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Eleftherios N. Economou

Green's Functions in Quantum Physics

Third Edition

With 60 Figures

Springer

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To Sophia

Preface to the Third Edition

In this third edition the book has been expanded in three directions:

1. Problems have been added at the end of each chapter (40% of which are solved in the last section of the book) together with suggestions for further reading. Furthermore, the number of appendices (marked with a grey stripe) has been substantially enlarged in order to make the book more self-sufficient. These additions, together with many clarifications in the text, render the book more suitable as a companion in a course on Green's functions and their applications.
2. The impressive developments of the 1980s and 1990s in mesoscopic physics, and in particular in transport properties, found their way – to a certain extent – in the new Chaps. 8 and 9 (which also contain some of the material of the old Chap. 7). This is a natural expansion, since Green's functions have played an important role as a theoretical tool in this new field of physics, a role that continues in nanoregime research (see, e.g., recent publications dealing with carbon nanotubes). Thus, the powerful and unifying formalism of Green's functions finds applications not only in standard physics subjects such as perturbation and scattering theory, bound-state formation, etc., but also at the forefront of current and, most likely, future developments.
3. Over the last 15 years or so Green's functions have found applications not only in condensed matter electronic motion but in classical wave propagation in both periodic and random media; photonic and phononic crystals are the outcomes of this line of research whose underlying basic theoretical principles are summarized in Sect. 7.2.4.

I would like to thank Ms. Mina Papadakis and Dr. Stamatis Stamatiadis whose help was invaluable during the writing and typesetting of this drastically revised third edition of my book.

Heraklion, Crete, March 2005 *E. N. Economou*

Preface to the Second Edition

In this edition, the second and main part of the book has been considerably expanded so as to cover important applications of the formalism of Green's functions.

In Chap. 5 a section was added outlining the extensive role of the tight-binding (or, equivalently, the linear combination of atomiclike orbitals) approach to many branches of solid-state physics. Some additional information (including a table of numerical values) regarding square and cubic lattice Green's functions were incorporated.

In Chap. 6 the difficult subjects of superconductivity and the Kondo effect are examined employing an appealingly simple connection to the question of the existence of a bound state in a very shallow potential well. The existence of such a bound state depends entirely on the form of the unperturbed density of states near the end of the spectrum: if the density of states blows up, there is always at least one bound state. If the density of states approaches zero continuously, a critical depth (and/or width) of the well must be reached in order to have a bound state. The borderline case of a finite discontinuity (which is very important to superconductivity and the Kondo effect) always produces a bound state with an exponentially small binding energy.

Chapter 7 has been expanded to cover details of the new and fast-developing field of wave propagation in disordered media. The coherent potential approximation (a simple but powerful method) is presented with an extensive list of references to the current literature. Then the electrical conductivity is examined both because it is an interesting quantity in its own right and because it plays a central role in demonstrating how disorder can create a qualitatively different behavior. Since the publication of the first edition of this book, significant advances in the field of random media have taken place. An effort has been made to present in a simple way the essential points of these advances (for the reader with a casual interest in this subject) and to review the current literature (for the benefit of the reader whose research activities are or will be related to the field of disordered systems).

In this edition, each chapter is preceded by a short outline of the material to be covered and concluded by a summary containing the most important equations numbered as in the main text.

I would like to thank A. Andriotis and A. Fertis for pointing out to me several misprints in the first edition. I would also like to express my gratitude to Exxon Research and Engineering Company for its hospitality during the final stages of this work.

Heraklion, Crete, January 1983 *E. N. Economou*

Preface to the First Edition

This text grew out of a series of lectures addressed to solid-state experimentalists and students beginning their research career in solid-state physics.

The first part, consisting of Chaps. 1 and 2, is a rather extensive mathematical introduction that covers material related to Green's functions usually included in a graduate course on mathematical physics. Emphasis is given to those topics that are important in quantum physics. On the other hand, little attention is given to the important question of determining the Green's functions associated with boundary conditions on surfaces at finite distances from the source. The second and main part of the book is, in my opinion, the first attempt at integrating, in a systematic but concise way, various topics of quantum physics, where Green's functions (as defined in Part I) can be successfully applied. Chapter 3 is a direct application of the formalism developed in Part I. In Chap. 4 the perturbation theory for Green's functions is presented and applied to scattering and to the question of bound-state formation. Next, the Green's functions for the so-called tight-binding Hamiltonian (TBH) are calculated. The TBH is of central importance for solid-state physics because it is the simplest example of wave propagation in periodic structures. It is also important for quantum physics in general because it is rich in physical phenomena (e.g., negative effective mass, creation of a bound state by a repulsive perturbation) and, at the same time, simple in its mathematical treatment. Thus one can derive simple, exact expressions for scattering cross sections and for bound and resonance levels. The multiple scattering formalism is presented within the framework of the TBH and applied to questions related to the behavior of disordered systems (such as amorphous semiconductors). The material of Part II is of interest not only to solid-state physicists but to students in a graduate-level course in quantum mechanics (or scattering theory) as well.

In Part III, with the help of the second quantization formalism, many-body Green's functions are introduced and utilized in extracting physical information about interacting many-particle systems. Many excellent books have been devoted to the material of Part III (e.g., Fetter and Walecka: Quantum Theory of Many-Particle Systems [20]). Thus the present treatment must be viewed as a brief introduction to the subject; this introduction may help the solid-state theorist approach the existing thorough treatments of the subject and the solid-state experimentalist become acquainted with the formalism.

I would like to thank the “Demokritos” Nuclear Research Center and the Greek Atomic Energy Commission for their hospitality during the writing of the second half of this book.

Athens, Greece, November 1978 *E. N. Economou*

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Part I

Green's Functions in Mathematical Physics

1

Time-Independent Green's Functions

Summary. In this chapter, the time-independent Green's functions are defined, their main properties are presented, methods for their calculation are briefly discussed, and their use in problems of physical interest is summarized.

1.1 Formalism

Green's functions can be defined as solutions of inhomogeneous differential equations of the type[1]

$$[z - L(\boldsymbol{r})]\, G(\boldsymbol{r}, \boldsymbol{r}'; z) = \delta(\boldsymbol{r} - \boldsymbol{r}') \ , \tag{1.1}$$

subject to certain boundary conditions (BCs) for $\boldsymbol{r}$ or $\boldsymbol{r}'$ lying on the surface S of the domain Ω of $\boldsymbol{r}$ and $\boldsymbol{r}'$. Here we assume that z is a complex variable with $\lambda \equiv \mathrm{Re}\{z\}$ and $s \equiv \mathrm{Im}\{z\}$ and that $L(\boldsymbol{r})$ is a time-independent, linear, hermitian[2] differential operator that possesses a complete set of eigenfunctions $\{\phi_n(\boldsymbol{r})\}$, i.e.,

$$L(\boldsymbol{r})\phi_n(\boldsymbol{r}) = \lambda_n \phi_n(\boldsymbol{r}) \ , \tag{1.2}$$

where $\{\phi_n(\boldsymbol{r})\}$ satisfy the same BCs as $G(\boldsymbol{r}, \boldsymbol{r}'; z)$. The subscript n may stand for more than one index specifying uniquely each eigenfunction and the corresponding eigenvalue. The set $\{\phi_n\}$ can be considered as orthonormal without loss of generality (see Problem 1.1s at the end of Chap. 1), i.e.,

$$\int_\Omega \phi_n^*(\boldsymbol{r})\phi_m(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} = \delta_{nm} \ . \tag{1.3}$$

[1] Several authors write the right-hand side (rhs) of (1.1) as $4\pi\delta(\boldsymbol{r} - \boldsymbol{r}')$ or $-4\pi\delta(\boldsymbol{r} - \boldsymbol{r}')$.

[2] A linear operator, L, acting on arbitrary complex functions, $\phi(\boldsymbol{r})$ and $\psi(\boldsymbol{r})$, defined on Ω and satisfying given BCs is called hermitian if $\int_\Omega \phi^*(\boldsymbol{r})[L\psi(\boldsymbol{r})]\mathrm{d}\boldsymbol{r} = \{\int_\Omega \psi^*(\boldsymbol{r})[L\phi(\boldsymbol{r})]\mathrm{d}\boldsymbol{r}\}^* = \int_\Omega [L\phi(\boldsymbol{r})]^* \psi(\boldsymbol{r})\mathrm{d}\boldsymbol{r}$.

The completeness of the set $\{\phi_n(\boldsymbol{r})\}$ means that (Problem 1.2s)

$$\sum_n \phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') \ . \tag{1.4}$$

(For the definition and properties of Dirac's delta function, δ, see Appendix A.)

Note that n may stand for a set of indices that can take either discrete values (for the discrete part of the spectrum of L, if any) and/or continuous values (for the continuous part of the spectrum of L, if any). Similarly, the symbol $\sum_n$ should be interpreted as $\sum_n{}' + \int \mathrm{d}c$, where $\sum_n{}'$ indicates a genuine summation over the eigenfunctions belonging to the discrete spectrum (if any) and $\int \mathrm{d}c$ denotes (multiple) integration over the continuous spectrum (if any).[3]

Working with Green's functions is greatly facilitated by introducing an abstract vector space, a particular representation of which is the various functions we are dealing with. The most convenient way of achieving this is by using Dirac's bra and ket notation, according to which one can write (Appendix B):

$$\phi_n(\boldsymbol{r}) = \langle \boldsymbol{r} \,|\, \phi_n \rangle \,, \quad \phi_n^*(\boldsymbol{r}) = \langle \phi_n \,|\, \boldsymbol{r} \rangle \,, \quad \text{etc.}\,, \tag{1.5}$$

$$\delta(\boldsymbol{r}-\boldsymbol{r}')\, L(\boldsymbol{r}) \equiv \langle \boldsymbol{r} \,|\, L \,|\, \boldsymbol{r}' \rangle \ , \tag{1.6}$$

$$G(\boldsymbol{r},\boldsymbol{r}';z) \equiv \langle \boldsymbol{r} \,|\, G(z) \,|\, \boldsymbol{r}' \rangle \ , \tag{1.7}$$

$$\langle \boldsymbol{r} \,|\, \boldsymbol{r}' \rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') \ , \tag{1.8}$$

$$\int \mathrm{d}\boldsymbol{r}\, |\boldsymbol{r}\rangle \langle \boldsymbol{r}| = 1 \ , \tag{1.9}$$

where $|\boldsymbol{r}\rangle$ is the eigenvector of the position operator; in the new notation we can write (1.1) to (1.4) as follows:

$$(z-L)G(z) = 1 \ , \tag{1.1$'$}$$

$$L\,|\phi_n\rangle = \lambda_n\,|\phi_n\rangle \ , \tag{1.2$'$}$$

$$\langle \phi_n \,|\, \phi_m \rangle = \delta_{nm} \ , \tag{1.3$'$}$$

$$\sum_n |\phi_n\rangle \langle \phi_n| = 1 \ . \tag{1.4$'$}$$

The ordinary $\boldsymbol{r}$-representation is recaptured by using (1.5)–(1.9); e.g., taking the $\langle \boldsymbol{r}|$, $|\boldsymbol{r}'\rangle$ matrix element of (1.1′) we have

$$\langle \boldsymbol{r} \,|\, (z-L)G(z) \,|\, \boldsymbol{r}' \rangle = \langle \boldsymbol{r} \,|\, 1 \,|\, \boldsymbol{r}' \rangle = \langle \boldsymbol{r} \,|\, \boldsymbol{r}' \rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') \ .$$

[3] The continuous spectrum and the integration $\int \mathrm{d}c$ can be obtained by considering a finite domain Ω and taking the limit as Ω becomes infinite. For example, for plane waves, $\phi_{\boldsymbol{k}} = \frac{1}{\sqrt{\Omega}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$, and in d-dimensional space, $\sum_{\boldsymbol{k}} \underset{\Omega\to\infty}{\longrightarrow} \left[\frac{\Omega}{(2\pi)^d}\right] \int \mathrm{d}\boldsymbol{k}$. (For a proof see Problem 1.5s.)

The left-hand side (lhs) of the last relation can be written as follows:

$$zG(\boldsymbol{r}, \boldsymbol{r}'; z) - \langle \boldsymbol{r} \,|\, LG(z) \,|\, \boldsymbol{r}' \rangle \ .$$

By introducing the unit operator, $\int \mathrm{d}\boldsymbol{r}'' \, |\boldsymbol{r}''\rangle \langle \boldsymbol{r}''|$, between L and G in the last expression we rewrite it in the form

$$zG(\boldsymbol{r}, \boldsymbol{r}'; z) - \int \mathrm{d}\boldsymbol{r}'' \, \langle \boldsymbol{r} \,|\, L \,|\, \boldsymbol{r}'' \rangle \langle \boldsymbol{r}'' \,|\, G(z) \,|\, \boldsymbol{r}' \rangle \ .$$

Finally, taking into account (1.6) we obtain

$$zG(\boldsymbol{r}, \boldsymbol{r}'; z) - L(\boldsymbol{r})G(\boldsymbol{r}, \boldsymbol{r}'; z) = \delta(\boldsymbol{r} - \boldsymbol{r}') \ ,$$

which is identical to (1.1). The usefulness of the bra and ket notation is that

(i) The intermediate algebraic manipulations are facilitated and
(ii) One is not restricted to the $\boldsymbol{r}$-representation (e.g., one can express all equations in the $\boldsymbol{k}$-representation, which is equivalent to taking the Fourier transform with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$ of the original equations).

If all eigenvalues of $z - L$ are nonzero, i.e., if $z \neq \{\lambda_n\}$, then one can solve (1.1′) formally as

$$G(z) = \frac{1}{z - L} \ . \tag{1.10}$$

Multiplying (1.10) by (1.4′) we obtain

$$G(z) = \frac{1}{z - L} \sum_n |\phi_n\rangle \langle \phi_n| = \sum_n \frac{1}{z - L} |\phi_n\rangle \langle \phi_n| = \sum_n \frac{|\phi_n\rangle \langle \phi_n|}{z - \lambda_n} \ . \tag{1.11}$$

The last step follows from (1.2′), and the general relation $F(L)\,|\phi_n\rangle = F(\lambda_n)\,|\phi_n\rangle$ valid by definition for any well-behaved function F. Equation (1.11) can be written more explicitly as

$$G(z) = \sum_n{}' \frac{|\phi_n\rangle \langle \phi_n|}{z - \lambda_n} + \int \mathrm{d}c \, \frac{|\phi_c\rangle \langle \phi_c|}{z - \lambda_c} \ , \tag{1.12}$$

or, in the $\boldsymbol{r}$-representation,

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = \sum_n{}' \frac{\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}')}{z - \lambda_n} + \int \mathrm{d}c \, \frac{\phi_c(\boldsymbol{r})\phi_c^*(\boldsymbol{r}')}{z - \lambda_c} \ . \tag{1.13}$$

Since L is a hermitian operator, all of its eigenvalues $\{\lambda_n\}$ are real. Hence, if $\operatorname{Im}\{z\} \neq 0$, then $z \neq \{\lambda_n\}$, which means that $G(z)$ is an analytic function in the complex z-plane except at those points or portions of the real z-axis that correspond to the eigenvalues of L. As can be seen from (1.12) or (1.13), $G(z)$ exhibits simple poles at the position of the discrete eigenvalues of L; the inverse is also true: *the poles of $G(z)$ give the discrete eigenvalues of L*. If

$z = \lambda$, where λ belongs to the continuous spectrum of L, $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ is not well defined since the integrand in (1.13) has a pole. Then one can attempt to define $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ by a limiting procedure. In the usual case, where the eigenstates associated with the continuous spectrum are propagating or extended (i.e., not decaying as $r \to \infty$), the side limits of $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda \pm \mathrm{i}s)$ as $s \to 0^+$ exist but are different from each other. Thus, this type of continuous spectrum produces a branch cut in $G(z)$ along part(s) of the real z-axis. We mention here in passing, and we shall return to the point in a later chapter, that in disordered systems there is the possibility of a continuous spectrum associated with localized eigenstates [i.e., states decaying fast enough as $r \to \infty$ so that the normalized $\{\phi_n(\boldsymbol{r})\}$ approach a nonzero limit as $\Omega \to \infty$]. For such an unusual spectrum even the side limits $\lim_{s \to 0^+} G(\boldsymbol{r}, \boldsymbol{r}'; \lambda \pm \mathrm{i}s)$ do not exist; the line of singularity corresponding to such a spectrum is not a branch cut but what is called a natural boundary. In what follows we restrict ourselves to the normal case of a continuous spectrum consisting of extended eigenstates. For λ belonging to such a spectrum we define two Green's functions as follows:

$$G^+(\boldsymbol{r}, \boldsymbol{r}'; \lambda) \equiv \lim_{s \to 0^+} G(\boldsymbol{r}, \boldsymbol{r}'; \lambda + \mathrm{i}s) \ , \tag{1.14}$$

$$G^-(\boldsymbol{r}, \boldsymbol{r}'; \lambda) \equiv \lim_{s \to 0^+} G(\boldsymbol{r}, \boldsymbol{r}'; \lambda - \mathrm{i}s) \ , \tag{1.15}$$

with similar definitions for the corresponding operators $G^+(\lambda)$, $G^-(\lambda)$. From (1.13) one can easily see that

$$G^*(\boldsymbol{r}, \boldsymbol{r}'; z) = G(\boldsymbol{r}', \boldsymbol{r}; z^*) \ . \tag{1.16}$$

If z is real, $z = \lambda$, and $\lambda \neq \{\lambda_n\}$, it follows from (1.16) that $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ is hermitian; in particular, $G(\boldsymbol{r}, \boldsymbol{r}; \lambda)$ is real. On the other hand, for λ belonging to the continuous spectrum, we have from (1.16) and definitions (1.14) and (1.15) that

$$G^-(\boldsymbol{r}, \boldsymbol{r}'; \lambda) = \left[G^+(\boldsymbol{r}', \boldsymbol{r}; \lambda)\right]^* \ , \tag{1.17}$$

which shows that

$$\mathrm{Re}\left\{G^-(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} = \ \ \mathrm{Re}\left\{G^+(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} \tag{1.18}$$

and

$$\mathrm{Im}\left\{G^-(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} = -\mathrm{Im}\left\{G^+(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} \ . \tag{1.19}$$

Using the identity (see the solution of Problem 1.3s)

$$\lim_{y \to 0^+} \frac{1}{x \pm \mathrm{i}y} = \mathrm{P}\frac{1}{x} \mp \mathrm{i}\pi\delta(x) \tag{1.20}$$

and (1.13) we can express the discontinuity, $\widetilde{G}(\lambda)$, in terms of delta function

$$\widetilde{G}(\lambda) \equiv G^+(\lambda) - G^-(\lambda) = -2\pi\mathrm{i}\delta(\lambda - L) \ , \tag{1.21}$$

or, in the $\boldsymbol{r}$, $\boldsymbol{r}'$ representation,

$$\begin{aligned}\widetilde{G}\left(\boldsymbol{r},\boldsymbol{r}';\lambda\right) &= -2\pi\mathrm{i}\sum_n \delta\left(\lambda-\lambda_n\right)\phi_n(\boldsymbol{r})\phi_n^*\left(\boldsymbol{r}'\right) \\ &= -2\pi\mathrm{i}{\sum_n}' \delta\left(\lambda-\lambda_n\right)\phi_n(\boldsymbol{r})\phi_n^*\left(\boldsymbol{r}'\right) \\ &\quad -2\pi\mathrm{i}\int \delta\left(\lambda-\lambda_c\right)\phi_c(\boldsymbol{r})\phi_c^*\left(\boldsymbol{r}'\right)\mathrm{d}c\,. \end{aligned} \tag{1.22}$$

For the diagonal matrix element we obtain from (1.13) and (1.20)

$$G^{\pm}\left(\boldsymbol{r},\boldsymbol{r};\lambda\right) = \mathrm{P}\sum_n \frac{\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r})}{\lambda-\lambda_n} \mp \mathrm{i}\pi\sum_n \delta\left(\lambda-\lambda_n\right)\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r})\,. \tag{1.23}$$

Integrating (1.23) over $\boldsymbol{r}$ we have

$$\begin{aligned}\int \mathrm{d}\boldsymbol{r}G^{\pm}\left(\boldsymbol{r},\boldsymbol{r};\lambda\right) &= \int \mathrm{d}\boldsymbol{r}\left\langle \boldsymbol{r}\,\middle|\,G^{\pm}(\lambda)\,\middle|\,\boldsymbol{r}\right\rangle \equiv \mathrm{Tr}\left\{G^{\pm}(\lambda)\right\} \\ &= \mathrm{P}\sum_n \frac{1}{\lambda-\lambda_n} \mp \mathrm{i}\pi\sum_n \delta\left(\lambda-\lambda_n\right)\,. \end{aligned} \tag{1.24}$$

The quantity $\sum_n \delta(\lambda-\lambda_n)$ is the density of states (DOS) at λ, $\mathcal{N}(\lambda)$; $\mathcal{N}(\lambda)\mathrm{d}\lambda$ gives the number of states in the interval $[\lambda,\lambda+\mathrm{d}\lambda]$. The quantity

$$\begin{aligned}\varrho(\boldsymbol{r};\lambda) &\equiv \sum_n \delta\left(\lambda-\lambda_n\right)\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}) \\ &= {\sum_n}' \delta\left(\lambda-\lambda_n\right)\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}) + \int \delta\left(\lambda-\lambda_c\right)\phi_c(\boldsymbol{r})\phi_c^*(\boldsymbol{r})\mathrm{d}c \end{aligned} \tag{1.25}$$

is the DOS per unit volume at point $\boldsymbol{r}$. Obviously,

$$\mathcal{N}(\lambda) = \int \varrho(\boldsymbol{r};\lambda)\mathrm{d}\boldsymbol{r}\,. \tag{1.26}$$

Using (1.22)–(1.25) we obtain

$$\varrho(\boldsymbol{r};\lambda) = \mp\frac{1}{\pi}\mathrm{Im}\left\{G^{\pm}(\boldsymbol{r},\boldsymbol{r};\lambda)\right\} = -\frac{1}{2\pi\mathrm{i}}\widetilde{G}(\boldsymbol{r},\boldsymbol{r};\lambda)\,, \tag{1.27}$$

and

$$\mathcal{N}(\lambda) = \mp\frac{1}{\pi}\mathrm{Im}\left\{\mathrm{Tr}\,G^{\pm}(\lambda)\right\}\,. \tag{1.28}$$

$G(z)$ can be expressed in terms of the discontinuity $\tilde{G}(\lambda) \equiv G^+(\lambda) - G^-(\lambda)$:

$$\begin{aligned}G(\boldsymbol{r},\boldsymbol{r}';z) &= \sum_n \frac{\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}')}{z-\lambda_n} = \int_{-\infty}^{\infty}\mathrm{d}\lambda\sum_n \delta\left(\lambda-\lambda_n\right)\frac{\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r})}{z-\lambda} \\ &= \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\lambda\frac{\widetilde{G}\left(\boldsymbol{r},\boldsymbol{r}';\lambda\right)}{z-\lambda}\,, \end{aligned} \tag{1.29}$$

where (1.22) was taken into account. In particular, for the diagonal matrix elements of G we have

$$G(\boldsymbol{r}, \boldsymbol{r}; z) = \int_{-\infty}^{\infty} \mathrm{d}\lambda' \frac{\varrho(\boldsymbol{r}; \lambda')}{z - \lambda'} . \tag{1.30}$$

Note that $\varrho(\boldsymbol{r}; \lambda')$ versus λ' may consist of a sum of δ functions (corresponding to the discrete spectrum of L) and a continuous function (corresponding to the continuous spectrum of L) as shown in (1.25). Equation (1.30) shows that the DOS per unit volume [i.e., the imaginary part of $\mp G^{\pm}(\boldsymbol{r}, \boldsymbol{r}; \lambda')/\pi$] enables us to calculate $G(\boldsymbol{r}, \boldsymbol{r}; z)$ (both $\mathrm{Re}\{G\}$ and $\mathrm{Im}\{G\}$) for all values of $z = \lambda + \mathrm{i}s$.

Consider the expression

$$\boldsymbol{E}(z) \equiv E_x(x, y) - \mathrm{i}E_y(x, y) = \int_C \mathrm{d}z' \frac{2\varrho(z')}{z - z'} , \tag{1.30'}$$

giving the x and y component of the electric field $\boldsymbol{E}(x, y)$ in two-dimensional (2-d) space in terms of the charge density $\varrho(z') \equiv \varrho(x', y')$ along line C. Comparing with (1.30) we see that $G(\boldsymbol{r}, \boldsymbol{r}; z)$ can be thought of as the electric field generated by a positive charge distribution on the x-axis given by one half the DOS per unit volume, $\varrho/2$. More explicitly, the correspondence is

$$\begin{aligned} \mathrm{Re}\{G(\boldsymbol{r}, \boldsymbol{r}; z)\} &\leftrightarrow \quad E_x(z) , \\ \mathrm{Im}\{G(\boldsymbol{r}, \boldsymbol{r}; z)\} &\leftrightarrow -E_y(z) ; \\ \varrho(\boldsymbol{r}; \lambda) &\leftrightarrow 2\varrho(z') , \\ z \equiv \lambda + \mathrm{i}s &\leftrightarrow z \ = x \ + \mathrm{i}y , \\ \lambda' &\leftrightarrow z' = x' + \mathrm{i}y' . \end{aligned}$$

This analogy is often helpful in visualizing the z dependence of $G(\boldsymbol{r}, \boldsymbol{r}; z)$ for complex values of z. For example, we see immediately that

$$\mathrm{Re}\left\{G^{+}(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} = \quad \mathrm{Re}\left\{G^{-}(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\}$$

while

$$\mathrm{Im}\left\{G^{+}(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} = -\mathrm{Im}\left\{G^{-}(\boldsymbol{r}, \boldsymbol{r}; \lambda)\right\} ,$$

with $\mathrm{Im}\{G^{+}(\boldsymbol{r}, \boldsymbol{r}; \lambda)\}$ being always negative or zero. Of course, when λ is not an eigenvalue of L, $G^{+}(\boldsymbol{r}, \boldsymbol{r}; \lambda)$ is real; it satisfies the relation

$$\frac{\mathrm{d}G(\boldsymbol{r}, \boldsymbol{r}; \lambda)}{\mathrm{d}\lambda} = -\left\langle \boldsymbol{r} \,\middle|\, (\lambda - L)^{-2} \,\middle|\, \boldsymbol{r} \right\rangle < 0 . \tag{1.31}$$

To prove (1.31) we write

$$\frac{\mathrm{d}G(\boldsymbol{r}, \boldsymbol{r}; \lambda)}{\mathrm{d}\lambda} = \frac{\mathrm{d}\left[\left\langle \boldsymbol{r} \,\middle|\, (\lambda - L)^{-1} \,\middle|\, \boldsymbol{r} \right\rangle\right]}{\mathrm{d}\lambda} = -\left\langle \boldsymbol{r} \,\middle|\, (\lambda - L)^{-2} \,\middle|\, \boldsymbol{r} \right\rangle ,$$

which is negative since, for λ real and not coinciding with any eigenvalue of L, $(\lambda - L)^{-2}$ is a positive definite operator.

To summarize our findings: $G(\boldsymbol{r}, \boldsymbol{r}'; z)$ is analytic on the complex z-plane except on portions or points of the real axis. The positions of the poles of $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ on the real axis give the discrete eigenvalues of L. The residue at each pole gives the product $\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}')$ if the corresponding nondegenerate eigenfunction is $\phi_n(\boldsymbol{r})$. Otherwise it gives the sum $\sum_m \phi_m(\boldsymbol{r})\phi_m^*(\boldsymbol{r}')$, where m runs over all eigenstates corresponding to the eigenvalue λ_n. The branch cuts of $G(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ along the real λ-axis correspond to the continuous spectrum of L, and the discontinuity of the diagonal matrix element $G(\boldsymbol{r}, \boldsymbol{r}; \lambda)$ across the branch cut gives the DOS per unit volume times $-2\pi\mathrm{i}$. Note that the analytic continuation of $G(\boldsymbol{r}, \boldsymbol{r}'; z)$ across the branch cut does not coincide with $G(\boldsymbol{r}, \boldsymbol{r}'; z)$, and it may develop singularities in the complex z-plane.

Knowledge of the Green's function $G(\boldsymbol{r}, \boldsymbol{r}'; z)$ permits us to obtain immediately the solution of the general inhomogeneous equation

$$[z - L(\boldsymbol{r})]\, u(\boldsymbol{r}) = f(\boldsymbol{r}) \,, \tag{1.32}$$

where the unknown function $u(\boldsymbol{r})$ satisfies on S the same BCs as $G(\boldsymbol{r}, \boldsymbol{r}'; z)$; $f(\boldsymbol{r})$ is a given function. By taking into account (1.1), it is easy to show that the solution of (1.32) is

$$u(\boldsymbol{r}) = \begin{cases} \displaystyle\int G(\boldsymbol{r}, \boldsymbol{r}'; z)\, f(\boldsymbol{r}')\, \mathrm{d}\boldsymbol{r}' \,, & z \neq \{\lambda_n\} \,, \quad (1.33\mathrm{a}) \\ \displaystyle\int G^{\pm}(\boldsymbol{r}, \boldsymbol{r}'; \lambda)\, f(\boldsymbol{r}')\, \mathrm{d}\boldsymbol{r}' + \phi(\boldsymbol{r}) \,, & z = \lambda \,, \quad (1.33\mathrm{b}) \end{cases}$$

where in (1.33b) λ belongs to the branch cut of $G(z)$ (i.e., λ belongs to the continuous spectrum of L) and $\phi(\boldsymbol{r})$ is the general solution of the corresponding homogeneous equation. If z coincides with a discrete eigenvalue of L, say, λ_n, there is no solution of (1.32) unless $f(\boldsymbol{r})$ is orthogonal to all eigenfunctions associated with λ_n (Problem 1.4). If $u(\boldsymbol{r})$ describes physically the response of a system to a source $f(\boldsymbol{r})$, then $G(\boldsymbol{r}, \boldsymbol{r}')$ describes the response of the same system to a unit point source located at $\boldsymbol{r}'$. Note that the symmetry relation (1.16) is a generalized reciprocity relation: the response at $\boldsymbol{r}$ from a source at $\boldsymbol{r}'$ is essentially the same as the response at $\boldsymbol{r}'$ from a source at $\boldsymbol{r}$. Equation (1.33a) means that the response to the general source $f(\boldsymbol{r})$ can be expressed as the sum of the responses to point sources distributed according to $f(\boldsymbol{r})$.

1.2 Examples

In this section we consider the case where $L(\boldsymbol{r}) = -\nabla^2$ and the domain Ω extends eventually over the whole real space. The BC is that the eigenfunctions of L must be finite at infinity. Then the eigenfunctions are

$$\langle \boldsymbol{r} \,|\, \boldsymbol{k} \rangle = \frac{1}{\sqrt{\Omega}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \,, \tag{1.34}$$

and the eigenvalues are

$$\lambda_n = \boldsymbol{k}^2 \,, \tag{1.35}$$

where the components of the vector $\boldsymbol{k}$ are real to satisfy the BCs. Thus, the spectrum is continuous, extending from 0 to $+\infty$. The Green's function can be obtained by either solving the defining equation, which in the present case is

$$\left(z + \nabla_r^2\right) G(\boldsymbol{r}, \boldsymbol{r}'; z) = \delta(\boldsymbol{r} - \boldsymbol{r}') \,, \tag{1.36}$$

or from (1.13), which in the present case can be written as

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = \sum_{\boldsymbol{k}} \frac{\langle \boldsymbol{r} \,|\, \boldsymbol{k} \rangle \, \langle \boldsymbol{k} \,|\, \boldsymbol{r}' \rangle}{z - k^2} = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d} \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{r} - \boldsymbol{r}')}}{z - k^2} \,, \tag{1.37}$$

where d is the dimensionality.[4] For $d = 3$ we will use (1.37) to evaluate G, while for $d = 2$ or 1 we will compute G from (1.36).

1.2.1 Three-Dimensional Case ($d = 3$)

If $\boldsymbol{\varrho}$ is the difference $\boldsymbol{r} - \boldsymbol{r}'$ and θ the angle between $\boldsymbol{k}$ and $\boldsymbol{\varrho}$, we can write (1.37) as

$$\begin{aligned} G(\boldsymbol{r}, \boldsymbol{r}'; z) &= \frac{1}{4\pi^2} \int_0^\infty \frac{k^2 \mathrm{d}k}{z - k^2} \int_0^\pi \mathrm{d}\theta \sin\theta \, \mathrm{e}^{\mathrm{i}k\varrho\cos\theta} \\ &= \frac{1}{4\pi^2} \int_0^\infty \frac{k^2 \mathrm{d}k}{z - k^2} \frac{\mathrm{e}^{\mathrm{i}k\varrho} - \mathrm{e}^{-\mathrm{i}k\varrho}}{\mathrm{i}k\varrho} \\ &= \frac{1}{4\mathrm{i}\pi^2 \varrho} \int_{-\infty}^\infty \frac{k\mathrm{e}^{\mathrm{i}k\varrho}}{z - k^2} \mathrm{d}k \,. \end{aligned} \tag{1.38}$$

The integration path can be closed by an infinite semicircle in the upper half plane. Unless z is real and nonnegative, one of the poles (denoted by $\sqrt{z}$) of the integrand in (1.38) has a positive imaginary part and hence lies within the integration contour, and the other (denoted by $-\sqrt{z}$) has a negative imaginary part and lies outside the integration contour. By employing the residue theorem we obtain from (1.38)

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = -\frac{\exp\left(\mathrm{i}\sqrt{z}\,|\boldsymbol{r} - \boldsymbol{r}'|\right)}{4\pi\,|\boldsymbol{r} - \boldsymbol{r}'|}; \qquad \mathrm{Im}\,\{z\} > 0 \,. \tag{1.39}$$

If $z = \lambda$, where $\lambda \geq 0$ (i.e., if z coincides with the eigenvalues of $-\nabla^2$), the two poles lie on the integration contour and G is not well defined. The side limits $G^{\pm}(\boldsymbol{r}, \boldsymbol{r}'; \lambda)$ are well defined and are given by

[4] Use was made of the relation $\sum_{\boldsymbol{k}} \to \left[\Omega/(2\pi)^d\right] \int \mathrm{d}\boldsymbol{k}$ as $\Omega \to \infty$. For a proof and comments see Problem 1.5s.

$$G^{\pm}(\boldsymbol{r},\boldsymbol{r}';\lambda) = -\frac{\mathrm{e}^{\pm\mathrm{i}\sqrt{\lambda}|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|}; \qquad \sqrt{\lambda},\lambda \geq 0\,. \tag{1.40}$$

For $z = \lambda$, where $\lambda < 0$, we obtain from (1.39)

$$G(\boldsymbol{r},\boldsymbol{r}';\lambda) = -\frac{\mathrm{e}^{-\sqrt{|\lambda|}|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|}; \qquad \lambda < 0, \qquad \sqrt{|\lambda|} > 0\,. \tag{1.41}$$

For the particular case $z = 0$ we have

$$G(\boldsymbol{r},\boldsymbol{r}';0) = -\frac{1}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|}\,. \tag{1.42}$$

As can be seen from (1.36), $G(\boldsymbol{r},\boldsymbol{r}';0)$ is the Green's function corresponding to a Laplace equation with a point source, i.e.,

$$\nabla_r^2 G(\boldsymbol{r},\boldsymbol{r}';0) = \delta\left(\boldsymbol{r}-\boldsymbol{r}'\right)\,. \tag{1.43}$$

By employing (1.33b) we can write the general solution of Poisson's equation

$$\nabla^2 V(\boldsymbol{r}) = -4\pi\varrho(\boldsymbol{r})$$

as

$$\begin{aligned} V(\boldsymbol{r}) &= \int G(\boldsymbol{r},\boldsymbol{r}';0)(-4\pi)\varrho\left(\boldsymbol{r}'\right)\mathrm{d}\boldsymbol{r}' + \text{const.} \\ &= \int \frac{\varrho\left(\boldsymbol{r}'\right)\mathrm{d}\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} + \text{const.} \end{aligned} \tag{1.44}$$

The constant has been added since the most general eigenfunction of $-\nabla^2$ corresponding to eigenvalue 0 is a constant, as can be seen from (1.34) and (1.35). Equation (1.44) is the basic result in electrostatics.

1.2.2 Two-Dimensional Case ($d = 2$)

Because of symmetry considerations, $G(\boldsymbol{r},\boldsymbol{r}';z)$ is a function of the magnitude of the 2-d vector $\boldsymbol{\varrho} = \boldsymbol{r} - \boldsymbol{r}'$ and z. Furthermore, it satisfies the homogeneous equation

$$(z + \nabla^2)G(\varrho;z) = 0 \qquad \text{for} \quad \varrho \neq 0\,. \tag{1.45}$$

The δ function source can be transformed into an equivalent BC as $\varrho \to 0$; indeed, by applying Gauss' theorem, $\int \nabla\cdot(\nabla G)\,\mathrm{d}\Omega = \int \nabla G\cdot\mathrm{d}\boldsymbol{S}$, which in the present 2-d case takes the form

$$\int_0^{\varrho} \nabla^2 G\; 2\pi\varrho'\,\mathrm{d}\varrho' = 2\pi\varrho\frac{\partial G}{\partial\varrho}\,,$$

we obtain from (1.36)

$$2\pi\varrho\frac{\partial G}{\partial\varrho} + 2\pi z\int_0^{\varrho} G\varrho'\mathrm{d}\varrho' = 1\ ,$$

which, as $\varrho \to 0$, leads to

$$G(\varrho) \underset{\varrho\to 0}{\longrightarrow} \frac{1}{2\pi}\ln\varrho + \text{const.} \tag{1.46}$$

Furthermore, $G(\varrho)$ must satisfy the condition

$$G(\varrho) \underset{\varrho\to\infty}{\longrightarrow} 0\ . \tag{1.47}$$

The only solution of (1.45) that is symmetric and satisfies BCs (1.46) and (1.47) is

$$G(\boldsymbol{r},\boldsymbol{r}';z) = -\frac{\mathrm{i}}{4}H_0^{(1)}\left(\sqrt{z}\,|\boldsymbol{r}-\boldsymbol{r}'|\right); \qquad \mathrm{Im}\left\{\sqrt{z}\right\} > 0\ , \tag{1.48}$$

where $H_0^{(1)}$ is the Hankel function of zero order of the first kind.[5] This can be seen from the fact that the general solution of (1.45) is a superposition of terms like $\left[A_nH_n^{(1)}(\sqrt{z}\varrho) + B_nH_n^{(2)}(\sqrt{z}\varrho)\right]\mathrm{e}^{\pm in\theta}$ (Appendix C). Since we are looking for a θ-independent solution, $n = 0$; furthermore, the Hankel function $H_0^{(2)}(\sqrt{z}\varrho)$, for $\mathrm{Im}\{\sqrt{z}\} > 0$, blows up as $\varrho \to \infty$ and must be excluded. Finally, (1.46) together with the relation $H_0^{(1)}(\sqrt{z}\varrho) \to (2\mathrm{i}/\pi)\ln(\varrho)$ as $\varrho \to 0$ fixes the coefficient A_0. For $z = \lambda$, where $\lambda \geq 0$, (i.e., for z coinciding with the spectrum of $-\nabla^2$) $\mathrm{Im}\{\sqrt{z}\} = 0$, and only the side limits are well defined as

$$G^{\pm}(\boldsymbol{r},\boldsymbol{r}';\lambda) = -\frac{\mathrm{i}}{4}H_0^{(1)}\left(\pm\sqrt{\lambda}\varrho\right); \qquad \sqrt{\lambda} > 0\ , \tag{1.49}$$

where[5]

$$H_0^{(1)}\left(-\sqrt{\lambda}\varrho\right) = -H_0^{(2)}\left(\sqrt{\lambda}\varrho\right)\ . \tag{1.50}$$

G^+ describes an outgoing wave, while G^- is an ingoing wave; this can be seen from the asymptotic form of $H_0^{(1)}$ and $H_0^{(2)}$.

Equation (1.48) for the particular case $z = -|\lambda|$ can be recast as

$$G^{\pm}(\boldsymbol{r},\boldsymbol{r}';-|\lambda|) = -\frac{1}{2\pi}K_0\left(\sqrt{|\lambda|}\,|\boldsymbol{r}-\boldsymbol{r}'|\right); \qquad \sqrt{|\lambda|} > 0\ , \tag{1.51}$$

where K_0 is the modified Bessel function of zero order.[5]

The Green's function corresponding to the 2-d Laplace equation can be obtained from (1.48) by letting $z \to 0$ and keeping the leading $|\boldsymbol{r}-\boldsymbol{r}'|$-dependent term. We find that

[5] For definitions and properties of Bessel and Hankel functions see the book by Abramowitz and Stegun [1].

$$G(\boldsymbol{r}, \boldsymbol{r}'; 0) = \frac{1}{2\pi} \ln |\boldsymbol{r} - \boldsymbol{r}'| + \text{const.} \tag{1.52}$$

The solution of Poisson's equation in 2-d is then

$$V(\boldsymbol{r}) = -2 \int \varrho\,(\boldsymbol{r}') \ln |\boldsymbol{r} - \boldsymbol{r}'|\, \mathrm{d}\boldsymbol{r}' + \text{const.} \tag{1.53}$$

Taking the $-\nabla$ of (1.53) we obtain the expression for the 2-d electric field given before in (1.30′).

1.2.3 One-Dimensional Case ($d = 1$)

The basic equation (1.36) becomes

$$\left(z + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) G\,(x, x'; z) = \delta\,(x - x')\ . \tag{1.54}$$

For $x < x'$ we have $G = A \exp\left(-\mathrm{i}\sqrt{z}x\right)$ with $\mathrm{Im}\left\{\sqrt{z}\right\} > 0$, while for $x > x'$ we obtain $G = B \exp(\mathrm{i}\sqrt{z}x)$; the choice of signs in the exponents ensures that $G \to 0$ as $|x| \to \infty$. By integrating (1.54) we find that $G(x'^{-}, x'; 0) = G(x'^{+}, x'; z)$ and $(\mathrm{d}G/\mathrm{d}x)_{x=x'^{+}} - (\mathrm{d}G/\mathrm{d}x)_{x=x'^{-}} = 1$. We thus determine the constants A and B. We obtain finally

$$G(x, x'; z) = \frac{\exp\left(\mathrm{i}\sqrt{z}\,|x - x'|\right)}{2\mathrm{i}\sqrt{z}}\ ; \qquad \mathrm{Im}\left\{\sqrt{z}\right\} > 0\ . \tag{1.55}$$

For $z = \lambda \geq 0$ (i.e., within the continuous spectrum of $-\mathrm{d}^2/\mathrm{d}x^2$) we have for the side limits

$$G^{\pm}(x, x'; \lambda) = \mp \frac{\mathrm{i}}{2\sqrt{\lambda}} \exp\left(\pm\mathrm{i}\sqrt{\lambda}\,|x - x'|\right)\ ; \quad \lambda > 0, \sqrt{\lambda} > 0\ . \tag{1.56}$$

For $z = -\,|\lambda|$ we obtain from (1.55)

$$G(x, x'; -\,|\lambda|) = -\frac{1}{2\sqrt{|\lambda|}} \exp\left(-\sqrt{|\lambda|}\,|x - x'|\right)\ ; \quad \sqrt{|\lambda|} > 0\ . \tag{1.57}$$

The Green's function for the 1-d Laplace equation can be found either by solving (1.54) for $z = 0$ directly or by taking the limit of $(G^{+} + G^{-})/2$ as $\lambda \to 0$. We find

$$G(x, x'; 0) = \frac{1}{2}\,|x - x'| + \text{const.} \tag{1.58}$$

1.2.4 Finite Domain Ω

The problem of determination of G becomes more tedious when the surface S bounding our domain Ω consists in part (or in whole) of pieces at a finite distance from the point $\boldsymbol{r}'$ of the source. One can then employ any of the following methods to determine G:

1. Use general equation (1.13) where the eigenvalues and eigenfunctions are the ones associated with the BCs on S.
2. Write G as $G = G^{\infty} + \phi$, where G^{∞} is the Green's function associated with the infinite domain (which is assumed to be known) and ϕ is the general solution of the corresponding homogeneous equation. Then determine the arbitrary coefficients in ϕ by requiring that $G^{\infty} + \phi$ satisfy the given BCs on S. It is then clear that G satisfies both the differential equation and the BCs.
3. Divide the domain Ω into two subdomains by a surface S' passing through the source point $\boldsymbol{r}'$. Then G in the interior of each subdomain satisfies a homogeneous equation. Find in each subdomain the general solution of the homogeneous equation subject to the given BCs on S. Next, match the two solutions on S' in a way obtained by integrating the differential equation for G around $\boldsymbol{r}'$. An elementary example of this technique was used in Sect. 1.2.3.
4. Write, e.g., in 3-d,

$$\begin{aligned}\delta(\boldsymbol{r}-\boldsymbol{r}') &= \frac{1}{r^2}\delta(r-r')\,\delta(\phi-\phi')\,\delta(\cos\theta-\cos\theta') \\ &= \frac{1}{r^2}\delta(r-r')\sum_{\ell m} Y_{\ell m}(\theta,\phi)Y^{*}_{\ell m}(\theta',\phi')\end{aligned}$$

   so as to reduce the problem to 1-d with respect to r and r'.

The interested reader may find a brief presentation of these techniques in the book by Mathews and Walker [2]. A more comprehensive and rigorous presentation is given in the second volume of the book by Byron and Fuller [3]; see also the books by Duffy [4], Barton [5], Roach [6], Stakgold [7] and Morse and Feshbach [8]. Several books on electromagnetism, such as those by Smythe [9] or Jackson [10], contain several interesting examples of Green's functions.

Finally, it should be mentioned that for more complicated operators L (such as those describing the quantum-mechanical motion of a particle in an external field), the determination of G is a very complicated problem. More often than not one has to employ approximate techniques such as perturbation expansions. We will return to this very interesting subject in Chap. 4. Examples of methods (1) to (4) mentioned above are presented in the solutions of the problems in Chap. 1 (see also Appendix C).

1.3 Summary

1.3.1 Definition

The Green's function, corresponding to the linear, hermitian, time-independent differential operator $L(\boldsymbol{r})$ and the complex variable $z = \lambda + \mathrm{i}s$, is defined