Multidimensional Green's Functions: Formalism

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The extensive study of Green's functions in one dimension in the last chapter has no doubt exhibited the power and elegance of their use in solving inhomogeneous differential equations. If the differential equation has a (unique) solution, the GF exists and contains all the information necessary to build it up. The solution results from operating on the inhomogeneous term with an integral operator whose kernel is the appropriate Green's function.

The Green's function's very existence depends on the type of BCs imposed. We encountered two types of problems in solving ODEs. The first, called initial value problems (IVPs), involves fixing (for an nth-order DE) the value of the solution and its first $n-1$ derivatives at a fixed point. Then the ODE, if it is sufficiently well-behaved, will determine the values of the solution in the neighborhood of the fixed point in a unique way. Because of this uniqueness, Green's functions always exist for IVPs.

The second type of problems, called boundary value problems (BVPs), consists—when the DE is second order—of determining a relation between the solution and its derivative evaluated at the boundaries of some interval $[a, b]$. These boundary values are relations that we denoted by $\mathbf{R}_i[u] = \gamma_i$, where $i = 1, 2$. In this case, the existence and uniqueness of the Green's function are not guaranteed.

There is a fundamental (topological) difference between a boundary in one dimension and a boundary in two and more dimensions. In one dimension a boundary consists of *only two points*; in 2 and higher dimensions a boundary has *infinitely many points*. The boundary of a region in $\mathbb{R}^2$ is a closed curve, in $\mathbb{R}^3$ it is a closed surface, and in $\mathbb{R}^m$ it is called a **hypersurface**. This fundamental difference makes the study of Green's functions in higher dimensions more complicated, but also richer and more interesting.

21.1 Properties of Partial Differential Equations

This section presents certain facts and properties of PDEs, in particular, how BCs affect their solutions. We shall discover the important difference between ODEs and PDEs: The existence of a solution to a PDE satisfying a given BC depends on the type of the PDE.

S. Hassani, *Mathematical Physics*, DOI 10.1007/978-3-319-01195-0_21,

We shall be concerned exclusively with a linear PDE. A linear PDE of order M in m variables is of the form

$$\mathbf{L}_{\mathbf{x}}[u] = f(\mathbf{x}) \quad \text{where} \quad \mathbf{L}_{\mathbf{x}} = \sum_{|J|=1}^{M} \sum_{J} a_J(\mathbf{x}) \frac{\partial^{|J|}}{\partial \mathbf{x}^J}, \tag{21.1}$$

where the following notation has been used:

$$\mathbf{x} = (x_1, \ldots, x_m), \qquad J = (j_1, \ldots, j_m),$$
$$|J| = j_1 + j_2 + \cdots + j_m, \qquad \frac{\partial^{|J|}}{\partial \mathbf{x}^J} = \frac{\partial^{|J|}}{\partial x_1^{j_1} \partial x_2^{j_2} \cdots \partial x_m^{j_m}};$$

the j_k are nonnegative integers; M, the order of the highest derivative, is called the **order** of the PDE. The outer sum in Eq. (21.1) is over $|J|$; once $|J|$ is fixed, the inner summation goes over individual j_k's with the restriction that their sum has to equal the given $|J|$.

principal part of a PDE

The **principal part** of $\mathbf{L}_{\mathbf{x}}$ is

$$\mathbf{L}_p = \sum_{|J|=M} a_J(x_1, \ldots, x_m) \frac{\partial^M}{\partial \mathbf{x}^J}. \tag{21.2}$$

The coefficients a_J and the inhomogeneous (or source) term f are assumed to be continuous functions of their arguments.

We consider Eq. (21.1) as an IVP with appropriate initial data. The most direct generalization of the IVP of ordinary differential equation theory is to specify the values of u and all its *normal derivatives* of order less than or equal to $M-1$ on a hypersurface Γ of dimension $m-1$. This type of initial data is called **Cauchy data**, and the resulting IVP is known as the **Cauchy problem** for $\mathbf{L}_{\mathbf{x}}$. The reason that the tangential derivatives do not come into play here is that once we know the values of u on Γ, we can evaluate u on two neighboring points on Γ, take the limit as the points get closer and closer, and evaluate the tangential derivatives.

Cauchy data and Cauchy problem

21.1.1 Characteristic Hypersurfaces

In contrast to the IVP in one dimension, the Cauchy problem for arbitrary Cauchy data may not have a solution, or if it does, the solution may not be unique.

Box 21.1.1 *The existence and uniqueness of the solution of the Cauchy problem depend crucially on the hypersurface* Γ *and on the type of PDE.*

We assume that Γ can be parametrized by a set of m functions of $m-1$ parameters. These parameters can be thought of as generalized coordinates of points of Γ.

Consider a point P on Γ. Introduce $m-1$ coordinates $\xi_2, \ldots, \xi_m$, called **tangential coordinates**, to label points on Γ. Choose, by translation if necessary, coordinates in such a way that P is the origin, with coordinates $(0, 0, \ldots, 0)$. Now let $\nu = \xi_1$ stand for the remaining coordinate normal to Γ. Usually ξ_i is taken to be the ith coordinate of the projection of the point on Γ onto the hyperplane tangent to Γ at P.

tangential coordinates

As long as we do not move too far away from P, the Cauchy data on Γ can be written as

$$u(0, \xi_2, \ldots, \xi_m), \qquad \frac{\partial u}{\partial \nu}(0, \xi_2, \ldots, \xi_m), \ldots, \frac{\partial^{M-1} u}{\partial \nu^{M-1}}(0, \xi_2, \ldots, \xi_m).$$

Using the chain rule, $\partial u/\partial x_i = \sum_{j=1}^{m} (\partial u/\partial \xi_j)(\partial \xi_j/\partial x_i)$, where $\xi_1 = \nu$, we can also determine the first $M-1$ derivatives of u with respect to x_i. The fundamental question is whether we can determine u uniquely using the above Cauchy data and the DE. To motivate the answer, let's look at the analogous problem in one dimension.

Consider the Mth-order linear ODE

$$\mathbf{L}_x[u] = a_M(x)\frac{d^M u}{dx^M} + \cdots + a_1(x)\frac{du}{dx} + a_0(x)u = f(x) \tag{21.3}$$

with the following initial data at x_0: $\{u(x_0), u'(x_0), \ldots, u^{(M-1)}(x_0)\}$. If the coefficients $\{a_k(x)\}_{k=0}^{M}$ and the inhomogeneous term $f(x)$ are continuous and if $a_M(x_0) \neq 0$, then Theorem 20.2.2 implies that there exists a unique solution to the IVP in a neighborhood of x_0.

For $a_M(x_0) \neq 0$, Eq. (21.3), the initial data, and a knowledge of $f(x_0)$ give $u^{(M)}(x_0)$ uniquely. Having found $u^{(M)}(x_0)$, we can calculate, with arbitrary accuracy (by choosing Δx small enough), the following set of *new* initial data at $x_1 = x_0 + \Delta x$:

$$u(x_1) = u(x_0) + u'(x_0)\Delta x, \ldots, u^{(M-1)}(x_1) = u^{(M-1)}(x_0) + u^{(M)}(x_0)\Delta x.$$

Using these new initial data and Theorem 20.2.2, we are assured of a unique solution at x_1. Since $a_M(x)$ is assumed to be continuous for x_1, for sufficiently small Δx, $a_M(x_0)$ is nonzero, and it is possible to find newer initial data at $x_2 = x_1 + \Delta x$. The process can continue until we reach a singularity of the DE, a point where $a_M(x)$ vanishes. We can thus construct the unique solution of the IVP in an interval (x_0, b) as long as $a_M(x)$ does not vanish anywhere in $[x_0, b]$. This procedure is analogous to the one used in the analytic continuation of a complex function.

For $a_M(x_0) = 0$, however, we cannot calculate $u^{(M)}(x_0)$ unambiguously. In such a case the LHS of (21.3) is completely determined from the initial data. If the LHS happens to be equal to $f(x_0)$, then the equation is satisfied for *any* $u^{(M)}(x_0)$, i.e., there exist infinitely many solutions for $u^{(M)}(x_0)$; if the LHS is not equal to $f(x_0)$, there are no solutions. The difficulty can be stated in another way, which is useful for generalization to the m-dimensional case: If $a_M(x_0) = 0$ in (21.3), then the initial data determine the function $\mathbf{L}_x[u]$.

Let us now return to the question of constructing u and investigate conditions under which the Cauchy problem may have a solution. We follow the same steps as for the IVP for ODEs. To construct the solution numerically for points near P but away from Γ (since the function is completely determined on Γ, not only its Mth derivative but derivatives of all orders are known on Γ), we must be able to calculate $\partial^M u/\partial \nu^M$ at P. This is not possible if the coefficient of $\partial^M u/\partial \nu^M$ in $\mathbf{L}_{\mathbf{x}}[u]$ is zero when $x_1, \ldots, x_m$ is written in terms of $\nu, \xi_2, \ldots, \xi_m$. When this happens, $\mathbf{L}_x[u]$ itself will be determined by the Cauchy data. This motivates the following definition.

characteristic hypersurface

Definition 21.1.2 If $\mathbf{L}_{\mathbf{x}}[u]$ can be evaluated at a point P on Γ from the Cauchy data alone, then Γ is said to be **characteristic** for $\mathbf{L}_{\mathbf{x}}$ at P. If Γ is characteristic for all its points, then it is called a **characteristic hypersurface** for $\mathbf{L}_{\mathbf{x}}$. The Cauchy problem does not have a solution at a point on the characteristic hypersurface.

The following theorem characterizes Γ:

Theorem 21.1.3 *Let Γ be a smooth $(m-1)$-dimensional hypersurface. Let $\mathbf{L}_{\boldsymbol{x}}[u] = f$ be an Mth-order linear PDE in m variables. Then Γ is characteristic at $P \in \Gamma$ if and only if the coefficient of $\partial^M u/\partial \nu^M$ vanishes when $\mathbf{L}_{\boldsymbol{x}}$ is expressed in terms of the normal–tangential coordinate system $(\nu, \xi_2, \ldots, \xi_m)$.*

One can rephrase the foregoing theorem as follows:

Box 21.1.4 *The hypersurface Γ is* not *characteristic at P if and only if all Mth-order partial derivatives of u with respect to $\{x_i\}_{i=1}^m$ are unambiguously determined at P by the DE and the Cauchy data on Γ.*

Characteristic "hypersurfaces" of ODEs are points!

In the one-dimensional case the difficulty arose when $a_M(x_0) = 0$. In the language being used here, we could call x_0 a "characteristic point." This makes sense because in this special case ($m = 1$), the hypersurfaces can only be of dimension 0. Thus, we can say that in the neighborhood of a characteristic point, the IVP has no well-defined solution.[1] For the general case ($m > 1$), we can similarly say that the Cauchy problem has no well-defined solution in the neighborhood of P if P happens to lie on a characteristic hypersurface of the differential operator. Thus, it is important to determine the characteristic hypersurfaces of PDEs.

Example 21.1.5 Let us consider the first-order PDE in two variables

$$\mathbf{L}_{\mathbf{x}}[u] = a(x, y)\frac{\partial u}{\partial x} + b(x, y)\frac{\partial u}{\partial y} + F(x, y, u) = 0 \tag{21.4}$$

[1] Here lies the crucial difference between ODEs and PDEs: All ODEs have a universal characteristic hypersurface, i.e., a point. PDEs, on the other hand, can have a variety of hypersurfaces.

where $F(x, y, u) \equiv c(x, y)u + d(x, y)$. For this discussion the form of F is irrelevant.

We wish to find the characteristic hypersurfaces (in this case, curves) of **L**. The Cauchy data consist of a simple determination of u on Γ. By Theorem 21.1.3, we need to derive relations that ensure that $\partial u/\partial x$ and $\partial u/\partial y$ cannot be unambiguously determined at $P = (x, y)$. Using an obvious notation, the PDE of Eq. (21.4) gives

$$-F\big(P, u(P)\big) = a(P)\frac{\partial u}{\partial x}(P) + b(P)\frac{\partial u}{\partial y}(P).$$

On the other hand, if $Q \equiv (x + dx, y + dy)$ lies on the curve Γ, then

$$u(Q) - u(P) = dx\frac{\partial u}{\partial x}(P) + dy\frac{\partial u}{\partial y}(P).$$

The Cauchy data determine the LHS of both of the preceding equations. Treating these equations as a system of two linear equations in two unknowns, $\partial u/\partial x(P)$ and $\partial u/\partial y(P)$, we conclude that the system has a unique solution if and only if the matrix of coefficients is invertible. Thus, by Box 21.1.4, Γ is a characteristic curve if and only if

$$\det\begin{pmatrix} dx & dy \\ a(P) & b(P) \end{pmatrix} = b(P)\,dx - a(P)\,dy = 0,$$

or $dy/dx = b(x, y)/a(x, y)$, assuming that $a(x, y) \neq 0$. Solving this FODE yields y as a function of x, thus determining the characteristic curve. Note that a general solution of this FODE involves an arbitrary constant, resulting in a family of characteristic curves.

Historical Notes

Sofia Vasilyevna Kovalevskaya (1850–1891) is considered the greatest woman mathematician prior to the twentieth century. She grew up in a well-educated family of the Russian nobility, her father being an artillery general and reputed to be a descendant of a Hungarian king, Mathias Korvin. Sonja was educated by a British governess and enjoyed life at the large country estate of her father's family, although the rather progressive thinking of the Kovalevsky sisters did not always meet with approval from their father.

Sonja has written of two factors that attracted her to the study of mathematics. The first was her Uncle Pyotr, who had studied the subject on his own and would speak of squaring the circle and of the asymptote, as well as of many other things that excited her imagination. The second was a curious "wallpaper" that was used to cover one of the children's rooms at Polibino, which turned out to be lecture notes on differential and integral calculus that had been purchased by her father in student days. These sheets fascinated her and she would spend hours trying to decipher separate phrases and to find the proper ordering of the pages.

In the autumn of 1867 Sonja went to St. Petersburg, where she studied calculus with Alexander Strannolyubsky, a teacher of mathematics at the naval school. While there, she consulted the prominent Russian mathematician Chebyshev about her mathematical studies, but since Russian universities were closed to women, there seemed to be no way that she could pursue advanced studies in her native land.

In order to escape the oppression of women common in Russia at the time, young ladies of ambition and ability would often arrange a marriage of convenience in order to allow study at a foreign university. At the age of 18, Sonya arranged such a marriage with Vladimir Kovalevsky, a paleontologist, and in 1869 the couple moved to Heidelberg, where Sonja took courses from Kirchhoff, Helmholtz, and others. Two years later

Sofia Vasilyevna Kovalevskaya 1850–1891

she went to Berlin, where she worked with Weierstrass, who tutored her privately, since she, as a woman, was not allowed to attend lectures.
The three papers she published in the next three years earned her a doctorate in absentia from the University of Göttingen. Unfortunately, even that distinction was not sufficient to gain her a university position anywhere in Europe, despite strong recommendation from the renowned Weierstrass. Her rejections resulted in a six-year period during which time she neither undertook research nor replied to Weierstrass's letters. She was bitter to discover that the best job she was offered was teaching arithmetic to elementary classes of schoolgirls, and remarked, "I was unfortunately weak in the multiplication table."
The existence and uniqueness of solutions to partial differential equations occupied the attention of many notable mathematicians of the last century, including Cauchy, who transformed the problem into his *method of majorant functions*. This method was later extended and refined by Kovalevskaya to include more general cases. The result was the now-famous *Cauchy–Kovalevskaya theorem*. She also contributed to the advancement of the study of Abelian integrals and functions and applied her knowledge of these topics to problems in physics, including her paper "On the Rotation of a Solid Body About a Fixed Point," for which she won a 5000-franc prize. She also performed some investigations into the dynamics of Saturn's rings, inspiring a sonnet in which she is named "Muse of the Heavens." In 1878, Kovalevskaya gave birth to a daughter, but from 1880 increasingly returned to her study of mathematics. In 1882 she began work on the refraction of light, and wrote three articles on the topic. In the spring of 1883, Vladimir, from whom Sonja had been separated for two years, committed suicide. After the initial shock, Kovalevskaya immersed herself in mathematical work in an attempt to rid herself of feelings of guilt. Mittag-Leffler managed to overcome opposition to Kovalevskaya in Stockholm, and obtained for her a position as privat docent. She began to lecture there in early 1884, was appointed to a five-year extraordinary professorship in June of that year, and in June 1889 became the third woman ever to hold a chair at a European university.
During Kovalevskaya's years at Stockholm she carried out important research, taught courses on the latest topics in analysis, and became an editor of the new journal *Acta Mathematica*. She was the liaison with the mathematicians of Paris and Berlin, and took part in the organization of international conferences. Interestingly, Kovalevskaya also nurtured a parallel career in literature, penning several novels and a drama, "The Struggle for Happiness" that was favorably received at the Korsh Theater in Moscow. She died at the pinnacle of her scientific career from a combination of influenza and pneumonia less than two years after her election to both the Swedish and the Russian Academies of Sciences. The latter membership being initiated by Chebyshev, in spite of the Tsarist government's repeated refusal to grant her a university position in her own country.

21.1.2 Second-Order PDEs in m Dimensions

Because of their importance in mathematical physics, the rest of this chapter and the next will be devoted to SOPDEs. This subsection classifies SOPDEs and the BCs associated with them.

The most general linear SOPDE in m variables can be written as

$$\sum_{j,k=1}^{m} A_{jk}(\mathbf{x})\frac{\partial^2 u}{\partial x_j \partial x_k} + \sum_{j=1}^{m} B_j(\mathbf{x})\frac{\partial u}{\partial x_j} + C(\mathbf{x})u = 0,$$

where A_{jk} can be assumed to be symmetric in j and k. We restrict ourselves to the simpler case in which the matrix (A_{jk}) is diagonal.[2] We therefore

[2]This is not a restriction because, by a change of variables and Theorem 6.6.6 (especially the comments after it) A_{jk} can be brought to a diagonal form.

consider the PDE

$$\sum_{j=1}^{m} a_j(\mathbf{x}) \frac{\partial^2 u}{\partial x_j^2} + F\left(\mathbf{x}, u, \frac{\partial u}{\partial \mathbf{x}}\right), \tag{21.5}$$

where the last term collects all the terms except the second derivatives. We classify SOPDEs as follows:

second-order PDE of elliptic type

1. Equation (21.5) is said to be of **elliptic type** at $\mathbf{x}_0$ if all the coefficients $a_j(\mathbf{x}_0)$ are nonzero and have the same sign.

second-order PDEs of hyperbolic and ultrahyperbolic type

2. Equation (21.5) is said to be of **ultrahyperbolic type** at $\mathbf{x}_0$ if all $a_j(\mathbf{x}_0)$ are nonzero but do not have the same sign. If only one of the coefficients has a sign different from the rest, the equation is said to be of **hyperbolic type**.

second-order PDE of parabolic type

3. Equation (21.5) is said to be of **parabolic type** at $\mathbf{x}_0$ if at least one of the coefficients $a_j(\mathbf{x}_0)$ is zero.

If a SOPDE is of a given type at every point of its domain, it is said to be of that given type. In particular, if the coefficients a_j are constants, the type of the PDE does not change from point to point.

Example 21.1.6 In this example, we study the SOPDE in two dimensions. The most general linear SOPDE is

$$\mathbf{L}[u] = a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0, \tag{21.6}$$

where a, b, and c are functions of x and y.

To determine the characteristic curves of $\mathbf{L}$, we seek conditions under which all second-order partial derivatives of u can be determined from the DE and the Cauchy data, which are values of u and all its first derivatives on Γ. Consider a point $Q \equiv (x + dx, y + dy)$ close to $P \equiv (x, y)$. We can write

$$\begin{aligned}
\frac{\partial u}{\partial x}(Q) - \frac{\partial u}{\partial x}(P) &= dx\frac{\partial^2 u}{\partial x^2}(P) + dy\frac{\partial^2 u}{\partial x \partial y}(P), \\
\frac{\partial u}{\partial y}(Q) - \frac{\partial u}{\partial y}(P) &= dx\frac{\partial^2 u}{\partial x \partial y}(P) + dy\frac{\partial^2 u}{\partial y^2}(P), \\
-F\left(P, u(P), \frac{\partial u}{\partial x}(P), \frac{\partial u}{\partial y}(P)\right) &= a(P)\frac{\partial^2 u}{\partial x^2}(P) + 2b(P)\frac{\partial^2 u}{\partial x \partial y}(P) \\
&\quad + c(P)\frac{\partial^2 u}{\partial y^2}(P).
\end{aligned}$$

This system of three linear equations in the three unknowns—the three second derivatives evaluated at P—has a unique solution if and only if the determinant of the coefficients is nonzero. Thus, by Box 21.1.4, Γ is a char-

acteristic curve if and only if

$$\det \begin{pmatrix} dx & dy & 0 \\ 0 & dx & dy \\ a(P) & 2b(P) & c(p) \end{pmatrix} = 0,$$

or $a(x, y)(dy)^2 - 2b(x, y)dxdy + c(x, y)(dx)^2 = 0$. It then follows, assuming that $a(x, y) \neq 0$, that

$$\frac{dy}{dx} = \frac{b \pm \sqrt{b^2 - ac}}{a}. \tag{21.7}$$

There are three cases to consider:

1. If $b^2 - ac < 0$, Eq. (21.7) has no solution, which implies that no characteristic curves exist at P. Problem 21.1 shows that the SOPDE is of elliptic type. Thus, the Laplace equation in two dimensions is elliptic because $b^2 - ac = -1$. In fact, it is elliptic in the whole plane, or, stated differently, it has no characteristic curve in the entire xy-plane. This may lead us to believe that the Cauchy problem for the Laplace equation in two dimensions has a unique solution. However, even though the absence of a characteristic hypersurface at P is a necessary condition for the existence of a solution to the Cauchy problem, it is not sufficient. Problem 21.4 presents a Cauchy problem that is **ill-posed**, meaning that the solution at any fixed point is not a continuous function of the initial data. Satisfying this continuity condition is required of a well-posed problem on both mathematical and physical grounds.

ill-posed Cauchy problem

2. If $b^2 - ac > 0$, Eq. (21.7) has two solutions; that is, there are two characteristic curves passing through P. Problem 21.1 shows that the SOPDE is of hyperbolic type. The wave equation is such an equation in the entire $\mathbb{R}^2$.
3. If $b^2 - ac = 0$, Eq. (21.7) has only one solution. In this case there is only one characteristic curve at P. The SOPDE is parabolic in this case. The one-dimensional diffusion equation is an example of an SOPDE that is parabolic in the entire $\mathbb{R}^2$.

appropriate BCs are determined by the type of PDE

The question of what type of BCs to use to obtain a unique solution for a PDE is a very intricate mathematical problem. As Problem 21.4 shows, even though it has no characteristic curves in the entire $\mathbb{R}^2$, the two-dimensional Laplace equation does not lead to a well-posed Cauchy problem. On the other hand, examples in Chap. 19 that dealt with electrostatic potentials and temperatures led us to believe that a specification of the solution u on a *closed* curve in 2D, and a closed surface in 3D, gives a unique solution. This has a sound physical basis. After all, specifying the temperature (or electrostatic potential) on a closed surface should be enough to give us information about the temperature (or electrostatic potential) in the region close to the curve.

Dirichlet boundary condition and boundary value problem

Definition 21.1.7 A boundary condition in which the value of the solution is given on a closed hypersurface is called a **Dirichlet boundary condition**, and the associated problem, a **Dirichlet BVP**.

There is another type of BC, which on physical grounds is appropriate for the Laplace equation. This condition is based on the fact that if the surface charge on a conductor is specified, then the electrostatic potential in the vicinity of the conductor can be determined uniquely. The surface charge on a conductor is proportional to the value of the electric field on the conductor. The electric field, on the other hand, is the normal derivative of the potential.

Neumann boundary condition and boundary value problem

Definition 21.1.8 A boundary condition in which the value of the normal derivative of the solution is specified on a closed hypersurface is called a **Neumann BC**, and the associated problem, a **Neumann boundary value problem**.

Thus, at least on physical grounds, either a Dirichlet BVP or a Neumann BVP is a well-posed problem for the Laplace equation.

For the heat (or diffusion) equation we are given an initial temperature distribution $f(x)$ on a bar along, say the x-axis, with end points held at constant temperatures. For a bar with end points at $x = a$ and $x = b$, this is equivalent to the data $u(0, x) = f(x)$, $u(t, a) = T_1$, and $u(t, b) = T_2$. These are not Cauchy data, so we need not worry about characteristic curves. The boundary curve consists of three parts: (1) $t = 0$ for $a \leq x \leq b$, (2) $t > 0$ for $x = a$, and (3) $t > 0$, for $x = b$. In the xt-plane, these form an open rectangle consisting of $\overline{ab}$ as one side and vertical lines at a and b as the other two. The problem is to determine u on the side that closes the rectangle, that is, on the side $a \leq x \leq b$ at $t > 0$.

The wave equation requires specification of both u and $\partial u/\partial t$ at $t = 0$. The displacement of the boundaries of the waving medium—a taut rope for example—must also be specified. Again the curve is open, as for the diffusion case, but the initial data are Cauchy. Thus, for the wave equation we do have a Cauchy problem with Cauchy data specified on an open curve. Since the curve, the open rectangle, is not a characteristic curve of the wave equation, the Cauchy problem is well-posed. We can generalize these BCs to m dimensions.

Boundary conditions for elliptic, hyperbolic, and parabolic PDEs

Box 21.1.9 *The following correspondences exist between SOPDEs with m variables and their appropriate BCs*:

1. *Elliptic SOPDE* $\leftrightarrow$ *Dirichlet or Neumann BCs on a closed hypersurface.*
2. *Hyperbolic SOPDE* $\leftrightarrow$ *Cauchy data on an open hypersurface.*
3. *Parabolic SOPDE* $\leftrightarrow$ *Dirichlet or Neumann BCs on an open hypersurface.*

21.2 Multidimensional GFs and Delta Functions

This section will discuss some of the characteristics of Green's functions in higher dimensions. These characteristics are related to the formal partial

differential operator associated with the Green's function and also to the delta functions.

Using the formal idea of several continuous indices, we can turn the operator equation $\mathbf{LG} = \mathbf{1}$ into the PDE

$$\mathbf{L}_{\mathbf{x}} G(\mathbf{x}, \mathbf{y}) = \frac{\delta(\mathbf{x} - \mathbf{y})}{w(\mathbf{x})}, \tag{21.8}$$

where $\mathbf{x}, \mathbf{y} \in \mathbb{R}^m$, $w(\mathbf{x})$ is a weight function that is usually set equal to one, and, *only in Cartesian coordinates*,

$$\delta(\mathbf{x} - \mathbf{y}) = \delta(x_1 - y_1)\delta(x_2 - y_2) \cdots \delta(x_m - y_m) = \prod_{i=1}^{m} \delta(x_i - y_i). \tag{21.9}$$

In most applications Cartesian coordinates are not the most convenient to use. Therefore, it is helpful to express Eqs. (21.8) and (21.9) in other coordinate systems. In particular, it is helpful to know how the delta function transforms under a general coordinate transformation.

Let $x_i = f_i(\xi_1, \ldots, \xi_m)$, $i = 1, 2, \ldots, m$, be a coordinate transformation. Let P be a point whose coordinates are $\mathbf{a} = (a_1, \ldots, a_m)$ and $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_m)$ in the x and ξ coordinate systems, respectively. Let J be the Jacobian of the transformation, that is, the absolute value of the determinant of a matrix whose elements are $\partial x_i / \partial \xi_j$. For a function $F(\mathbf{x})$ the definition of the delta function gives

$$\int d^m x \, F(\mathbf{x}) \delta(\mathbf{x} - \mathbf{a}) = F(\mathbf{a}).$$

Expressing this equation in terms of the ξ coordinate system, recalling that $d^m x = J d^m \xi$ and $a_i = f_i(\boldsymbol{\alpha})$, and introducing the notation $H(\boldsymbol{\xi}) \equiv F(f_1(\boldsymbol{\xi}), \ldots, f_m(\boldsymbol{\xi}))$, we obtain

$$\int d^m \xi \, J H(\boldsymbol{\xi}) \prod_{i=1}^{m} \delta\big(f_i(\boldsymbol{\xi}) - f_i(\boldsymbol{\alpha})\big) = H(\boldsymbol{\alpha}). \tag{21.10}$$

This suggests that

$$J \prod_{i=1}^{m} \delta\big(f_i(\boldsymbol{\xi}) - f_i(\boldsymbol{\alpha})\big) = \prod_{i=1}^{m} \delta(\xi_i - \alpha_i),$$

or, in more compact notation,

$$J \delta(\mathbf{x} - \mathbf{a}) = \delta(\boldsymbol{\xi} - \boldsymbol{\alpha}).$$

It is, of course, understood that $J \neq 0$ at P. What happens when $J = 0$ at P?

singular point of a transformation

A point at which the Jacobian vanishes is called a **singular point** of the transformation. Thus, all points on the z-axis, including the origin, are singular points of Cartesian–spherical transformation. Since J is a determinant, its vanishing at a point signals lack of invertibility at that point. Thus, in the transformation from Cartesian to spherical coordinates, all spherical coordinates $(5, \pi, \varphi)$, with arbitrary φ, are mapped to the Cartesian coordinates

$(0, 0, -5)$. Similarly, the point $(0, 0, 0)$ in the Cartesian coordinate system goes to $(0, \theta, \varphi)$ in the spherical system, with θ and φ arbitrary. A coordinate whose value is not determined at a singular point is called an **ignorable coordinate** at that point. Thus, at the origin both θ and φ are ignorable.

ignorable coordinates

Among the ξ coordinates, let $\{\xi_i\}_{i=k+1}^{m}$ be ignorable at P with Cartesian coordinates $\mathbf{a}$. This means that any function, when expressed in terms of ξ's, will be independent of the ignorable coordinates. A reexamination of Eq. (21.10) reveals that (see Problem 21.8)

$$\delta(\mathbf{x}-\mathbf{a}) = \frac{1}{|J_k|}\prod_{i=1}^{k}\delta(\xi_i-\alpha_i), \quad \text{where} \quad J_k = \int J\, d\xi_{k+1}\cdots d\xi_m. \tag{21.11}$$

In particular, if the transformation is invertible, $k = m$ and $J_m = J$, and we recover $J\delta(\mathbf{x}-\mathbf{a}) = \delta(\boldsymbol{\xi}-\boldsymbol{\alpha})$.

Example 21.2.1 In two dimensions the transformation between Cartesian and polar coordinates is given by $x_1 \equiv x = r\cos\theta \equiv \xi_1\cos\xi_2$, $x_2 \equiv y = r\sin\theta \equiv \xi_1\sin\xi_2$ with the Jacobian

$$J = \det\begin{pmatrix} \partial x_1/\partial\xi_1 & \partial x_1/\partial\xi_2 \\ \partial x_2/\partial\xi_1 & \partial x_2/\partial\xi_2 \end{pmatrix} = \det\begin{pmatrix} \cos\xi_2 & -\xi_1\sin\xi_2 \\ \sin\xi_2 & \xi_1\cos\xi_2 \end{pmatrix} = \xi_1 = r,$$

which vanishes at the origin. The angle θ is the only ignorable coordinate at the origin. Thus, $k = 2-1 = 1$, and

$$J_1 = \int_0^{2\pi} J\, d\theta = \int_0^{2\pi} r\, d\theta = 2\pi r \quad \Rightarrow \quad \delta(\mathbf{x}) \equiv \delta(x)\delta(y) = \frac{\delta(r)}{2\pi r}.$$

In three dimensions, the transformation between Cartesian and spherical coordinates yields the Jacobian $J = r^2\sin\theta$. This vanishes at the origin regardless of the values of θ and φ. We thus have two ignorable coordinates at the origin (therefore, $k = 3-2 = 1$), over which we integrate to obtain

$$J_1 = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta r^2\sin\theta = 4\pi r^2 \quad \Rightarrow \quad \delta(\mathbf{x}) = \frac{\delta(r)}{4\pi r^2}.$$

21.2.1 Spherical Coordinates in m Dimensions

In discussing Green's functions in m dimensions, a particular curvilinear coordinate system will prove useful. This system is the generalization of spherical coordinates in three dimensions. The m-dimensional spherical coordinate system is defined as

$$x_k = r\left(\prod_{j=1}^{m-k}\sin\theta_j\right)\cos\theta_{m-k+1}, \quad k = 1, \ldots, m, \tag{21.12}$$

where, by definition, we set $\theta_m = 0$ and $\prod_{j=1}^{0}\sin\theta_j = 1$. (Note that for $m = 3$, the first two Cartesian coordinates are switched compared to their usual definitions.)

It is not hard to show (see Example 21.2.2) that the Jacobian of the transformation (21.12) is

$$J = r^{m-1}(\sin\theta_1)^{m-2}(\sin\theta_2)^{m-3}\cdots(\sin\theta_k)^{m-k-1}\cdots\sin\theta_{m-2} \tag{21.13}$$

and that the volume element in terms of these coordinates is

$$d^m x = J\, dr\, d\theta_1 \cdots d\theta_{m-1} = r^{m-1} dr\, d\Omega_m, \tag{21.14}$$

element of the m-dimensional solid angle

where

$$d\Omega_m = (\sin\theta_1)^{m-2}(\sin\theta_2)^{m-3}\cdots\sin\theta_{m-2} d\theta_1 d\theta_2 \cdots d\theta_{m-1} \tag{21.15}$$

is the element of the **m-dimensional solid angle**.

Example 21.2.2 For $m = 4$ we have

$$x_1 = r\sin\theta_1\sin\theta_2\sin\theta_3, \qquad x_2 = r\sin\theta_1\sin\theta_2\cos\theta_3,$$
$$x_3 = r\sin\theta_1\cos\theta_2, \qquad x_4 = r\cos\theta_1,$$

and the Jacobian is given by

$$J = \det\begin{pmatrix} \partial x_1/\partial r & \partial x_1/\partial\theta_1 & \partial x_1/\partial\theta_2 & \partial x_1/\partial\theta_3 \\ \partial x_2/\partial r & \partial x_2/\partial\theta_1 & \partial x_2/\partial\theta_2 & \partial x_2/\partial\theta_3 \\ \partial x_3/\partial r & \partial x_3/\partial\theta_1 & \partial x_3/\partial\theta_2 & \partial x_3/\partial\theta_3 \\ \partial x_4/\partial r & \partial x_4/\partial\theta_1 & \partial x_4/\partial\theta_2 & \partial x_4/\partial\theta_3 \end{pmatrix} = r^3\sin^2\theta_1\sin\theta_2.$$

It is readily seen (one can use mathematical induction to prove it rigorously) that the Jacobians for $m = 2$ ($J = r$), $m = 3$ ($J = r^2\sin\theta_1$), and $m = 4$ ($J = r^3\sin^2\theta_1\sin\theta_2$) generalize to Eq. (21.13).

Using the integral

$$\int_0^\pi \sin^n\theta\, d\theta = \sqrt{\pi}\frac{\Gamma[(n+1)/2]}{\Gamma[(n+2)/2]},$$

the total solid angle in m dimensions can be found to be

$$\Omega_m = \frac{2\pi^{m/2}}{\Gamma(m/2)}. \tag{21.16}$$

An interesting result that is readily obtained is an expression of the delta function in terms of spherical coordinates at the origin. Since $r = 0$, Eq. (21.12) shows that all the angles are ignorable. Thus, we have

$$J_1 = \int J\, d\theta_1 \cdots d\theta_{m-1} = r^{m-1}\int d\Omega_m = r^{m-1}\Omega_m,$$

which yields

$$\delta(\mathbf{x}) = \delta(x_1)\cdots\delta(x_m) = \frac{\delta(r)}{\Omega_m r^{m-1}} = \frac{\Gamma(m/2)\delta(r)}{2\pi^{m/2}r^{m-1}}. \tag{21.17}$$

21.2.2 Green's Function for the Laplacian

With the machinery developed above, we can easily obtain the (indefinite) Green's function for the Laplacian in m dimensions. We will ignore questions of BCs and simply develop a function that satisfies $\nabla^2 G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y})$. Without loss of generality we let $\mathbf{y} = 0$; that is, we translate the axes so that $\mathbf{y}$ becomes the new origin. Then we have $\nabla^2 G(\mathbf{x}) = \delta(\mathbf{x})$. In spherical coordinates this becomes

$$\nabla^2 G(\mathbf{x}) = \frac{\delta(r)}{\Omega_m r^{m-1}} \tag{21.18}$$

by (21.17). Since the RHS is a function of r only, we expect G to behave in the same way. We now have to express ∇^2 in terms of spherical coordinates. In general, this is difficult; however, for a function of $r = \sqrt{x_1^2 + \cdots + x_m^2}$ alone, such as $F(r)$, we have

$$\frac{\partial F}{\partial x_i} = \frac{\partial F}{\partial r}\frac{\partial r}{\partial x_i} = \frac{\partial F}{\partial r}\frac{x_i}{r} \quad \text{and} \quad \frac{\partial^2 F}{\partial {x_i}^2} = \frac{\partial^2 F}{\partial r^2}\frac{x_i^2}{r^2} + \frac{\partial F}{\partial r}\left(\frac{1}{r} - \frac{x_i^2}{r^3}\right),$$

so that

$$\nabla^2 F(r) = \sum_{i=1}^{m} \frac{\partial^2 F}{\partial {x_i}^2} = \frac{\partial^2 F}{\partial r^2} + \frac{m-1}{r}\frac{\partial F}{\partial r} = \frac{1}{r^{m-1}}\frac{\partial}{\partial r}\left(r^{m-1}\frac{\partial F}{\partial r}\right).$$

For the Green's function, therefore, we get

$$\frac{d}{dr}\left(r^{m-1}\frac{dG}{dr}\right) = \frac{\delta(r)}{\Omega_m}. \tag{21.19}$$

The solution, for $m \geq 3$, is (see Problem 21.9)

$$G(r) = -\frac{\Gamma(m/2)}{2(m-2)\pi^{m/2}}\left(\frac{1}{r^{m-2}}\right) \quad \text{for } m \geq 3. \tag{21.20}$$

We can restore the vector $\mathbf{y}$, at which we placed the origin, by noting that $r = |\mathbf{r}| = |\mathbf{x} - \mathbf{y}|$. Thus, we get

$$\begin{aligned} G(\mathbf{x}, \mathbf{y}) &= -\frac{\Gamma(m/2)}{2(m-2)\pi^{m/2}}\left(\frac{1}{|\mathbf{x} - \mathbf{y}|^{m-2}}\right) \\ &= -\frac{\Gamma(m/2)}{2(m-2)\pi^{m/2}}\left[\sum_{i=1}^{m}(x_i - y_i)^2\right]^{-(m-2)/2} \quad \text{for } m \geq 3. \end{aligned} \tag{21.21}$$

Green's function for the Laplacian

Similarly, we obtain

$$G(\mathbf{x}, \mathbf{y}) = \frac{1}{2\pi}\ln|\mathbf{x} - \mathbf{y}| = \frac{1}{4\pi}\ln\left[(x_1 - y_1)^2 + (x_2 - y_2)^2\right] \quad \text{for } m = 2. \tag{21.22}$$

solution of Poisson equation in m dimensions

Having found the Green's function for the Laplacian, we can find a solution to the inhomogeneous equation, the *Poisson equation*, $\nabla^2 u = -\rho(\mathbf{x})$. Thus, for $m \geq 3$, we get

$$u(\mathbf{x}) = -\int d^m y G(\mathbf{x}, \mathbf{y})\rho(\mathbf{y}) = \frac{\Gamma(m/2)}{2(m-2)\pi^{m/2}} \int d^m y \frac{\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{m-2}}.$$

In particular, for $m = 3$, we obtain

$$u(\mathbf{x}) = \frac{1}{4\pi} \int d^3 y \frac{\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|},$$

which is the electrostatic potential due to a charge density $\rho(\mathbf{y})$.

21.3 Formal Development

The preceding section was devoted to a discussion of the Green's function for the Laplacian with no mention of the BCs. This section will develop a formalism that not only works for more general operators, but also incorporates the BCs.

21.3.1 General Properties

Basic to a study of GFs is Green's identity, whose 1-dimensional version we encountered in Chap. 20. Here, we generalize it to m dimensions. Suppose there exist two differential operators, $\mathbf{L}_\mathbf{x}$ and $\mathbf{L}_\mathbf{x}^\dagger$, which for any two functions u and v, satisfy the following relation:[3]

$$v^* \mathbf{L}_\mathbf{x}[u] - u\big(\mathbf{L}_\mathbf{x}^\dagger[v]\big)^* = \boldsymbol{\nabla} \cdot \mathbf{Q}\big[u, v^*\big] \equiv \sum_{i=1}^{m} \frac{\partial Q_i}{\partial x_i}\big[u, v^*\big]. \tag{21.23}$$

The differential operator $\mathbf{L}_\mathbf{x}^\dagger$ is—as in the one-dimensional case—called the formal adjoint of $\mathbf{L}_\mathbf{x}$. Integrating (21.23) over a closed domain D in $\mathbb{R}^m$ with boundary ∂D, and using the divergence theorem, we obtain

$$\int_D d^m x \big\{ v^* \mathbf{L}_\mathbf{x}[u] - u\big(\mathbf{L}_\mathbf{x}^\dagger[v]\big)^* \big\} = \int_{\partial D} \mathbf{Q} \cdot \hat{\mathbf{e}}_n \, da, \tag{21.24}$$

where $\hat{\mathbf{e}}_n$ is an m-dimensional unit vector normal to ∂D, and da is an element of "area" of the m-dimensional hypersurface ∂D. Equation (21.24) is the **generalized Green's identity** for m dimensions. Note that the weight function is set equal to one for simplicity.

generalized Green's identity

[3] The notions of divergence and divergence theorem require the machinery of differential geometry to which we shall come back later. Here, we are simply using a direct and most obvious generalization of the notions from three to m dimensions.

The differential operator $\mathbf{L}_\mathbf{x}$ is said to be formally self-adjoint if the RHS of Eq. (21.24), the surface term, vanishes. In such a case, we have $\mathbf{L}_\mathbf{x} = \mathbf{L}_\mathbf{x}^\dagger$ as in one dimension. This relation is a necessary condition for the surface term to vanish because u and v are, by assumption, arbitrary. $\mathbf{L}_\mathbf{x}$ is called self-adjoint (or, somewhat imprecisely, hermitian) if $\mathbf{L}_\mathbf{x} = \mathbf{L}_\mathbf{x}^\dagger$ and the domains of the two operators, as determined by the vanishing of the surface term, are identical.

We can use Eq. (21.24) to study the pair of PDEs

$$\mathbf{L}_\mathbf{x}[u] = f(\mathbf{x}) \quad \text{and} \quad \mathbf{L}_\mathbf{x}^\dagger[v] = h(\mathbf{x}). \tag{21.25}$$

As in one dimension, we let $G(\mathbf{x}, \mathbf{y})$ and $g(\mathbf{x}, \mathbf{y})$ denote the Green's functions for $\mathbf{L}_\mathbf{x}$ and $\mathbf{L}_\mathbf{x}^\dagger$, respectively. Let us assume that the BCs are such that the surface term in Eq. (21.24) vanishes. Then we get Green's identity

$$\int_D d^m x v^* \mathbf{L}_\mathbf{x}[u] = \int_D d^m x u \big(\mathbf{L}_\mathbf{x}^\dagger[v]\big)^*. \tag{21.26}$$

If in this equation we let $u = G(\mathbf{x}, \mathbf{t})$ and $v = g(\mathbf{x}, \mathbf{y})$, where $\mathbf{t}, \mathbf{y} \in D$, we obtain

$$\int_D d^m x g^*(\mathbf{x}, \mathbf{y}) \delta(\mathbf{x} - \mathbf{t}) = \int_D d^m x G(\mathbf{x}, \mathbf{t}) \delta(\mathbf{x} - \mathbf{y}),$$

or $g^*(\mathbf{t}, \mathbf{y}) = G(\mathbf{y}, \mathbf{t})$. In particular, when $\mathbf{L}_\mathbf{x}$ is formally self-adjoint, we have $G^*(\mathbf{t}, \mathbf{y}) = G(\mathbf{y}, \mathbf{t})$, or $G(\mathbf{t}, \mathbf{y}) = G(\mathbf{y}, \mathbf{t})$, if all the coefficient functions of $\mathbf{L}_\mathbf{x}$ are real. That is, the Green's function will be symmetric.

Green's functions are symmetric functions of their arguments

If we let $v = g(\mathbf{x}, \mathbf{y})$ and use the first equation of (21.25) in (21.26), we get $u(\mathbf{y}) = \int_D d^m x g^*(\mathbf{x}, \mathbf{y}) f(\mathbf{x})$, which, using $g^*(\mathbf{t}, \mathbf{y}) = G(\mathbf{y}, \mathbf{t})$ and interchanging $\mathbf{x}$ and $\mathbf{y}$, becomes $u(\mathbf{x}) = \int_D d^m y G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})$. It can similarly be shown that $v(\mathbf{x}) = \int_D d^m y g(\mathbf{x}, \mathbf{y}) h(\mathbf{y})$.

21.3.2 Fundamental (Singular) Solutions

The inhomogeneous term of the differential equation to which $G(\mathbf{x}, \mathbf{y})$ is a solution is the delta function, $\delta(\mathbf{x} - \mathbf{y})$. It would be surprising if $G(\mathbf{x}, \mathbf{y})$ did not "take notice" of this catastrophic source term and did not adapt itself to behave differently at $\mathbf{x} = \mathbf{y}$ than at any other "ordinary" point. We noted the singular behavior of the Green's function at $x = y$ in one dimension when we proved Theorem 20.3.5. There we introduced $h(x, y)$—which was discontinuous at $x = y$—as a part of the Green's function. Similarly, when we discussed the Green's functions for the Laplacian in two and m dimensions earlier in this chapter, we noted that they behaved singularly at $\mathbf{r} = 0$ or $\mathbf{x} = \mathbf{y}$. In this section, we study similar properties of the GFs for other differential operators.

Next to the Laplacian in difficulty is the formally self-adjoint elliptic PDO $\mathbf{L}_\mathbf{x} = \nabla^2 + q(\mathbf{x})$ discussed in Problem 21.10. Substituting this operator in the generalized Green's identity and using the expression for $\mathbf{Q}$ given in

Problem 21.10, we obtain

$$\int_D d^m x \left\{ v \mathbf{L}_{\mathbf{x}}[u] - u\big(\mathbf{L}_{\mathbf{x}}[v]\big) \right\} = \int_{\partial D} (v \hat{\mathbf{e}}_n \cdot \boldsymbol{\nabla} u - u \hat{\mathbf{e}}_n \cdot \boldsymbol{\nabla} v)\, da.$$

Letting $v = G(\mathbf{x}, \mathbf{y})$ and denoting $\hat{\mathbf{e}}_n \cdot \boldsymbol{\nabla}$ by $\partial/\partial n$ gives

$$\int_D d^m x [G \mathbf{L}_{\mathbf{x}} u - u \mathbf{L}_{\mathbf{x}} G] = \int_{\partial D} \left[G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right] da. \tag{21.27}$$

We want to use this equation to find out about the behavior of $G(\mathbf{x}, \mathbf{y})$ as $|\mathbf{x} - \mathbf{y}| \to 0$. Therefore, assuming that $\mathbf{y} \in D$, we divide the domain D into two parts: one part is a region D_ϵ bounded by an infinitesimal hypersphere S_ϵ with radius ϵ and center at $\mathbf{y}$; the other is the rest of D. Instead of D we use the region $D' \equiv D - D_\epsilon$. The following facts are easily deduced for D':

(1) $\mathbf{L}_{\mathbf{x}} G(\mathbf{x}, \mathbf{y}) = 0$ because $\mathbf{x} \neq \mathbf{y}$ in D';
(2) $\int_D = \lim_{\epsilon \to 0} \int_{D'}$;
(3) $\partial D' = \partial D \cup S_\epsilon$.

Suppose that we are interested in finding a solution to

$$\mathbf{L}_{\mathbf{x}}[u] = \big[\nabla^2 + q(\mathbf{x})\big] u(\mathbf{x}) = f(\mathbf{x})$$

subject to certain, as yet unspecified, BCs. Using the three facts listed above, Eq. (21.27) yields

$$\begin{aligned}
&\int_D d^m x [G \mathbf{L}_{\mathbf{x}} u - u \mathbf{L}_{\mathbf{x}} G] \\
&= \lim_{\epsilon \to 0} \int_{D'} d^m x [G \underbrace{\mathbf{L}_{\mathbf{x}} u}_{=f} - u \underbrace{\mathbf{L}_{\mathbf{x}} G}_{=0}] \\
&= \lim_{\epsilon \to 0} \int_{D'} d^m x G(\mathbf{x}, \mathbf{y}) f(\mathbf{x}) = \int_D d^m x G(\mathbf{x}, \mathbf{y}) f(\mathbf{x}) \\
&= \int_{\partial D} \left(G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right) da + \int_{S_\epsilon} \left(G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right) da.
\end{aligned}$$

We assume that the BCs are such that the integral over ∂D vanishes. This is a generalization of the one-dimensional case (recall from Chap. 20 that this is a necessary condition for the existence of Green's functions). Moreover, for an m-dimensional sphere, $da = r^{m-1} d\Omega_m$, which for S_ϵ reduces to $\epsilon^{m-1} d\Omega_m$. Substituting in the preceding equation yields

$$\int_D d^m x G(\mathbf{x}, \mathbf{y}) f(\mathbf{x}) = \int_{S_\epsilon} \left(G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right) \epsilon^{m-1} d\Omega_m.$$

We would like the RHS to be $u(\mathbf{y})$. This will be the case if

$$\lim_{\epsilon \to 0} \int_{S_\epsilon} G(\mathbf{x}, \mathbf{y}) \frac{\partial u}{\partial n} \epsilon^{m-1} d\Omega_m = 0 \quad \text{and} \quad \lim_{\epsilon \to 0} \int_{S_\epsilon} u \frac{\partial G}{\partial n} \epsilon^{m-1} d\Omega_m = u(\mathbf{y})$$

for *arbitrary* u. This will happen only if

$$\lim_{r\to 0} G(\mathbf{y}+\mathbf{r},\mathbf{y})r^{m-1}=0, \qquad \lim_{r\to 0}\frac{\partial G}{\partial r}(\mathbf{y}+\mathbf{r},\mathbf{y})r^{m-1}=\text{const.} \quad (21.28)$$

A solution to these two equations is

$$G(\mathbf{x},\mathbf{y})=\begin{cases} -\frac{F(\mathbf{x},\mathbf{y})}{2\pi}\ln(|\mathbf{x}-\mathbf{y}|)+H(\mathbf{x},\mathbf{y}) & \text{if } m=2,\\ -\frac{1}{(m-2)\Omega_m}\frac{F(\mathbf{x},\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{m-2}}+H(\mathbf{x},\mathbf{y}) & \text{if } m\geq 3, \end{cases} \quad (21.29)$$

where $H(\mathbf{x},\mathbf{y})$ and $F(\mathbf{x},\mathbf{y})$ are well behaved at $\mathbf{x}=\mathbf{y}$. The introduction of these functions is necessary because Eq. (21.28) determines the behavior of $G(\mathbf{x},\mathbf{y})$ only when $\mathbf{x}\approx\mathbf{y}$. Such behavior does not uniquely determine $G(\mathbf{x},\mathbf{y})$. For instance, $e^{|\mathbf{x}-\mathbf{y}|}\ln(|\mathbf{x}-\mathbf{y}|)$ and $\ln(|\mathbf{x}-\mathbf{y}|)$ behave in the same way as $|\mathbf{x}-\mathbf{y}|\to 0$.

Equation (21.29) shows that for $\mathbf{L}_\mathbf{x}=\nabla^2+q(\mathbf{x})$, the Green's function consists of two parts. The first part determines the singular behavior of the Green's function as $\mathbf{x}\to\mathbf{y}$. The nature of this singularity (how badly the GF "blows up" as $\mathbf{x}\to\mathbf{y}$) is extremely important, because it is a prerequisite for our ability to write the solution in terms of an integral representation with the Green's function as its kernel. Due to their importance in such representations, the first terms on the RHS of Eq. (21.29) are called the **fundamental solution** of the differential equation, or the **singular part** of the Green's function.

fundamental solution is the singular part of GF

What about the second part of the Green's function? What role does it play in obtaining a solution? So far we have been avoiding consideration of BCs. Here $H(\mathbf{x},\mathbf{y})$ can help. We choose $H(\mathbf{x},\mathbf{y})$ in such a way that $G(\mathbf{x},\mathbf{y})$ satisfies the appropriate BCs. Let us discuss this in greater detail and generality.

If BCs are ignored, the Green's function for a SOPDO $\mathbf{L}_\mathbf{x}$ cannot be determined uniquely. In particular, if $G(\mathbf{x},\mathbf{y})$ is a Green's function, that is, if $\mathbf{L}_\mathbf{x}G(\mathbf{x},\mathbf{y})=\delta(\mathbf{x}-\mathbf{y})$, then so is $G(\mathbf{x},\mathbf{y})+H(\mathbf{x},\mathbf{y})$ as long as $H(\mathbf{x},\mathbf{y})$ is a solution of the homogeneous equation $\mathbf{L}_\mathbf{x}H(\mathbf{x},\mathbf{y})=0$. Thus, we can break the Green's function into two parts:

homogeneous solution is the regular part of GF

$$G=G_s+H, \quad \text{where} \quad \mathbf{L}_\mathbf{x}G_s(\mathbf{x},\mathbf{y})=\delta(\mathbf{x}-\mathbf{y}), \quad \mathbf{L}_\mathbf{x}H(\mathbf{x},\mathbf{y})=0 \quad (21.30)$$

with G_s the singular part of the Green's function. H is called the **regular part** of the Green's function. Neither G_s nor H (nor G, therefore) is unique. However, the appropriate BCs, which depend on the type of $\mathbf{L}_\mathbf{x}$, will determine G uniquely.

regular part of the Green's function

To be more specific, let us assume that we want to find a Green's function for $\mathbf{L}_\mathbf{x}$ that vanishes at the boundary ∂D. That is, we wish to find $G(\mathbf{x},\mathbf{y})$ such that $G(\mathbf{x}_b,\mathbf{y})=0$, where $\mathbf{x}_b$ is an arbitrary point of the boundary. All that is required is to find a G_s and an H satisfying Eq. (21.30) with the BC $H(\mathbf{x}_b,\mathbf{y})=-G_s(\mathbf{x}_b,\mathbf{y})$. The latter problem, involving a homogeneous differential equation, can be handled by the methods of Chap. 19. Since any discussion of BCs is tied to the type of PDE, we have reserved the discussion of such specifics for the next chapter.

21.4 Integral Equations and GFs

Integral equations are best applied in combination with Green's functions. In fact, we can use a Green's function to turn a DE into an integral equation. If this integral equation is compact or has a compact resolvent, then the problem lends itself to the methods described in Chaps. 17 and 18.

Let $\mathbf{L_x}$ be a SOPDO in m variables. We are interested in solving the SOPDE

$$\mathbf{L_x}[u] + \lambda V(\mathbf{x})u(\mathbf{x}) = f(\mathbf{x})$$

subject to some BCs. Here λ is an arbitrary constant, and $V(\mathbf{x})$ is a well-behaved function on $\mathbb{R}^m$. Transferring the second term on the LHS to the RHS and then treating the RHS as an inhomogeneous term, we can write the "solution" to the PDE as

$$u(\mathbf{x}) = H(\mathbf{x}) + \int_D d^m y G_0(\mathbf{x}, \mathbf{y})\big[f(\mathbf{y}) - \lambda V(\mathbf{y})u(\mathbf{y})\big],$$

where D is the domain of $\mathbf{L_x}$ and G_0 is the Green's function for $\mathbf{L_x}$ with some, as yet unspecified, BCs. The function H is a solution to the homogeneous equation, and it is present to guarantee the appropriate BCs.

Combining the first term in the integral with $H(\mathbf{x})$, we have

$$u(\mathbf{x}) = F(\mathbf{x}) - \lambda \int_D d^m y G_0(\mathbf{x}, \mathbf{y}) V(\mathbf{y})u(\mathbf{y}). \tag{21.31}$$

Equation (21.31) is an m-dimensional Fredholm equation whose solution can be obtained in the form of a Neumann series.

Example 21.4.1 Consider the bound-state Schrödinger equation in one dimension:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\Psi}{dx^2} + V(x)\Psi(x) = E\Psi(x), \quad E < 0.$$

We rewrite this equation as

$$\mathbf{L}_x[\Psi] \equiv \left(\frac{d^2}{dx^2} - \kappa^2\right)\Psi(x) = \frac{2\mu}{\hbar^2}V(x)\Psi(x),$$

where $\kappa^2 = -2\mu E/\hbar^2 > 0$. Equation (21.31) gives the equivalent integral equation

$$\Psi(x) = \Psi_0(x) + \frac{2\mu}{\hbar^2}\int_{-\infty}^{\infty} G_0(x, y)V(y)\Psi(y)\,dy$$

where $\Psi_0(x)$ is the solution of $\mathbf{L}_x[\Psi_0] = 0$, which is easily found to be of the general form $\Psi_0(x) = Ae^{\kappa x} + Be^{-\kappa x}$. If we assume that $\Psi_0(x)$ remains finite as $x \to \pm\infty$, $\Psi_0(x)$ will be zero. Furthermore, it can be shown that $G_0(x, y) = -e^{-\kappa|x-y|}/2\kappa$ (see Problem 20.12). Therefore,

$$\Psi(x) = -\frac{\mu}{\hbar^2\kappa}\int_{-\infty}^{\infty} e^{-\kappa|x-y|}V(y)\Psi(y)\,dy.$$

Now consider an attractive delta-function potential with center at a:

$$V(x) = -V_0\delta(x-a), \quad V_0 > 0.$$

For such a potential, the integral equation yields

$$\Psi(x) = \frac{\mu}{\hbar^2\kappa}\int_{-\infty}^{\infty} e^{-\kappa|x-y|}V_0\delta(y-a)\Psi(y)\,dy = \frac{\mu V_0}{\hbar^2\kappa}e^{-\kappa|x-a|}\Psi(a).$$

For this equation to be consistent, i.e., to get an identity when $x = a$, we must have

$$\frac{\mu V_0}{\hbar^2\kappa} = 1 \quad \Rightarrow \quad \kappa = \frac{\mu V_0}{\hbar^2} \quad \Rightarrow \quad E = -\frac{\mu V_0}{2\hbar^2}.$$

There is only one nondegenerate quantum state for an attractive delta function potential.

Therefore, there is only one bound state and one energy level for an attractive delta-function potential.

To find a Neumann-series solution we can substitute the expression for u given by the RHS of Eq. (21.31) in the integral of that equation. The resulting equation will have two integrals, in the second of which u appears. Substituting the new u in the second integral and continuing the process N times yields

$$u(\mathbf{x}) = F(\mathbf{x}) + \sum_{n=1}^{N-1}(-\lambda)^n\int_D d^m y\,K^n(\mathbf{x},\mathbf{y})F(\mathbf{y}) + (-\lambda)^N\int_D d^m y\,K^N(\mathbf{x},\mathbf{y})u(\mathbf{y}),$$

where

$$\begin{aligned} K(\mathbf{x},\mathbf{y}) &\equiv V(\mathbf{x})G_0(\mathbf{x},\mathbf{y}), \\ K^n(\mathbf{x},\mathbf{y}) &\equiv \int_D d^m t\,K^{n-1}(\mathbf{x},\mathbf{t})K(\mathbf{t},\mathbf{y}) \quad \text{for } n \geq 2. \end{aligned} \tag{21.32}$$

The Neumann series is obtained by letting $N \to \infty$:

$$u(\mathbf{x}) = F(\mathbf{x}) + \sum_{n=1}^{\infty}(-\lambda)^n\int_D d^m y\,K^n(\mathbf{x},\mathbf{y})F(\mathbf{y}). \tag{21.33}$$

Except for the fact that here the integrations are in m variables, Eq. (21.33) is the same as the Neumann series derived in Sect. 18.1. In exact analogy, therefore, we abbreviate (21.33) as

$$|u\rangle = |F\rangle + \sum_{n=1}^{\infty}(-\lambda)^n\mathbf{K}^n|F\rangle. \tag{21.34}$$

Equations (21.33) and (21.34) have meaning only if the Neumann series converges, i.e., if

$$|\lambda|\left[\int_D d^m y\int_D d^m x\left|K(\mathbf{x},\mathbf{y})\right|^2\right]^{1/2} < 1. \tag{21.35}$$

Feynman's diagrammatic representation of GF

We will briefly discuss an intuitive physical interpretation of the Neumann series due to Feynman. Although Feynman developed this *diagrammatic technique* for quantum electrodynamics, it has been useful in other areas, such as statistical and condensed matter physics. In most cases of interest, the SOPDE is homogeneous, so $f(\mathbf{x}) = 0$. In that case, $\mathbf{L_x}$ and $V(\mathbf{x})$ are called the *free operator* and the *interacting potential*, respectively. The solution to $\mathbf{L_x}[u] = 0$ is called the *free solution* and denoted by $u_f(\mathbf{x})$.

Let us start with Eq. (21.31) written as

$$u(\mathbf{x}) = u_f(\mathbf{x}) - \lambda \int_{\mathbb{R}^m} d^m y G_0(\mathbf{x}, \mathbf{y}) V(\mathbf{y}) u(\mathbf{y}), \tag{21.36}$$

where G_0 stands for the Green's function for the free operator $\mathbf{L_x}$. The full Green's function, that is, that for $\mathbf{L_x} + \lambda V$, will be denoted by G. Moreover, as is usually the case, the region D has been taken to be all of $\mathbb{R}^m$. This implies that no boundary conditions are imposed on u, which in turn permits us to use the singular part of the Green's function in the integral. Because of the importance of the full Green's function, we are interested in finding a series for G in terms of G_0, which is supposed to be known. To obtain such a series we start with the abstract operator equation and write $\mathbf{G} = \mathbf{G}_0 + \mathbf{A}$, where $\mathbf{A}$ is to be determined. Operating on both sides with $\mathbf{L}$ ("inverse" of $\mathbf{G}_0$), we obtain $\mathbf{LG} = \mathbf{LG}_0 + \mathbf{LA} = \mathbf{1} + \mathbf{LA}$. On the other hand, $(\mathbf{L} + \lambda \mathbf{V})\mathbf{G} = \mathbf{1}$, or $\mathbf{LG} = \mathbf{1} - \lambda \mathbf{VG}$. These two equations give

$$\mathbf{LA} = -\lambda \mathbf{VG} \quad \Rightarrow \quad \mathbf{A} = -\lambda \mathbf{L}^{-1} \mathbf{VG} = -\lambda \mathbf{G}_0 \mathbf{VG}.$$

Therefore,

$$\mathbf{G} = \mathbf{G}_0 - \lambda \mathbf{G}_0 \mathbf{VG}. \tag{21.37}$$

Sandwiching both sides between $\langle \mathbf{x}|$ and $|\mathbf{z}\rangle$, inserting $\mathbf{1} = \int |\mathbf{y}\rangle \langle \mathbf{y}| \, d^m y$ between $\mathbf{G}_0$ and $\mathbf{V}$ and $\mathbf{1} = \int |\mathbf{t}\rangle \langle \mathbf{t}| \, d^m t$ between $\mathbf{V}$ and $\mathbf{G}$, and assuming that $\mathbf{V}$ is local [i.e., $V(\mathbf{y}, \mathbf{t}) = V(\mathbf{y}) \delta(\mathbf{y} - \mathbf{t})$], we obtain

$$G(\mathbf{x}, \mathbf{z}) = G_0(\mathbf{x}, \mathbf{z}) - \lambda \int d^m y G_0(\mathbf{x}, \mathbf{y}) V(\mathbf{y}) G(\mathbf{y}, \mathbf{z}). \tag{21.38}$$

This equation is the analogue of (21.31) and, just like that equation, is amenable to a Neumann series expansion. The result is

$$G(\mathbf{x}, \mathbf{y}) = G_0(\mathbf{x}, \mathbf{y}) + \sum_{n=1}^{\infty} (-\lambda)^n \int_{\mathbb{R}^m} d^m z G_0(\mathbf{x}, \mathbf{z}) K^n(\mathbf{z}, \mathbf{y}), \tag{21.39}$$

where $K^n(\mathbf{x}, \mathbf{z})$ is as given in Eq. (21.32).

GF as propagator

Feynman's idea is to consider $G(\mathbf{x}, \mathbf{y})$ as an interacting **propagator** between points $\mathbf{x}$ and $\mathbf{y}$ and $G_0(\mathbf{x}, \mathbf{y})$ as a free propagator. The first term on the RHS of (21.39) is simply a free propagation from $\mathbf{x}$ to $\mathbf{y}$. Diagrammatically, it is represented by a line joining the points $\mathbf{x}$ and $\mathbf{y}$ [see Fig. 21.1(a)]. The second term is a free propagation from $\mathbf{x}$ to $\mathbf{y}_1$ (also called a **vertex**), interaction at $\mathbf{y}_1$ with a potential $-\lambda V(\mathbf{y}_1)$, and subsequent free propagation to $\mathbf{y}$ [see Fig. 21.1(b)]. According to the third term, the particle or wave

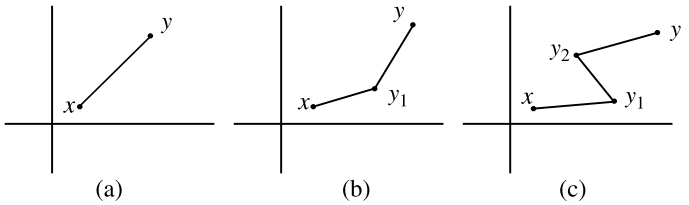

Fig. 21.1 Contributions to the full propagator in (**a**) the zeroth order, (**b**) the first order, and (**c**) the second order. At each vertex one introduces a factor of $-\lambda V$ and integrates over all values of the variable of that vertex

[represented by $u_f(\mathbf{x})$] propagates freely from $\mathbf{x}$ to $\mathbf{y}_1$, interacts at $\mathbf{y}_1$ with the potential $-\lambda V(\mathbf{y}_1)$, propagates freely from $\mathbf{y}_1$ to $\mathbf{y}_2$, interacts for a second time with the potential $-\lambda V(\mathbf{y}_2)$, and finally propagates freely from $\mathbf{y}_2$ to $\mathbf{y}$ [Fig. 21.1(c)]. The interpretation of the rest of the series in (21.39) is now clear: The nth-order term of the series has n vertices between $\mathbf{x}$ and $\mathbf{y}$ with a factor $-\lambda V(\mathbf{y}_k)$ and an integration over $\mathbf{y}_k$ at vertex k. Between any two consecutive vertices $\mathbf{y}_k$ and $\mathbf{y}_{k+1}$ there is a factor of the free propagator $G_0(\mathbf{y}_k, \mathbf{y}_{k+1})$.

Feynman diagrams are used extensively in relativistic quantum field theory, for which $m = 4$, corresponding to the four-dimensional space–time. In this context λ is determined by the strength of the interaction. For quantum electrodynamics, for instance, λ is the fine-structure constant, $e^2/\hbar c = 1/137$.

21.5 Perturbation Theory

Few operator equations lend themselves to an exact solution, and due to the urgency of finding a solution to such equations in fundamental physics, various techniques have been developed to approximate solutions to operator equations. We have already seen instances of such techniques in, for example, the WKB method. This section is devoted to a systematic development of perturbation theory, which is one of the main tools of calculation in quantum mechanics. For a thorough treatment of perturbation theory along the lines presented here, see [Mess 66, pp. 712–720].

The starting point is the resolvent (Definition 17.7.1) of a Hamiltonian $\mathbf{H}$, which, using z instead of λ, we write as $\mathbf{R}_z(\mathbf{H})$. For simplicity, we assume that the eigenvalues of $\mathbf{H}$ are discrete. This is a valid assumption if the Hamiltonian is compact or if we are interested in approximations close to one of the discrete eigenvalues. Denoting the eigenvalues of $\mathbf{H}$ by $\{E_i\}_{i=0}^{\infty}$, we have

$$\mathbf{H}\mathbf{P}_i = E_i \mathbf{P}_i, \tag{21.40}$$

where $\mathbf{P}_i$ is the projection operator to the ith eigenspace. We can write the resolvent in terms of the projection operators by using Eq. (17.6):

$$\mathbf{R}_z(\mathbf{H}) = \sum_{i=0}^{\infty} \frac{\mathbf{P}_i}{E_i - z}. \tag{21.41}$$

The projection operator $\mathbf{P}_i$ can be written as a contour integral as in Eq. (17.11). Any sum of these operators can also be written as a contour integral. For instance, if Γ is a circle enclosing the first $n+1$ eigenvalues, then

$$\mathbf{P}_\Gamma \equiv \sum_{i=0}^{n} \mathbf{P}_i = -\frac{1}{2\pi i} \oint_\Gamma \mathbf{R}_z(\mathbf{H})\, dz. \tag{21.42}$$

Multiplying Eq. (21.42) by $\mathbf{H}$ and using the definition of the resolvent, one can show that

$$\mathbf{H}\mathbf{P}_\Gamma = -\frac{1}{2\pi i} \oint_\Gamma z\mathbf{R}_z(\mathbf{H})\, dz. \tag{21.43}$$

When Γ includes *all* eigenvalues of $\mathbf{H}$, $\mathbf{P}_\Gamma = \mathbf{1}$, and Eq. (21.43) reduces to (17.10) with $\mathsf{A} \to \mathbf{T}$ and $f(x) \to x$.

perturbing potential

To proceed, let us assume that $\mathbf{H} = \mathbf{H}_0 + \lambda\mathbf{V}$ where $\mathbf{H}_0$ is a Hamiltonian with known eigenvalues and eigenvectors, and $\mathbf{V}$ is a *perturbing potential*; λ is a (small) parameter that keeps track of the order of approximation. Let us also use the abbreviations

$$\mathbf{G}(z) \equiv -\mathbf{R}_z(\mathbf{H}) \quad \text{and} \quad \mathbf{G}_0(z) \equiv -\mathbf{R}_z(\mathbf{H}_0). \tag{21.44}$$

Then a procedure very similar to that leading to Eq. (21.37) yields

$$\mathbf{G}(z) = \mathbf{G}_0(z) + \lambda\mathbf{G}_0(z)\mathbf{V}\mathbf{G}(z), \tag{21.45}$$

which can be expanded in a Neumann series by iteration:

$$\mathbf{G}(z) = \sum_{n=0}^{\infty} \lambda^n \mathbf{G}_0(z)\big[\mathbf{V}\mathbf{G}_0(z)\big]^n. \tag{21.46}$$

Degeneracy is the dimension of the eigenspace of the Hamiltonian.

Let $\{E_a^0\}$, $\{\mathcal{M}_a^0\}$, and m_a denote, respectively, the eigenvalues of $\mathbf{H}_0$, their corresponding eigenspaces, and the latter's dimensions.[4] In the context of perturbation theory, m_a is called the **degeneracy** of E_a^0, and E_a^0 is called m_a-**fold degenerate**, with a similar terminology for the perturbed Hamiltonian. We assume that all eigenspaces have finite dimensions.

It is clear that eigenvalues and eigenspaces of $\mathbf{H}$ will tend to those of $\mathbf{H}_0$ when $\lambda \to 0$. So, let us collect all eigenspaces of $\mathbf{H}$ that tend to $\mathcal{M}_a^0$ and denote them by $\{\mathcal{M}_i^a\}_{i=1}^{r_a}$. Similarly, we use E_i^a and $\mathbf{P}_i^a$ to denote, respectively, the energy eigenvalue and the projector to the eigenspace $\mathcal{M}_i^a$. Since dimension is a discrete quantity, it cannot depend on λ, and we have

$$\sum_{i=1}^{r_a} \dim \mathcal{M}_i^a = \dim \mathcal{M}_a^0 = m_a. \tag{21.47}$$

[4] We use the beginning letters of the Latin alphabet for the unperturbed Hamiltonian. Furthermore, we attach a superscript "0" to emphasize that the object belongs to $\mathbf{H}_0$.

We also use the notation $\mathbf{P}$ for the projector onto the direct sum of $\mathcal{M}_i^a$'s. We thus have

$$\mathbf{P} \equiv \sum_{i=1}^{r_a} \mathbf{P}_i^a \quad \text{and} \quad \lim_{\lambda \to 0} \mathbf{P} = \mathbf{P}_a^0, \tag{21.48}$$

where we have used an obvious notation for the projection operator onto $\mathcal{M}_a^0$.

The main task of perturbation theory is to find the eigenvalues and eigenvectors of the perturbed Hamiltonian in terms of a series in powers of λ of the corresponding unperturbed quantities. Since the eigenvectors—or, more appropriately, the projectors onto eigenspaces—and their corresponding eigenvalues of the perturbed Hamiltonian are related via Eq. (21.40), this task reduces to writing $\mathbf{P}$ as a series in powers of λ whose coefficients are operators expressible in terms of unperturbed quantities.

For sufficiently small λ, there exists a contour in the z-plane enclosing E_a^0 and all E_i^a's but excluding all other eigenvalues of $\mathbf{H}$ and $\mathbf{H}_0$. Denote this contour by Γ_a and, using Eq. (21.42), write

$$\mathbf{P} = \frac{1}{2\pi i} \oint_{\Gamma_a} \mathbf{G}(z)\, dz.$$

It follows from Eq. (21.46) that

$$\mathbf{P} = \mathbf{P}_a^0 + \sum_{n=1}^{\infty} \lambda^n \mathbf{A}^{(n)}, \quad \text{where}$$

$$\mathbf{A}^{(n)} \equiv \frac{1}{2\pi i} \oint_{\Gamma_a} \mathbf{G}_0(z) \big[\mathbf{V}\mathbf{G}_0(z)\big]^n dz. \tag{21.49}$$

This equation shows that perturbation expansion is reduced to the calculation of $\mathbf{A}^{(n)}$, which is simply the residue of $\mathbf{G}_0(z)[\mathbf{V}\mathbf{G}_0(z)]^n$. The only singularity of the integrand in Eq. (21.49) comes from $\mathbf{G}_0(z)$, which, by (21.44) and (21.41), has a pole at E_a^0. So, to calculate this residue, we simply expand $\mathbf{G}_0(z)$ in a Laurent series about E_a^0:

$$\begin{aligned}
\mathbf{G}_0(z) &= \sum_b \frac{\mathbf{P}_b^0}{z - E_b^0} \\
&= \frac{\mathbf{P}_a^0}{z - E_a^0} + \sum_{b \neq a} \frac{\mathbf{P}_b^0}{z - E_b^0} \\
&= \frac{\mathbf{P}_a^0}{z - E_a^0} + \sum_{b \neq a} \frac{\mathbf{P}_b^0}{(E_a^0 - E_b^0)(1 + \frac{z - E_a^0}{E_a^0 - E_b^0})} \\
&= \frac{\mathbf{P}_a^0}{z - E_a^0} + \sum_{b \neq a} \sum_{k=0}^{\infty} (-1)^k \frac{(z - E_a^0)^k \mathbf{P}_b^0}{(E_a^0 - E_b^0)^{k+1}}.
\end{aligned}$$

Switching the order of the two sums, and noting that our space is the Hilbert space of $\mathbf{H}_0$ whose basis can be chosen to consist of eigenstates of $\mathbf{H}_0$, we can write $\mathbf{H}_0$ instead of E_b^0 in the denominator to obtain

$$\sum_{b\neq a}\frac{\mathbf{P}_b^0}{(E_a^0-E_b^0)^{k+1}}=\sum_{b\neq a}\frac{\mathbf{P}_b^0}{(E_a^0-\mathbf{H}_0)^{k+1}}$$

$$=\frac{\sum_{b\neq a}\mathbf{P}_b^0}{(E_a^0-\mathbf{H}_0)^{k+1}}=\frac{\overbrace{\mathbf{1}-\mathbf{P}_a^0}^{\equiv\mathbf{Q}_a^0}}{(E_a^0-\mathbf{H}_0)^{k+1}}$$

$$=\frac{\mathbf{Q}_a^0}{(E_a^0-\mathbf{H}_0)^{k+1}}\equiv\mathbf{G}_0^{k+1}\big(E_a^0\big)\mathbf{Q}_a^0=\mathbf{Q}_a^0\mathbf{G}_0^{k+1}\big(E_a^0\big)\mathbf{Q}_a^0,$$

where we have used the completeness relation for the $\mathbf{P}_b^0$'s, the fact that $\mathbf{Q}_a^0$ commutes with $\mathbf{H}_0$ [and, therefore, with $\mathbf{G}_0^{k+1}(E_a^0)$], and, in the last equality, the fact that $\mathbf{Q}_a^0$ is a projection operator.[5] It follows that

$$\mathbf{G}_0(z)=\frac{\mathbf{P}_a^0}{z-E_a^0}+\sum_{k=0}^{\infty}(-1)^k\big(z-E_a^0\big)^k\mathbf{Q}_a^0\mathbf{G}_0^{k+1}\big(E_a^0\big)\mathbf{Q}_a^0$$

$$=\sum_{k=0}^{\infty}(-1)^k\big(z-E_a^0\big)^{k-1}\mathbf{S}^k, \tag{21.50}$$

where we have introduced the notation

$$\mathbf{S}^k\equiv\begin{cases}\mathbf{P}_a^0 & \text{if } k=0,\\ -\mathbf{Q}_a^0\mathbf{G}_0^k(E_a^0)\mathbf{Q}_a^0 & \text{if } k\geq 1.\end{cases}$$

By substituting Eq. (21.50) in $\mathbf{G}_0(z)[\mathbf{V}\mathbf{G}_0(z)]^n$ we obtain a Laurent expansion whose coefficient of $(z-E_a^0)^{-1}$ is $\mathbf{A}^{(n)}$. The reader may check that such a procedure yields

$$\mathbf{A}^{(n)}=(-1)^{n+1}\sum_{(n)}\mathbf{S}^{k_1}\mathbf{V}\mathbf{S}^{k_2}\mathbf{V}\cdots\mathbf{V}\mathbf{S}^{k_{n+1}}, \tag{21.51}$$

where by definition, $\sum_{(p)}$ extends over all nonnegative integers $\{k_i\}_{i=1}^{n+1}$ such that

$$\sum_{i=1}^{n+1}k_i=p\quad\forall p\geq 0.$$

[5] Note that although $\mathbf{G}_0(z)$ has a pole at E_a^0, the expressions in the last line of the equation above make sense because $\mathbf{Q}_a^0$ annihilates all states with eigenvalue E_a^0. The reason for the introduction of $\mathbf{Q}_a^0$ on both sides is to ensure that $\mathbf{G}_0^{k+1}(E_a^0)$ will not act on an eigenstate of E_a^0 on either side.

It turns out that for perturbation expansion, not only do we need the expansion of $\mathbf{P}$ [Eqs. (21.49) and (21.51)], but also an expansion for $\mathbf{HP}$. Using Eqs. (21.43) and (21.44), with Γ replaced by Γ_a, we have

$$\begin{aligned}\mathbf{HP} &= \frac{1}{2\pi i}\oint_{\Gamma_a} z\mathbf{G}(z)\,dz = \frac{1}{2\pi i}\oint_{\Gamma_a}\big(z - E_a^0 + E_a^0\big)\mathbf{G}(z)\,dz \\ &= \frac{1}{2\pi i}\oint_{\Gamma_a}\big(z - E_a^0\big)\mathbf{G}(z)\,dz + E_a^0\mathbf{P}.\end{aligned}$$

Substituting for $\mathbf{G}(z)$ from Eq. (21.46), we can rewrite this equation as

$$\big(\mathbf{H} - E_a^0\big)\mathbf{P} = \sum_{n=1}^{\infty}\lambda^n\mathbf{B}^{(n)}, \tag{21.52}$$

where

$$\mathbf{B}^{(n)} = (-1)^{n-1}\sum_{(n-1)}\mathbf{S}^{k_1}\mathbf{V}\mathbf{S}^{k_2}\mathbf{V}\cdots\mathbf{V}\mathbf{S}^{k_{n+1}}. \tag{21.53}$$

Equations (21.52) and (21.53) can be used to approximate the eigenvectors and eigenvalues of the perturbed Hamiltonian in terms of those of the unperturbed Hamiltonian. It is convenient to consider two cases: the nondegenerate case in which $m_a = 1$, and the degenerate case in which $m_a \geq 2$.

21.5.1 The Nondegenerate Case

In the nondegenerate case, we let $|_a^0\rangle$ denote the original unperturbed eigenstate, and use Eq. (21.47) to conclude that the perturbed eigenstate is also one-dimensional. In fact, it follows from (21.40) that $\mathbf{P}|_a^0\rangle$ is the desired eigenstate. Denoting the latter by $|\psi\rangle$ and using Eq. (21.49), we have

$$|\psi\rangle = \mathbf{P}|_a^0\rangle = \mathbf{P}_a^0|_a^0\rangle + \sum_{n=1}^{\infty}\lambda^n\mathbf{A}^{(n)}|_a^0\rangle = |_a^0\rangle + \sum_{n=1}^{\infty}\lambda^n\mathbf{A}^{(n)}|_a^0\rangle \tag{21.54}$$

because $\mathbf{P}_a^0$ is the projection operator onto $|_a^0\rangle$.

More desirable is the energy of the perturbed state E_a, which obeys the relation $\mathbf{HP} = E_a\mathbf{P}$. Taking the trace of this relation and noting that $\operatorname{tr}\mathbf{P} = \operatorname{tr}\mathbf{P}_a^0 = 1$, we obtain

$$\begin{aligned}E_a &= \operatorname{tr}(\mathbf{HP}) = \operatorname{tr}\left(E_a^0\mathbf{P} + \sum_{n=1}^{\infty}\lambda^n\mathbf{B}^{(n)}\right) \\ &= E_a^0 + \sum_{n=1}^{\infty}\lambda^n\underbrace{\operatorname{tr}\mathbf{B}^{(n)}}_{\equiv\varepsilon_n} = E_a^0 + \sum_{n=1}^{\infty}\lambda^n\varepsilon_n,\end{aligned} \tag{21.55}$$

where we used Eq. (21.52). Since λ is simply a parameter to keep track of the order of perturbation, one usually includes it in the definition of the perturbing potential $\mathbf{V}$. The nth-order correction to the energy is then written

as

$$\varepsilon_n = \operatorname{tr} \mathbf{B}^{(n)}. \tag{21.56}$$

Since each term of $\mathbf{B}^{(n)}$ contains $\mathbf{P}_a^0$ at least once, and since

$$\operatorname{tr}\big(\mathbf{U}\mathbf{P}_a^0\mathbf{T}\big) = \operatorname{tr}\big(\mathbf{T}\mathbf{U}\mathbf{P}_a^0\big)$$

for any pair of operators $\mathbf{U}$ and $\mathbf{T}$ (or products thereof), one can cast ε_n into the form of an expectation value of some product of operators in the unperturbed state $|_a^0\rangle$. For example,

first-order correction to energy

$$\varepsilon_1 = \operatorname{tr} \mathbf{B}^{(1)} = \sum_b \langle_b^0 | \mathbf{P}_a^0 \mathbf{V} \mathbf{P}_a^0 |_b^0\rangle = \langle_a^0 | \mathbf{V} |_a^0\rangle \tag{21.57}$$

because $\mathbf{P}_a^0 |_b^0\rangle = 0$ unless $b = a$. This is the familiar expression for the **first order correction** to the energy in nondegenerate perturbation theory. Similarly,

$$\begin{aligned}\varepsilon_2 &= \operatorname{tr} \mathbf{B}^{(2)} = -\operatorname{tr}\big(\mathbf{P}_a^0 \mathbf{V} \mathbf{P}_a^0 \mathbf{V}\big[-\mathbf{Q}_a^0 \mathbf{G}_0^k(E_a^0)\mathbf{Q}_a^0\big] \\ &\quad + \mathbf{P}_a^0 \mathbf{V}\big[-\mathbf{Q}_a^0 \mathbf{G}_0^k(E_a^0)\mathbf{Q}_a^0\big]\mathbf{V}\mathbf{P}_a^0 + \big[-\mathbf{Q}_a^0 \mathbf{G}_0^k(E_a^0)\mathbf{Q}_a^0\big]\mathbf{V}\mathbf{P}_a^0\mathbf{V}\mathbf{P}_a^0\big) \\ &= \langle_a^0 | \mathbf{V}\mathbf{Q}_a^0 \mathbf{G}_0^k(E_a^0)\mathbf{Q}_a^0 \mathbf{V} |_a^0\rangle.\end{aligned}$$

The first and the last terms in parentheses give zero because in the trace sum, $\mathbf{P}_a^0$ gives a nonzero contribution only if the state is $|_a^0\rangle$, which is precisely the state annihilated by $\mathbf{Q}_a^0$. Using the completeness relation $\sum_b |_b^0\rangle\langle_b^0| = \mathbf{1} = \sum_c |_c^0\rangle\langle_c^0|$ for the eigenstates of the unperturbed Hamiltonian, we can rewrite ε_2 as

second-order correction to energy

$$\varepsilon_2 = \sum_{b,c} \langle_a^0 | \mathbf{V} |_b^0\rangle \underbrace{\overbrace{\langle_b^0 | \mathbf{Q}_a^0}^{0 \text{ if } b=a}\ \mathbf{G}_0^k(E_a^0)\ \overbrace{\mathbf{Q}_a^0 |_c^0\rangle}^{0 \text{ if } c=a}}_{\delta_{bc}/(E_a^0 - E_b^0)} \langle_c^0 | \mathbf{V} |_a^0\rangle = \sum_{b\neq a} \frac{|\langle_a^0 | \mathbf{V} |_b^0\rangle|^2}{E_a^0 - E_b^0}.$$

This is the familiar expression for the **second-order correction** to the energy in nondegenerate perturbation theory.

21.5.2 The Degenerate Case

The degenerate case can also start with Eqs. (21.54) and (21.55). The difference is that ε_n cannot be determined as conveniently as the nondegenerate case. For example, the expression for ε_1 will involve a sum over a basis of $\mathcal{M}_a^0$ because $\mathbf{P}_a^0 |_b^0\rangle$ is no longer just $|_a^0\rangle$, but some general vector in $\mathcal{M}_a^0$. Instead of pursuing this line of approach, we present a more common method, which concentrates on the way $\mathcal{M}_a^0$ and the corresponding eigenspaces of the perturbed Hamiltonian, denoted by $\mathcal{M}_a$, enter in the calculation of eigenvalues and eigenvectors.

The projector $\mathbf{P}_a^0$ acts as a unit operator when restricted to $\mathcal{M}_a^0$. In particular, it is invertible. In the limit of small λ, the projection operator $\mathbf{P}$ is close to $\mathbf{P}_a^0$; therefore, it too must be invertible, i.e., $\mathbf{P} : \mathcal{M}_a^0 \to \mathcal{M}_a$ is an isomorphism. Similarly, $\mathbf{P}_a^0 : \mathcal{M}_a \to \mathcal{M}_a^0$ is also an isomorphism—not necessarily the inverse of the first one. It follows that for each vector in $\mathcal{M}_a^0$ there is a unique vector in $\mathcal{M}_a$ and vice versa.

The eigenvalue equation $\mathbf{H}|E_a\rangle = E_a|E_a\rangle$ can thus be written as

$$\mathbf{H}\mathbf{P}_a\big|E_a^0\big\rangle = E_a\mathbf{P}_a\big|E_a^0\big\rangle,$$

where $|E_a^0\rangle$ is the unique vector mapped onto $|E_a\rangle$ by $\mathbf{P}_a$. Multiplying both sides by $\mathbf{P}_a^0$, we obtain

$$\mathbf{P}_a^0\mathbf{H}\mathbf{P}_a\big|E_a^0\big\rangle = E_a\mathbf{P}_a^0\mathbf{P}_a\big|E_a^0\big\rangle,$$

which is completely equivalent to the previous equation because $\mathbf{P}_a^0$ is invertible. If we define

$$\mathbf{H}_a \equiv \mathbf{P}_a^0\mathbf{H}\mathbf{P}_a\mathbf{P}_a^0 : \mathcal{M}_a^0 \to \mathcal{M}_a^0, \qquad \mathbf{K}_a \equiv \mathbf{P}_a^0\mathbf{P}_a\mathbf{P}_a^0 : \mathcal{M}_a^0 \to \mathcal{M}_a^0, \tag{21.58}$$

the preceding equation becomes

$$\mathbf{H}_a\big|E_a^0\big\rangle = E_a\mathbf{K}_a\big|E_a^0\big\rangle. \tag{21.59}$$

As operators on $\mathcal{M}_a^0$ both $\mathbf{H}_a$ and $\mathbf{K}_a$ are hermitian. In fact, $\mathbf{K}_a$, which can be written as the product of $\mathbf{P}_a^0\mathbf{P}_a$ and its hermitian conjugate, is a positive definite operator. Equation (21.59) is a generalized eigenvalue equation whose eigenvalues E_a are solutions of the equation

$$\det(\mathbf{H}_a - x\mathbf{K}_a) = 0. \tag{21.60}$$

The eigenvectors of this equation, once projected onto $\mathcal{M}_a$ by $\mathbf{P}_a$, give the desired eigenvectors of $\mathbf{H}$.

The expansions of $\mathbf{H}_a$ and $\mathbf{K}_a$ are readily obtained from those of $\mathbf{H}\mathbf{P}_a$ and $\mathbf{P}_a$ as given in Eqs. (21.49) and (21.52). We give the first few terms of each expansion:

$$\begin{aligned}\mathbf{K}_a &= \mathbf{P}_a^0 - \lambda^2\mathbf{P}_a^0\mathbf{V}\mathbf{Q}_a^0\mathbf{G}_0^2\big(E_a^0\big)\mathbf{Q}_a^0\mathbf{V}\mathbf{P}_a^0 + \cdots,\\ \mathbf{H}_a &= E_a^0\mathbf{K}_a + \lambda\mathbf{P}_a^0\mathbf{V}\mathbf{P}_a^0 + \lambda^2\mathbf{P}_a^0\mathbf{V}\mathbf{Q}_a^0\mathbf{G}_0\big(E_a^0\big)\mathbf{Q}_a^0\mathbf{V}\mathbf{P}_a^0 + \cdots.\end{aligned} \tag{21.61}$$

To any given order of approximation, the eigenvalues E_a are obtained by terminating the series in (21.61) at that order, plugging the resulting finite sum in Eq. (21.60), and solving the determinant equation.

21.6 Problems

21.1 Show that the definitions of the three types of SOPDEs discussed in Example 21.1.6 are equivalent to the definitions based on Eq. (21.5). Hint: Diagonalize the matrix of coefficients of the SOPDE:

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x\partial y} + c\frac{\partial^2 u}{\partial y^2} + F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0,$$

where a, b, and c are functions of x and y. Write the eigenvalues as $(a + c \pm \Delta)/2$ and consider the three cases $|\Delta| < |a + c|$, $|\Delta| > |a + c|$, and $|\Delta| = |a + c|$.

21.2 Find the characteristic curves for $\mathbf{L}_x[u] = \partial u/\partial x$.

21.3 Find the characteristic curves for the two-dimensional wave equation and the two-dimensional diffusion equation.

21.4 Solve the Cauchy problem for the two-dimensional Laplace equation subject to the Cauchy data $u(0, y) = 0$, $(\partial u/\partial x)(0, y) = \epsilon \sin ky$, where ϵ and k are constants. Show that the solution does not vary continuously as the Cauchy data vary. In particular, show that for any $\epsilon \neq 0$ and any preassigned $x > 0$, the solution $u(x, y)$ can be made arbitrarily large by choosing k large enough.

21.5 Show that the x_i in Eq. (21.12) describe an m-dimensional sphere of radius r, that is, $\sum_{i=1}^{m} x_i^2 = r^2$.

21.6 Use $J\delta(\mathbf{x} - \mathbf{a}) = \delta(\boldsymbol{\xi} - \boldsymbol{\alpha})$ and the coordinate transformation from the spherical coordinate system to Cartesian coordinates to express the 3D Cartesian delta function in terms of the corresponding spherical delta function at a point $P = (x_0, y_0, z_0) = (r_0, \theta_0, \varphi_0)$ where the Jacobian J is nonvanishing.

21.7 Find the volume of an m-dimensional sphere.

21.8 Prove Eq. (21.11). First, note that the RHS of Eq. (21.10) is a function of only k of the α's. This means that

$$H(\boldsymbol{\xi})|_{\boldsymbol{\xi}=\boldsymbol{\alpha}} = H(\alpha_1, \ldots, \alpha_k).$$

(a) Rewrite Eq. (21.10) by separating the integral into two parts, one involving $\{\xi_i\}_{i=1}^{k}$ and the other involving $\{\xi_i\}_{i=k+1}^{m}$. Compare the RHS with the LHS and show that

$$\int J d\xi_{k+1} \cdots d\xi_m \delta(\mathbf{x} - \mathbf{a}) = \prod_{i=1}^{k} \delta(\xi_i - \alpha_i).$$

(b) Show that this equation implies that $\delta(\mathbf{x} - \mathbf{a})$ is independent of $\{\xi_i\}_{i=k+1}^{m}$. Thus, one can take the delta function out of the integral.

21.9 Find the m-dimensional Green's function for the Laplacian as follows.

(a) Solve Eq. (21.19) assuming that $r \neq 0$ and demanding that $G(r) \to 0$ as $r \to \infty$ (this can be done only for $m \geq 3$).

(b) Use the divergence theorem in m dimensions and (21.18) to show that

$$\iint_S \frac{dG}{dr}\, da = 1,$$

where S is a spherical hypersurface of radius r. Now use this and the result of part (a) to find the remaining constant of integration.

21.10 Consider the operator $\mathbf{L}_\mathbf{x} = \nabla^2 + \mathbf{b}\cdot\boldsymbol{\nabla} + c$ for which $\{b_i\}_{i=1}^m$ and c are functions of $\{x_i\}_{i=1}^m$.

(a) Show that $\mathbf{L}_\mathbf{x}^\dagger[v] = \nabla^2 v - \boldsymbol{\nabla}\cdot(\mathbf{b}v) + cv$, and

$$\mathbf{Q}\big[u, v^*\big] = \mathbf{Q}[u, v] = v\boldsymbol{\nabla}u - u\boldsymbol{\nabla}v + \mathbf{b}uv.$$

(b) Show that a necessary condition for $\mathbf{L}_\mathbf{x}$ to be self-adjoint is $2\mathbf{b}\cdot\boldsymbol{\nabla}u + u(\boldsymbol{\nabla}\cdot\mathbf{b}) = 0$ for arbitrary u.

(c) By choosing some u's judiciously, show that (b) implies that $b_i = 0$. Conclude that $\mathbf{L}_\mathbf{x} = \nabla^2 + c(\mathbf{x})$ is formally self-adjoint.

21.11 Solve the integral form of the Schrödinger equation for an attractive double delta-function potential

$$V(x) = -V_0\big[\delta(x-a_1) + \delta(x-a_2)\big], \quad V_0 > 0.$$

Find the eigenfunctions and obtain a transcendental equation for the eigenvalues (see Example 21.4.1).

21.12 Show that the integral equation associated with the damped harmonic oscillator DE $\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0$, having the BCs $x(0) = x_0$, $(dx/dt)_{t=0} = 0$, can be written in either of the following forms.

(a) $$x(t) = x_0 - \frac{\omega_0^2}{2\gamma}\int_0^t \big[1 - e^{-2\gamma(t-t')}\big]x\big(t'\big)\,dt'.$$

(b) $$x(t) = x_0\cos\omega_0 t + \frac{2\gamma x_0}{\omega_0}\sin\omega_0 t - 2\gamma\int_0^t \cos\big[\omega_0\big(t-t'\big)\big]x\big(t'\big)\,dt'.$$

Hint: Take $\omega_0^2 x$ or $2\gamma\dot{x}$, respectively, as the inhomogeneous term.

21.13 Show that for scattering problems ($E > 0$)

(a) the integral form of the Schrödinger equation in one dimension is

$$\Psi(x) = e^{ikx} - \frac{i\mu}{\hbar^2 k}\int_{-\infty}^{\infty} e^{ik|x-y|}V(y)\Psi(y)\,dy.$$

(b) Divide $(-\infty, +\infty)$ into three regions $R_1 = (-\infty, -a)$, $R_2 = (-a, +a)$ and $R_3 = (a, \infty)$. Let $\psi_i(x)$ be $\psi(x)$ in region R_i. Assume that the potential $V(x)$ vanishes in R_1 and R_3. Show that

$$\psi_1(x) = e^{ikx} - \frac{i\mu}{\hbar^2 k}e^{-ikx}\int_{-a}^{a} e^{iky}V(y)\psi_2(y)\,dy,$$

$$\psi_2(x) = e^{ikx} - \frac{i\mu}{\hbar^2 k}\int_{-a}^{a} e^{ik|x-y|}V(y)\psi_2(y)\,dy,$$

$$\psi_3(x) = e^{ikx} - \frac{i\mu}{\hbar^2 k}e^{ikx}\int_{-a}^{a} e^{-iky}V(y)\psi_2(y)\,dy.$$

This shows that determining the wave function in regions where there is no potential requires the wave function in the region where the potential acts.

(c) Let

$$V(x) = \begin{cases} V_0 & \text{if } |x| < a, \\ 0 & \text{if } |x| > a, \end{cases}$$

and find $\psi_2(x)$ by the method of successive approximations. Show that the nth term is less than $(2\mu V_0 a/\hbar^2 k)^{n-1}$ (so the Neumann series will converge) if $(2V_0 a/\hbar v) < 1$, where v is the velocity and $\mu v = \hbar k$ is the momentum of the wave. Therefore, for large velocities, the Neumann series expansion is valid.

21.14 (a) Show that $\mathbf{H}\mathbf{R}_z(\mathbf{H}) = \mathbf{1} + z\mathbf{R}_z(\mathbf{H})$. (b) Use (a) to prove Eq. (21.43).