabla operator the total time derivative in Eq. (1.16) can be written as

$$\mathrm{d}_t F\big(\mathbf{r}(t), t\big) = \partial_t F + (\mathbf{v} \cdot \boldsymbol{\nabla}) F. \tag{1.19}$$

Since $\boldsymbol{\nabla}$ is a differential operator, the order of the factors does matter in a scalar product containing it. So, whereas $\mathbf{v} \cdot \boldsymbol{\nabla}$ in the previous equation is a differential operator, the product $\boldsymbol{\nabla}\cdot\mathbf{v}$ with the reversed order of the factors is a scalar quantity. It appears so often in mathematical physics that it has acquired its own name, namely the divergence of the vector field,

$$\nabla\cdot\mathbf{v} \equiv \partial_x v_x + \partial_y v_y + \partial_z v_z = \partial_i v_i. \tag{1.20}$$

Concerning integrals, we denote the 3D integral measure by $\mathrm{d}\mathbf{r}$, so that in Cartesian co-ordinates we have $\mathrm{d}\mathbf{r} = \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$, in cylindrical co-ordinates $\mathrm{d}\mathbf{r} = r\mathrm{d}r\,\mathrm{d}\phi\,\mathrm{d}z$, and in spherical co-ordinates $\mathrm{d}\mathbf{r} = r^2\mathrm{d}r\,\sin\theta\mathrm{d}\theta\,\mathrm{d}z$. We also consider definite integrals as operators acting on integrands, thus we keep the integral sign and the associated integral measure together to the left of the integrand. As an example, the integral over a spherical body with radius a of the scalar function $S(\mathbf{r})$ is written as

$$\int_{\text{sphere}} S(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = \int_{\text{sphere}} \mathrm{d}\mathbf{r}\,S(\mathbf{r}) = \int_0^a r^2\mathrm{d}r \int_0^\pi \sin\theta\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\,S(r,\theta,\phi). \tag{1.21}$$

When working with vectors and tensors it is advantageous to use the following two special symbols: the Kronecker delta δ_{ij},

$$\delta_{ij} = \begin{cases} 1, & \text{for } i = j, \\ 0, & \text{for } i \neq j, \end{cases} \tag{1.22}$$

and the Levi–Civita symbol ϵ_{ijk},

$$\epsilon_{ijk} = \begin{cases} +1, & \text{if } (ijk) \text{ is an even permutation of } (123) \text{ or } (xyz), \\ -1, & \text{if } (ijk) \text{ is an odd permutation of } (123) \text{ or } (xyz), \\ 0, & \text{otherwise.} \end{cases} \tag{1.23}$$

In the index notation, the Levi–Cevita symbol appears directly in the definition of the cross-product of two vectors $\mathbf{u}$ and $\mathbf{v}$,

$$(\mathbf{u} \times \mathbf{v})_i \equiv \epsilon_{ijk}\, u_j v_k, \tag{1.24}$$

and in the definition of the rotation $\boldsymbol{\nabla}\times\mathbf{v}$ of a vector $\mathbf{v}$. The expression for the ith component of the rotation is:

$$(\boldsymbol{\nabla} \times \mathbf{v})_i \equiv \epsilon_{ijk}\, \partial_j v_k. \tag{1.25}$$

To calculate in the index notation the rotation of a rotation, such as $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{v})$, or the rotation of a cross-product it is very helpful to know the following expression for the product of two Levi–Civita symbols with one pair of repeated indices (here k):

$$\epsilon_{ijk}\, \epsilon_{lmk} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}. \tag{1.26}$$

Note the plus sign when pairing index 1 with 1 and 2 with 2 (direct pairing), while a minus sign appears when pairing index 1 with 2 and 2 with 1 (exchange pairing).

Let us end this short introduction to the index notation by an explicit example, namely the proof of the expression for the rotation of a rotation of a vector field $\mathbf{v}$,

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{v}) = \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{v}) - \nabla^2\mathbf{v}, \tag{1.27a}$$

or the equivalent expression for the gradient of the divergence,

$$\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{v}) = \nabla^2\mathbf{v} + \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\mathbf{v}). \tag{1.27b}$$

These expressions are used in hydrodynamics, acoustics and electromagnetism. First we write out the ith component of the left-hand side of Eq. (1.27a) using the Levi–Civita symbol for each cross-product, one at a time,

$$\big(\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{v}\big)_i = \epsilon_{ijk}\partial_j\big(\boldsymbol{\nabla}\times\mathbf{v}\big)_k = \epsilon_{ijk}\partial_j\big(\epsilon_{klm}\partial_l v_m\big) = \epsilon_{ijk}\epsilon_{klm}\,\partial_j\partial_l v_m. \tag{1.28a}$$

Then we permute the indices in the second Levy–Civita symbol and apply Eq. (1.26),

$$\big(\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{v}\big)_i = \epsilon_{ijk}\epsilon_{lmk}\,\partial_j\partial_l v_m = \big(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\big)\,\partial_j\partial_l v_m = \delta_{il}\delta_{jm}\,\partial_j\partial_l v_m - \delta_{im}\delta_{jl}\,\partial_j\partial_l v_m. \tag{1.28b}$$

Finally, we perform the sum over the indices appearing in the Kronecker deltas

$$\big(\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{v}\big)_i = \partial_j\partial_i v_j - \partial_j\partial_j v_i = \partial_i\big(\partial_j v_j\big) - \big(\partial_j\partial_j\big)v_i = \partial_i\big(\boldsymbol{\nabla}\cdot\mathbf{v}\big) - \nabla^2 v_i = \big[\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{v}) - \nabla^2\mathbf{v}\big]_i, \tag{1.28c}$$

which indeed proves Eq. (1.27a) and therefore also Eq. (1.27b).

Finally, we use upright letters for the two mathematical constants

$$\mathrm{e} \equiv \text{the exponential constant } \exp(1), \quad \text{and} \quad \mathrm{i} \equiv \text{the imaginary unit } \sqrt{-1}. \tag{1.29}$$

1.5 Perturbation theory

As we shall see shortly, the governing differential equations of microfluidics can only be solved analytically in a few idealized cases. Given sufficiently powerful computers, it is of course possible to solve almost any problem numerically, however, it is often of great value also to find analytical approximations to these solutions. One general applicable approximation scheme is the so-called perturbation theory, which we shall se examples of throughout the book. Here, we give a short introduction to the method.

Imagine that a given problem can be formulated in terms of some partial differential operator $\mathcal{D}$ acting on the field $f(\mathbf{r},t)$ as

$$\mathcal{D}f = 0. \tag{1.30}$$

The goal is to determine f. Now, assume that the differential operator can be written as a series expansion

$$\mathcal{D} = \mathcal{D}_0 + \alpha\mathcal{D}_1 + \alpha^2\mathcal{D}_2 + \cdots, \tag{1.31}$$

where $\mathcal{D}_0$ is a differential operator, which represents a simpler problem that we can solve, where α is a small dimensionless parameter, known as the perturbation parameter, which describes how far the actual problem deviates from the simpler solvable problem, and where $\mathcal{D}_i$ for $i > 0$ are known differential operators. The simpler problem is also denoted the unperturbed problem, while terms proportional to α and higher powers in α are denoted the perturbation terms. For $\alpha = 0$ the actual problem is identical to the simpler problem, and can thus be solved, while for $0 < |\alpha| \ll 1$ the actual problem deviates slightly from the simpler problem. The idea is to calculate the field f by successively finding the higher-order terms in the expansion

$$f = f_0 + \alpha f_1 + \alpha^2 f_2 + \cdots . \tag{1.32}$$

Inserting the perturbation series for $\mathcal{D}$ and f results, under the assumption of proper convergence, in the following expression for $\mathcal{D}f$,

$$\begin{aligned} \mathcal{D}f &= (\mathcal{D}_0 + \alpha\mathcal{D}_1 + \alpha^2\mathcal{D}_2 + \cdots)(f_0 + \alpha f_1 + \alpha^2 f_2 + \cdots) \\ &= \mathcal{D}_0 f_0 + \alpha(\mathcal{D}_1 f_0 + \mathcal{D}_0 f_1) + \alpha^2(\mathcal{D}_2 f_0 + \mathcal{D}_1 f_1 + \mathcal{D}_0 f_2) + \cdots . \end{aligned} \tag{1.33}$$

The original problem Eq. (1.30), $\mathcal{D}f = 0$ is consequently reformulated as

$$\mathcal{D}_0 f_0 + \alpha(\mathcal{D}_1 f_0 + \mathcal{D}_0 f_1) + \alpha^2(\mathcal{D}_2 f_0 + \mathcal{D}_1 f_1 + \mathcal{D}_0 f_2) + \cdots = 0. \tag{1.34}$$

For this to be true for any value of α each term must be zero, and we get the following infinite system of equations to solve,

$$\begin{aligned} \mathcal{D}_0 f_0 &= 0, && \text{order } \alpha^0 \text{ terms}, && (1.35\text{a}) \\ \mathcal{D}_0 f_1 &= -\mathcal{D}_1 f_0, && \text{order } \alpha^1 \text{ terms}, && (1.35\text{b}) \\ \mathcal{D}_0 f_2 &= -\mathcal{D}_2 f_0 - \mathcal{D}_1 f_1, && \text{order } \alpha^2 \text{ terms}, && (1.35\text{c}) \\ &\vdots && \vdots . \end{aligned}$$

By assumption, the homogeneous zero-order equation (1.35a) is the unperturbed, solvable problem, and f_0 can therefore be found. This implies that the first-order equation (1.35b) becomes an inhomogeneous differential equation for the first-order contribution f_1 with a known right-hand side, so in principle we can now find f_1. This in turn means that the second-order equation (1.35c) has become an inhomogeneous differential equation for f_2 with a known right-hand side determined by the, at this point known, lower-order fields f_0 and f_1, and in principle f_2 can be found. In this way the perturbation scheme allows for consecutive determination of f_n once all lower-order contributions f_i, for $i < n$ have been found.

In practice, it is only possible or worthwhile to calculate a few of the terms, rarely going beyond the second order contribution. The series is therefore truncated, i.e. neglecting all terms $\mathcal{O}(\alpha^3)$ with α^3 and higher powers, and an approximate result has been found,

$$f = f_0 + \alpha f_1 + \alpha^2 f_2 + \mathcal{O}(\alpha^3) \approx f_0 + \alpha f_1 + \alpha^2 f_2. \tag{1.36}$$

In some cases it may be advantageous to absorb the perturbation parameter α into the operators and functions as $\alpha^n\mathcal{D}_n \rightarrow \mathcal{D}_n$ and $\alpha^n f_n \rightarrow f_n$. The perturbation expansions Eqs. (1.31) and (1.32) become

$$\mathcal{D} = \mathcal{D}_0 + \mathcal{D}_1 + \mathcal{D}_2 + \cdots , \tag{1.37a}$$

$$f = f_0 + f_1 + f_2 + \cdots . \tag{1.37b}$$

In the differential equation $\mathcal{D}f = 0$, terms of order n are those where the sum of indices is n, e.g. $\mathcal{D}_k f_{n-k}$, so the expanded differential equation (1.34) is now written as

$$(\mathcal{D}_0 f_0) + (\mathcal{D}_1 f_0 + \mathcal{D}_0 f_1) + (\mathcal{D}_2 f_0 + \mathcal{D}_1 f_1 + \mathcal{D}_0 f_2) + \cdots = 0, \tag{1.38}$$

where the parentheses contain the zero-order term, the first-order terms, the second-order terms, *etc.* The infinite system of equations (1.35) is unaffected by making the perturbation parameter α implicit.

1.6 Eigenfunction expansion

A second general approach involves expansion of the hydrodynamic fields in certain basis functions or eigenfunctions $\phi_n(\mathbf{r})$, which are found as the eigenfunctions to simpler differential equation eigenvalue problems related to the problem to be solved. Often, the basis functions $\phi_n(\mathbf{r})$ are determined from the Helmholtz equation with Dirichlet boundary conditions involving the Laplace operator with eigenvalues k_n^2 in a domain Ω with the boundary $\partial\Omega$,

$$\nabla^2 \phi_n(\mathbf{r}) = -k_n^2\, \phi_n(\mathbf{r}), \quad \text{for } \mathbf{r} \in \Omega \text{ and } n = 1, 2, 3, \dots, \tag{1.39a}$$

$$\phi_n(\mathbf{r}) = 0, \qquad \text{for } \mathbf{r} \in \partial\Omega. \tag{1.39b}$$

For a 1D domain the expansion is the standard Fourier expansion in sine functions, while for a 2D circular domain it is the Fourier–Bessel expansion in Bessel functions. Any field $f(\mathbf{r})$ can be expanded in the basis- or eigenfunctions as

$$f(\mathbf{r}) = \sum_{n=1}^{\infty} a_n \phi_n(\mathbf{r}), \tag{1.40}$$

and the problem is solved once the coefficients a_n are determined.

The basis- or eigenfunctions are mutually orthogonal in the sense that the integral over the domain Ω is zero for a product of two different eigenfunctions is zero, and by proper normalization the integral over the square of a single eigenfunction is unity,

$$\int_\Omega \mathrm{d}\mathbf{r}\, \phi_n(\mathbf{r})\phi_m(\mathbf{r}) = \delta_{nm}, \tag{1.41}$$

where we have used the Kronecker delta Eq. (1.22). This special orthonormality property of the eigenfunctions forms the basis for the so-called Hilbert space theory of functions, where functions can be thought of as abstract vectors in a linear vector space. In physics, Hilbert spaces are used particularly in quantum physics, and the reader unfamiliar with the concept is referred to any basic textbook on quantum theory for further reading. We shall briefly use some of the concepts in fluid dynamics mainly as a convenient shorthand notation. First, we introduce the Dirac bra-ket notation for real-valued functions and integrals,

$$\langle f| \equiv f(\mathbf{r}), \qquad \text{the bra of } f, \tag{1.42a}$$

$$|g\rangle \equiv g(\mathbf{r}), \qquad \text{the ket of } g, \tag{1.42b}$$

$$\langle f|g\rangle \equiv \int_\Omega \mathrm{d}\mathbf{r}\, f(\mathbf{r})\, g(\mathbf{r}), \text{ the bra(c)ket of } f\, g. \tag{1.42c}$$

For complex-valued functions the function f associated with the bra-vector is to be complex conjugated. The bra(c)ket $\langle f|g\rangle$ is also known as the inner product of f and g, and the bra-ket notation makes it possible to interpret the involved operation of "*multiplying by a function f followed by integration over the domain*" as a simple "*multiply from the left by the bra $\langle f|$*". From the linearity of integrals it is easy to show, see Exercise 1.6, that

$$\langle a_1 f_1 + a_2 f_2 | b_1 g_1 + b_2 g_2\rangle = a_1 b_1 \langle f_1|g_1\rangle + a_1 b_2 \langle f_1|g_2\rangle + a_2 b_1 \langle f_2|g_1\rangle + a_2 b_2 \langle f_2|g_2\rangle. \tag{1.43}$$

In the Dirac notation the expansion Eq. (1.40) becomes

$$|f\rangle = \sum_{n=1}^{\infty} a_n |\phi_n\rangle, \tag{1.44}$$

and the othonormality property Eq. (1.41) appears as

$$\langle \phi_n|\phi_m\rangle = \delta_{nm}. \tag{1.45}$$

If we assume that the function $f(\mathbf{r})$ is known, then we can determine the expansion coefficients a_n by multiplying Eq. (1.44) from the left by $\langle\phi_m|$ and utilizing the linearity of the inner product as well as the othonormality of the eigenfunctions,

$$\langle \phi_m|f\rangle = \langle\phi_m| \left[\sum_{n=1}^{\infty} a_n |\phi_n\rangle\right]\rangle = \sum_{n=1}^{\infty} a_n \langle\phi_m|\phi_n\rangle = a_m. \tag{1.46}$$

This simple result is the generalization of the familiar method of determining Fourier coefficients. We note that by combining Eqs. (1.44) and (1.46) we obtain

$$|f\rangle = \sum_{n=1}^{\infty} \langle\phi_n|f\rangle\, |\phi_n\rangle = \sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n|f\rangle = \left[\sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n|\right] |f\rangle, \tag{1.47}$$

and consequently the parenthesis on the right-hand side must be unity, and we have derived the so-called completeness condition

$$\sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n| \equiv 1. \tag{1.48}$$

As a simple example of how to use the eigenfunction expansion to solve problems, let us consider the Poisson equation for the unknown field $f(\mathbf{r})$ with a known source term $g(\mathbf{r})$,

$$\nabla^2 f(\mathbf{r}) = -g(\mathbf{r}). \tag{1.49}$$

Inserting the expansions $|f\rangle = \sum_{n=1}^{\infty} a_n|\phi_n\rangle$ and $|g\rangle = \sum_{n=1}^{\infty}\langle\phi_n|g\rangle|\phi_n\rangle$ into the Poisson equation leads to

$$\sum_{n=1}^{\infty} a_n \nabla^2 |\phi_n\rangle = -\sum_{n=1}^{\infty} \langle\phi_n|g\rangle\, |\phi_n\rangle. \tag{1.50}$$

Employing the fundamental relation Eq. (1.39a) and multiplying from the left by $\langle\phi_m|$ leads, as shown in Exercise 1.6 to the determination of the coefficients a_m, and the solution can be written as

$$|f\rangle = \sum_{n=1}^{\infty} \frac{\langle\phi_n|g\rangle}{k_n^2}\, |\phi_n\rangle. \tag{1.51}$$

This simple example points to the usefulness of the eigenfunction-expansion approach. The eigenvalues k_n^2 are increasing rapidly for increasing values of n, so for many practical purposes it suffices to truncate the infinite sum and include only the first few terms.

In Section 3.4.1 we shall use eigenfunction expansion to study liquid flow through straight channels of constant but arbitrarily shaped cross-sections. In this context the domain Ω is the 2D cross-section, and issues related to the area and areal coverage become important. In the Dirac notation the area $\mathcal{A}$ of the domain Ω is written as

$$\mathcal{A} = \int_\Omega \mathrm{d}\mathbf{r}\; 1 = \int_\Omega \mathrm{d}\mathbf{r}\; 1^2 = \langle 1|1\rangle. \tag{1.52}$$

Likewise, when integrating over an eigenfunction $\phi_n(\mathbf{r})$ over the domain we get a measure of how much area this eigenfunction effectively covers. However, since $\langle 1|1\rangle = \mathcal{A}$ and $\langle \phi_n|\phi_n\rangle = 1$ the dimension of $\langle 1|\phi_n\rangle$ is seen to be length. Therefore the so-called effective area $\mathcal{A}_n$ of eigenfunction $\phi_n(\mathbf{r})$ is defined as the square of the area integral,

$$\mathcal{A}_n = \Big[\int_\Omega \mathrm{d}\mathbf{r}\; \phi_n(\mathbf{r})\Big]^2 = \Big[\int_\Omega \mathrm{d}\mathbf{r}\; \phi_n(\mathbf{r})\, \phi_n(\mathbf{r})\Big]^2 = \big[\langle 1|\phi_n\rangle\big]^2 = \langle \phi_n|1\rangle\langle 1|\phi_n\rangle. \tag{1.53}$$

1.7 Further reading

Two classic textbooks on the fundamentals of fluid dynamics are Landau and Lifshitz (1993) and Batchelor (2000), and more are listed in Section 2.4. Books focusing in particular on microfluidics or lab-on-a-chip systems are Karniadakis and Beskok (2002), Geschke, Klank and Telleman (2004), Tabeling (2005), and Berthier and Silberzan (2006); these titles are well supplemented by the review papers on microfluidics by Stone, Stroock and Ajdari (2004) and Squires and Quake (2005). For perturbation theory in fluid mechanics see Van Dyke (1975), while eigenfunction expansion in the Dirac notation is treated in quantum mechanics textbooks such as Merzbacher (1998) and Bruus and Flensberg (2004).

1.8 Exercises

Exercise 1.1
The intermolecular distance in air

Assume that air at room temperature and a pressure of 1000 hPa is an ideal gas. Estimate the average intermolecular distance. Compare the result with that of liquids.

Exercise 1.2
The Lennard-Jones potential for intermolecular pair-interaction

An approximative but quite useful expression for intermolecular pair-interactions is the so-called Lennard-Jones potential,

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\bigg[\Big(\frac{\sigma}{r}\Big)^{12} - \Big(\frac{\sigma}{r}\Big)^{6}\bigg]. \tag{1.54}$$

Let r_0 be the distance at which the pair of molecules experience the smallest possible interaction energy.

(a) Determine r_0 in units of the collision diameter σ and calculate the corresponding interaction energy $V(r_0)$ in units of the maximum attraction energy ε.

(b) Calculate $V_{\mathrm{LJ}}(3\sigma)$ and use the result to discuss the applicability of the ideal-gas model to air, given that for nitrogen $\sigma_{\mathrm{N_2}} = 0.3667$ nm and $\varepsilon_{\mathrm{N_2}}/k_{\mathrm{B}} = 99.8$ K.

Exercise 1.3
The size of the fundamental fluid particle in a liquid

Consider a small cube of side length λ^* in the middle of some liquid. The typical average intermolecular distance in the liquid is the one discussed in Section 1.3.1. Due to random thermal fluctuations the molecules inside the cube are continuously exchanged with the surrounding liquid, but on average there are N molecules inside the cube. For sufficiently small fluctuations the cube can play the role of a fundamental fluid particle.

(a) Use the standard result from basic statistics that the standard deviation of the counting number of uncorrelated random events (here, the number N of molecules inside the cube) is given by $\sqrt{N}$ to estimate the side length λ, such that the relative uncertainty $\sqrt{N}/N$ of the number of molecules is 1%.

(b) Determine λ^* such that the relative uncertainty of the number of molecules is 0.1%.

Exercise 1.4
The index notation

To become familiar with the index notation try to work out the following problems.

(a) Use the index notation to prove that $\partial_k\big(p\,\delta_{ik}\big) = (\boldsymbol{\nabla} p)_i$.

(b) Use the index notation to prove that $\boldsymbol{\nabla}\cdot(\rho\mathbf{v}) = (\boldsymbol{\nabla}\rho)\cdot\mathbf{v} + \rho\boldsymbol{\nabla}\cdot\mathbf{v}$.

(c) Prove that Eq. (1.25) for the rotation of a vector is correct.

(d) Use Eqs. (1.24) and (1.26) to prove that $\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c}$.

Exercise 1.5
First-order perturbation of the damped, harmonic oscillator

Consider the 1D, damped, harmonic oscillator of mass m, force constant k, damping coefficient γ and position co-ordinate $x(t)$ described by the equation of motion

$$m\,\partial_t^2 x = -kx - m\gamma\,\partial_t x. \tag{1.55}$$

The initial condition is given by $x(0) = \ell$ and $\partial_t x(0) = 0$. We study the solution of this problem using perturbation theory using the damping as the perturbation. The unperturbed oscillator has $\gamma = 0$ and the solution $x_0(t) = \ell\,\cos(\omega_0 t)$ with $\omega_0 \equiv \sqrt{k/m}$.

(a) Introduce the following dimensionless variable $\tilde{x}$ and $\tilde{t}$ by the definitions $x \equiv \ell\,\tilde{x}$ and $t \equiv \tilde{t}/\omega_0$, and let $\alpha = \gamma/\omega_0$ be the dimensionless perturbation parameter. Calculate the first-order perturbation result $\tilde{x} = \tilde{x}_0 + \alpha\,\tilde{x}_1$.

(b) Find the exact solution using a trial solution of the complex form $\tilde{x} = \exp(\mathrm{i}\beta\tilde{t})$, and compare a first-order expansion in α of the result with the first-order perturbation result.

Exercise 1.6
The Dirac bra-ket notation

The Dirac bra-ket notation is a compact notation that makes it possible to maintain the overview in a complex calculation without getting swamped by details.

(a) Prove the linearity relation for the inner product given in Eq. (1.43):
$\langle a_1 f_1 + a_2 f_2 | b_1 g_1 + b_2 g_2\rangle = a_1 b_1\langle f_1|g_1\rangle + a_1 b_2\langle f_1|g_2\rangle + a_2 b_1\langle f_2|g_1\rangle + a_2 b_2\langle f_2|g_2\rangle$.

(b) Use the Dirac notation expansions $|f\rangle = \sum_{n=1}^{\infty} a_n|\phi_n\rangle$ and $|g\rangle = \sum_{n=1}^{\infty}\langle\phi_n|g\rangle|\phi_n\rangle$ to solve the Poisson equation for the unknown field $f(\mathbf{r})$ with a known source term $g(\mathbf{r})$.

1.9 Solutions

Solution 1.1

The intermolecular distance in air

A single air molecule occupies the volume $\lambda^3 = \mathcal{V}/N$, where $\mathcal{V}$ is the volume of air containing N molecules. The length scale λ thus represents the average intermolecular distance. Using $p\mathcal{V} = Nk_\mathrm{B}T$, with $p = 10^5$ Pa and $T = 300$ K, we find

$$\lambda = \left(\frac{\mathcal{V}}{N}\right)^{\frac{1}{3}} = \left(\frac{k_\mathrm{B}T}{p}\right)^{\frac{1}{3}} = 3.5 \text{ nm}. \tag{1.56}$$

Thus the intermolecular distance in air is roughly one order of magnitude larger than the intermolecular distance in a typical liquid.

Solution 1.2

The Lennard-Jones potential for intermolecular pair interaction

(a) The minimum is found by solving $\partial_r V_\mathrm{LJ}(r) = 0$, which yields $r_0 = 2^{\frac{1}{6}}\sigma \approx 1.12\sigma$, and a corresponding interaction energy of $V_\mathrm{LJ}(r_0) = -\varepsilon$.

(b) $V_\mathrm{LJ}(3\sigma) = -0.0055\varepsilon$. For nitrogen this means that in the distance $3\sigma_{\mathrm{N}_2} = 1.1$ nm the interaction energy in kelvin is $V_\mathrm{LJ}(3\sigma_{\mathrm{N}_2})/k_\mathrm{B} = -0.5$ K. The average intermolecular distance is 3.5 nm, while the average kinetic translation energy in kelvin is $\frac{3}{2}T = 450$ K. Thus, the interaction effects are minute and can be neglected.

Solution 1.3

The size of the fundamental fluid particle in a liquid

Consider a cube of liquid with side length λ^* in which $\alpha = \sqrt{N}/N$ is a given relative uncertainty in the number of molecules inside the cube. Each molecule occupies the volume λ^3, where $\lambda = 0.3$ nm is a typical value of the intermolecular distance in a liquid. Clearly $(\lambda^*)^3 = N\lambda^3$ and $N = \alpha^{-2}$ and thus $\lambda^*(\alpha) = \alpha^{-\frac{2}{3}}\lambda$.

(a) With $\alpha = 10^{-2}$ we find $\lambda^* = 6.5$ nm.

(b) With $\alpha = 10^{-3}$ we find $\lambda^* = 30$ nm. For a gas λ^* is roughly ten times larger.

Solution 1.4

The index notation

(a) Since δ_{ij} is a constant we have $\partial_k\delta_{ij} \equiv 0$ for any value of i, j and k.
We thus find $\partial_k\big(p\delta_{ij}\big) = \big(\partial_k p\big)\delta_{ij} + p\big(\partial_k\delta_{ij}\big) = \partial_i p + 0 = \big(\boldsymbol{\nabla} p\big)_i$.

(b) For the divergence of the current density we get
$\boldsymbol{\nabla}\cdot\big(\rho\mathbf{v}\big) = \partial_j\big(\rho\mathbf{v}_j\big) = \big(\partial_j\rho\big)v_j + \rho\big(\partial_j v_j\big) = \big(\boldsymbol{\nabla}\rho\big)\cdot\mathbf{v} + \rho\boldsymbol{\nabla}\cdot\mathbf{v}$

(c) Let us consider the z component of the rotation. By definition we have $\big(\boldsymbol{\nabla}\times\mathbf{v}\big)_z = \partial_x v_y - \partial_y v_x$. Using index notation we obtain $\big(\boldsymbol{\nabla}\times\mathbf{v}\big)_z = \epsilon_{zjk}\partial_j v_k$. The only non-zero terms are carrying the indices $(j,k) = (x,y)$ or $(j,k) = (y,x)$, and since $\epsilon_{zxy} = +1$ and $\epsilon_{zyx} = -1$ we get the desired result: $\big(\boldsymbol{\nabla}\times\mathbf{v}\big)_z = \epsilon_{zjk}\partial_j v_k = \partial_x v_y - \partial_y v_x$. Likewise, for the x and y components of the rotation.

(d) For the double cross-product identity we get $\big[\mathbf{a}\times(\mathbf{b}\times\mathbf{c})\big]_{\;i} = \epsilon_{ijk}a_j(\mathbf{b}\times\mathbf{c})_k = \epsilon_{ijk}a_j\big(\epsilon_{klm}b_l c_m\big) = \epsilon_{ijk}\epsilon_{lmk}\,a_j b_l c_m$, where in the last equation we have made an even permutation of the indices in the second Levi–Civita symbol, $\epsilon_{klm} = \epsilon_{lmk}$. Finally, we use Eq. (1.26) to express the product of the two Levi–Civita symbols as a linear combination of Kronecker deltas, $\epsilon_{ijk}\epsilon_{lmk}\,a_j b_l c_m = \big(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\big)\,a_j b_l c_m = a_j c_j b_i - a_j b_j c_i = (\mathbf{a}\cdot\mathbf{c})b_i - (\mathbf{a}\cdot\mathbf{b})c_i = \big[(\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c}\big]_i$, which proves the relation.

Solution 1.5
First-order perturbation of the damped, harmonic oscillator

Introducing the dimensionless variables yields the following equation of motion,

$$\partial_{\tilde{t}}^2 \tilde{x} = -\tilde{x} - \alpha\, \partial_{\tilde{t}} \tilde{x}. \tag{1.57}$$

(a) With $\tilde{x} = \tilde{x}_0 + \alpha \tilde{x}_1$ the zero-order equation becomes $\partial_{\tilde{t}}^2 \tilde{x}_0 = -\tilde{x}_0$ with the solution $\tilde{x}_0(\tilde{t}) = \cos(\tilde{t})$. The first-order equation becomes $\partial_{\tilde{t}}^2 \tilde{x}_1 = -\tilde{x}_1 - \partial_{\tilde{t}} \tilde{x}_0 = -\tilde{x}_1 + \sin(\tilde{t})$ with the solution $\tilde{x}_1(\tilde{t}) = -\frac{1}{2}\, \tilde{t}\, \cos(\tilde{t})$. So the complete first-order perturbation result is

$$\tilde{x}(\tilde{t}) = \cos(\tilde{t}) \Big[1 - \tfrac{1}{2} \alpha \tilde{t} \Big] + \mathcal{O}(\alpha^2). \tag{1.58}$$

(b) Insertion of the trial function $\tilde{x} = \exp(\mathrm{i}\beta\tilde{t})$ into Eq. (1.57) leads to the simple algebraic equation $-\beta^2 = -1 - \mathrm{i}\,\alpha\beta$ with the solution $\beta = \sqrt{1 - (\alpha/2)^2} + \mathrm{i}\,\alpha/2 \approx 1 + \mathrm{i}\,\alpha/2$. Hence

$$\mathrm{Re}\Big[\mathrm{e}^{\mathrm{i}\beta\tilde{t}} \Big] \approx \mathrm{Re}\Big[\mathrm{e}^{\mathrm{i}\tilde{t}}\; \mathrm{e}^{-\alpha\tilde{t}/2} \Big] = \cos(\tilde{t})\, \mathrm{e}^{-\alpha\tilde{t}/2} \approx \cos(\tilde{t})\, \Big[1 - \tfrac{1}{2} \alpha \tilde{t} \Big] \tag{1.59}$$

in agreement with the first-order result Eq. (1.58).

Solution 1.6
The Dirac bra-ket notation

(a) Use the basic definition Eq. (1.42c) to obtain

$$\begin{aligned}
&\langle a_1 f_1 + a_2 f_2 | b_1 g_1 + b_2 g_2 \rangle \\
&\quad = \int_\Omega \mathrm{d}\mathbf{r}\; \big[a_1 f_1(\mathbf{r}) + a_2 f_2(\mathbf{r}) \big] \; \big[b_1 g_1(\mathbf{r}) + b_2 g_2(\mathbf{r}) \big] \\
&\quad = \int_\Omega \mathrm{d}\mathbf{r}\; \big[a_1 b_1 f_1(\mathbf{r}) g_1(\mathbf{r}) + a_1 b_2 f_1(\mathbf{r}) g_2(\mathbf{r}) + a_2 b_1 f_2(\mathbf{r}) g_1(\mathbf{r}) + a_2 b_2 f_2(\mathbf{r}) g_2(\mathbf{r}) \big] \\
&\quad = a_1 b_1 \langle f_1 | g_1 \rangle + a_1 b_2 \langle f_1 | g_2 \rangle + a_2 b_1 \langle f_2 | g_1 \rangle + a_2 b_2 \langle f_2 | g_2 \rangle.
\end{aligned} \tag{1.60}$$

(b) With the expansion $|f\rangle = \sum_{n=1}^{\infty} a_n |\phi_n\rangle$ we get

$$\nabla^2 |f\rangle = \sum_{n=1}^{\infty} a_n \nabla^2 |\phi_n\rangle = \sum_{n=1}^{\infty} a_n (-k_n^2) |\phi_n\rangle, \tag{1.61}$$

and with $|g\rangle = \sum_{n=1}^{\infty} \langle \phi_n | g \rangle |\phi_n\rangle$ the Poisson equation $\nabla^2 f(\mathbf{r}) = -g(\mathbf{r})$ therefore becomes

$$\sum_{n=1}^{\infty} a_n k_n^2 |\phi_n\rangle = \sum_{n=1}^{\infty} \langle \phi_n | g \rangle \; |\phi_n\rangle. \tag{1.62}$$

When multiplied by $\langle \phi_m |$ and using the orthonormality property Eq. (1.45) this reduces to

$$a_m k_m^2 = \langle \phi_m | g \rangle. \tag{1.63}$$

Division by k_m^2 leads to an expression for a_m and thus a determination of the solution $|f\rangle$,

$$|f\rangle = \sum_{m=1}^{\infty} a_m |\phi_m\rangle = \sum_{m=1}^{\infty} \frac{\langle \phi_n | g \rangle}{k_m^2} \, |\phi_m\rangle. \tag{1.64}$$