Supplements to Mathematical Methods in Science and Engineering
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CHAPTER 19: GREEN'S FUNCTIONS

I. Perturbation Theory:

A Short Introduction To Integral Equations (from the supplements of Chapter 18**):**

We often encounter cases where a given second-order linear differential operator,

$$\pounds = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q^{(0)}(x) + q^{(1)}(x),\ x \in [a,b], \tag{0.1}$$

differs from an exactly solvable Sturm-Liouville operator,

$$\pounds_0 = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q^{(0)}(x), \tag{0.2}$$

by a small term, $q^{(1)}(x)$, compared to $q^{(0)}(x)$. Since the eigenvalue problem for $\pounds_0$ is exactly solvable, it yields a complete and orthonormal set of eigenfunctions, u_i, which satisfy the eigenvalue equation

$$\pounds_0 u_i + \lambda_i u_i = 0, \tag{0.3}$$

where λ_i are the eigenvalues. We now consider the eigenvalue equation for the general operator $\pounds$:

$$\pounds\Psi(x) + \lambda\Psi(x) = 0, \tag{0.4}$$

and write it as

$$\pounds_0\Psi(x) + \lambda\Psi(x) = -q^{(1)}\Psi(x). \tag{0.5}$$

In general, the above equation is given as

$$\pounds_0\Psi(x) + \lambda\Psi(x) = f(x, \Psi(x)), \tag{0.6}$$

where the inhomogeneous term usually corresponds to sources or interactions. We confine our discussion to cases where $f(x, \Psi)$ is separable:

$$f(x, \Psi(x)) = h(x)\Psi(x). \tag{0.7}$$

Mathematical Methods in Science and Engineering. By Selçuk Ş. Bayın.

This covers a wide range of physically interesting cases. For example, in scattering problems the time independent Schrödinger equation is written as

$$\overrightarrow{\nabla}^2\Psi(\overrightarrow{r}) + \frac{2mE}{\hbar^2}\Psi(\overrightarrow{r}) = \frac{2m}{\hbar^2}V(\overrightarrow{r})\Psi(\overrightarrow{r}), \tag{0.8}$$

where $V(\overrightarrow{r})$ is the scattering potential.

As we discussed in Chapters 18 and 19 of Bayin (2006), the general solution of Equation (0.5) can be written as

$$\begin{aligned}\Psi(x) &= \Psi^{(0)}(x) + \int dx' G(x,x')h(x')\Psi(x') \\ &= \Psi^{(0)}(x) + \int dx' K(x,x')\Psi(x'),\end{aligned} \tag{0.9}$$

where $G(x,x')$ is the Green's function, $K(x,x') = G(x,x')h(x')$ is called the kernel of the integral equation and $\Psi^{(0)}(x)$ is the known solution of the homogeneous equation:

$$\pounds_0\Psi(x) + \lambda\Psi(x) = 0. \tag{0.10}$$

Introducing the linear integral operator $\mathbb{K}$,

$$\mathbb{K} = \int_a^b dx' K(x,x'), \tag{0.11}$$

$$\mathbb{K}(\alpha\Psi_1 + \beta\Psi_2) = \alpha\mathbb{K}\Psi_1 + \beta\mathbb{K}\Psi_2, \tag{0.12}$$

where α, β are constants, we can write Equation (0.9) as

$$(\mathbf{I} - \mathbb{K})\Psi(x) = \Psi^{(0)}(x), \tag{0.13}$$

where $\mathbf{I}$ is the identity operator. Assuming that $K(x,x')$ is small, we can write

$$\Psi(x) = \frac{\Psi^{(0)}(x)}{(\mathbf{I} - \mathbb{K})} \tag{0.14}$$

$$= (\mathbf{I} + \mathbb{K} + \mathbb{K}^2 + \cdots)\Psi^{(0)}(x). \tag{0.15}$$

A similar expansion can be written for $\Psi(x)$ as

$$\Psi(x) = \Psi^{(0)}(x) + \Psi^{(1)}(x) + \cdots, \tag{0.16}$$

which when substituted into Equation (0.15) yields the zeroth-order term of the approximation as

$$\Psi(x) \simeq \Psi^{(0)}(x), \tag{0.17}$$

and the subsequent terms of the expansion as

$$\Psi^{(1)}(x) = \int dx' K(x,x')\Psi^{(0)}(x), \tag{0.18}$$

$$\Psi^{(2)}(x) = \mathbb{K}\Psi^{(1)}(x) = \mathbb{K}^2\Psi^{(0)}(x) = \int dx'' K(x,x'') \int dx' K(x'',x')\Psi^{(0)}(x'), \tag{0.19}$$

$$\vdots$$

We can now write the following Neumann series [Eq. (18.51)]:

$$\Psi(x) = \Psi^{(0)}(x) + \int dx' K(x,x')\Psi^{(0)}(x') + \int dx' K(x,x')\Psi^{(1)}(x') + \cdots, \tag{0.20}$$

that is,

$$\begin{aligned}\Psi(x) = {} & \Psi^{(0)}(x) \\ & + \int dx' K(x,x')\Psi^{(0)}(x') \\ & + \int dx' K(x,x') \int dx'' K(x',x'')\Psi^{(0)}(x'') \\ & + \int dx' K(x,x') \int dx'' K(x',x'') \int dx''' K(x'',x''')\Psi^{(0)}(x''') \\ & + \cdots .\end{aligned} \tag{0.21}$$

If we approximate $\Psi(x)$ with the first N terms,

$$\Psi(x) \simeq \Psi^{(0)}(x) + \Psi^{(1)}(x) + \cdots + \Psi^{(N)}(x), \tag{0.22}$$

we can write Equation (0.13) as

$$(\mathbf{I} - \mathbb{K})(\Psi^{(0)} + \Psi^{(1)} + \cdots + \Psi^{(N)}) \simeq \Psi^{(0)}, \tag{0.23}$$

$$\Psi^{(0)} - \Psi^{(N+1)} \simeq \Psi^{(0)}. \tag{0.24}$$

For the convergence of Neumann series, for a given small positive number ε_0, we should be able to find a number N_0, independent of x and such that for

$$N + 1 > N_0, \tag{0.25}$$

$$\left|\Psi^{(N+1)}\right| < \varepsilon_0. \tag{0.26}$$

To obtain the sufficient condition for convergence let

$$\max|K(x,x')| = M \tag{0.27}$$

for

$$x, x' \in [a, b], \tag{0.28}$$

and take

$$\int_a^b dx' \left| \Psi^{(0)}(x) \right| = C. \tag{0.29}$$

We can now write the inequality

$$\left| \Psi^{(n+1)}(x) \right| < CM^{N+1}(b-a)^N = CM[M(b-a)]^N, \tag{0.30}$$

which yields the error committed by approximating $\Psi(x)$ with the first $N+1$ terms of the Neumann series [Eq. (0.21)] as

$$\left| \Psi(x) - \sum_{n=0}^{N} \Psi^{(n)}(x) \right| \leq \left| \Psi^{N+1}(x) \right| + \left| \Psi^{N+2}(x) \right| + \cdots \tag{0.31}$$

$$\leq CM[M(b-a)]^N \{1 + M(b-a) + M^2(b-a)^2 + \cdots\}. \tag{0.32}$$

If

$$M(b-a) < 1, \tag{0.33}$$

which is sufficient but not necessary, we can write

$$\left| \Psi(x) - \sum_{n=0}^{N} \Psi^{(n)}(x) \right| \leq \frac{CM[M(b-a)^N}{[1 - M(b-a)]} < \varepsilon_0 \tag{0.34}$$

for all $N > N_0$ independent of x.

Nondegenerate Perturbation Theory:

We now consider the following problem [Eq. (0.5)]:

$$\{\pounds_0 + \lambda\} \Psi(x) = \varepsilon h(x) \Psi(x), \tag{0.35}$$

where $\pounds_0$ is an exactly solvable Sturm-Liouville operator and where we have introduced a small parameter, ε, that allows us to keep track of the order of terms in our equations. In the limit as $\varepsilon \to 0$ and assuming that $h(x)$ is bounded, the solution, $\Psi(x)$, and the parameter λ, reduce to the exact eigenfunctions, $\Phi_n(x)$, and the exact eigenvalues, λ_n,of the unperturbed operator $\pounds_0$:

$$\{\pounds_0 + \lambda_n\} \Phi_n(x) = 0. \tag{0.36}$$

That is, as $\varepsilon \to 0$,

$$\Psi(x) \to \Psi^{(0)}(x) = \Phi_n(x), \tag{0.37}$$

$$\lambda \to \lambda_n. \tag{0.38}$$

We now write the perturbed eigenvalues as

$$\lambda = \lambda_n + \Delta\lambda, \tag{0.39}$$

thus Equation (0.35) becomes

$$\{\mathcal{L}_0 + \lambda_n\}\,\Psi(x) = [\varepsilon h(x) - \Delta\lambda]\Psi(x) = f(x, \Psi(x)), \tag{0.40}$$

Since the eigenfunctions of the unperturbed operator, $\mathcal{L}_0$, form a complete and orthonormal set:

$$\int_a^b dx\ \Phi_n(x)\Phi_m(x) = \delta_{nm}, \tag{0.41}$$

we can write the expansions

$$f(x) = \sum_k c_k \Phi_k(x), \tag{0.42}$$

$$c_k = \int_a^b dx' \Phi_k^*(x') f(x') \tag{0.43}$$

and

$$\Psi(x) = \sum_k a_k \Phi_k(x), \tag{0.44}$$

$$a_k = \int_a^b dx' \Phi_k^*(x') \Psi(x'). \tag{0.45}$$

Using these in Equation (0.40):

$$\sum_k a_k(\lambda_n - \lambda_k)\Phi_k = \sum_k c_k \Phi_k, \tag{0.46}$$

we obtain

$$a_k = \frac{c_k}{(\lambda_n - \lambda_k)}. \tag{0.47}$$

When $n = k$ we insist that $c_k = 0$. We now substitute a_k [Eq. (0.47)] and c_k [Eq. (0.43)] into the expansion of $\Psi(x)$ [Eq. (0.44)] to get

$$\Psi(x) = \sum_k \frac{1}{(\lambda_n - \lambda_k)} \int_a^b dx' \Phi_k^*(x')\Phi_k(x) f(x'), \tag{0.48}$$

which after rearranging becomes

$$\Psi(x) = \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right] [\varepsilon h(x') - \Delta\lambda]\Psi(x'). \tag{0.49}$$

The quantity inside the square brackets is the Green's function

$$G(x,x') = \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right]. \tag{0.50}$$

For the general solution of the differential equation [Eq. (0.40)] we also add the solution of the homogeneous equation, that is, the unperturbed solution, to write

$$\Psi(x) = \Phi_n(x) + \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right][\varepsilon h(x') - \Delta\lambda]\Psi(x'). \tag{0.51}$$

Comparing with the form in Equation (0.9), we write the kernel as

$$K(x,x') = G(x,x')[\varepsilon h(x') - \Delta\lambda]. \tag{0.52}$$

This is an integral equation and the unknown, $\Psi(x)$, appears on both sides of the equation. To obtain the perturbed solution in terms of known quantities, we expand $\Psi(x)$ and $\Delta\lambda$ in terms of the small parameter ε as, respectively,

$$\Psi(x) = \Phi_n(x) + \varepsilon\Psi^{(1)}(x) + \varepsilon^2\Psi^{(2)}(x) + \cdots \tag{0.53}$$

and

$$\lambda = \lambda_n + \varepsilon[\Delta\lambda^{(1)} + \varepsilon\Delta\lambda^{(2)} + \varepsilon^2\Delta\lambda^{(3)} + \cdots], \tag{0.54}$$

which gives

$$\Delta\lambda = \varepsilon[\Delta\lambda^{(1)} + \varepsilon\Delta\lambda^{(2)} + \varepsilon^2\Delta\lambda^{(3)} + \cdots]. \tag{0.55}$$

We now substitute these expansions into Equation (0.51) and simplify:

$$\begin{aligned}\Psi(x) = \Phi_n(x) &+ \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right]\left[\left(\varepsilon h(x') - \varepsilon\Delta\lambda^{(1)}\right) - \varepsilon^2\Delta\lambda^{(2)} + \cdots\right] \\ &\times \left[\Phi_n(x') + \varepsilon\Psi^{(1)}(x') + \varepsilon^2\Psi^{(2)}(x') + \cdots\right],\end{aligned} \tag{0.56}$$

$$\begin{aligned}\Psi(x) = \Phi_n(x) &+ \varepsilon\int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right]\left[\left(h(x') - \Delta\lambda^{(1)}\right) - \varepsilon\Delta\lambda^{(2)} + \cdots\right] \\ &\times \left[\Phi_n(x') + \varepsilon\Psi^{(1)}(x') + \varepsilon^2\Psi^{(2)}(x') + \cdots\right],\end{aligned} \tag{0.57}$$

$$\begin{aligned}\Psi(x) = \Phi_n(x) &+ \varepsilon\int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)}\right]\left[h(x') - \Delta\lambda^{(1)}\right]\Phi_n(x') \\ &+ \varepsilon\int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)}\right]\left[-\varepsilon\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\varepsilon\Psi^{(1)}(x')\right] \\ &+ 0(\varepsilon^3).\end{aligned} \tag{0.58}$$

Collecting terms with equal powers of ε we get

$$\Psi(x) = \Phi_n(x) + \varepsilon \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] \left[h(x') - \Delta\lambda^{(1)} \right] \Phi_n(x')$$
$$+ \varepsilon^2 \int_a^b dx' \left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right] \left[-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x') \right]$$
$$+ 0(\varepsilon^3) \qquad (0.59)$$

Comparing the right-hand side with the expansion of the left-hand side:

$$\Psi(x) = \Psi^{(0)}(x) + \varepsilon\Psi^{(1)}(x) + \varepsilon^2\Psi^{(2)}(x) + \cdots , \qquad (0.60)$$

we obtain

$$\Psi^{(0)}(x) = \Phi_n(x), \qquad (0.61)$$
$$\Psi^{(1)}(x) = \int_a^b dx' \left[\sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} \right] [h(x') - \Delta\lambda^{(1)}]\Phi_n(x'), \qquad (0.62)$$
$$\Psi^{(2)}(x) = \int_a^b dx' \sum_j \left[\frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)} \right]$$
$$\times \left[-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x') \right], \qquad (0.63)$$
$$\vdots$$

In the first-order term [Eq. (0.62)], the numerator has to vanish for $k = n$, thus

$$\Phi_n(x) \int_a^b dx' \Phi_n^*(x')[h(x') - \Delta\lambda^{(1)}]\Phi_n(x') = 0, \qquad (0.64)$$
$$\Phi_n(x) \int_a^b dx' \Phi_n^*(x') h(x') \Phi_n(x') = \Phi_n(x)\Delta\lambda^{(1)} \int_a^b dx' \Phi_n^*(x')\Phi_n(x'), \qquad (0.65)$$
$$\int_a^b dx' \Phi_n^*(x') h(x') \Phi_n(x') = \Delta\lambda^{(1)} \int_a^b dx' \Phi_n^*(x')\Phi_n(x'). \qquad (0.66)$$

Using the orthogonality relation:

$$\int_a^b dx' \Phi_k^*(x')\Phi_n(x') = \delta_{kn}, \qquad (0.67)$$

we obtain the first order correction to the nth eigenvalue, λ_n, as

$$\Delta\lambda^{(1)} = \int_a^b dx' \Phi_n^*(x') h(x') \Phi_n(x') = h_{nn}. \tag{0.68}$$

We can now write the first-order correction to the eigenfunction as

$$\begin{aligned}
\Psi^{(1)}(x) &= \sum_{k\neq n} \int_a^b dx' \frac{\Phi_k(x)\Phi_k^*(x')}{(\lambda_n - \lambda_k)} [h(x') - \Delta\lambda^{(1)}]\Phi_n(x') && (0.69)\\
&= \sum_{k\neq n} \frac{\Phi_k(x)}{(\lambda_n - \lambda_k)} && (0.70)\\
&\times \left[\int_a^b dx' \Phi_k^*(x') h(x') \Phi_n(x') - \Delta\lambda^{(1)} \int_a^b dx' \Phi_k^*(x')\Phi_n(x')\right].
\end{aligned}$$

We again use the orthogonality relation [Eq. (0.67)] to write

$$\begin{aligned}
\Psi^{(1)}(x) &= \sum_{k\neq n} \frac{\Phi_k(x)}{(\lambda_n - \lambda_k)} \left[\int_a^b dx' \Phi_k^*(x') h(x') \Phi_n(x')\right] && (0.71)\\
&= \sum_{k\neq n} \frac{\Phi_k(x)\ h_{kn}}{(\lambda_n - \lambda_k)}, && (0.72)
\end{aligned}$$

where h_{kn} is the Hermitian matrix $h_{kn} = \int_a^b dx' \Phi_k^*(x') h(x') \Phi_n(x')$.

Let us now turn to the second-order term. Substituting $\Psi^{(1)}(x)$ [Eq. (0.72)] into $\Psi^{(2)}(x)$ [Eq. (0.63)]:

$$\begin{aligned}
\Psi^{(2)}(x) = \int_a^b dx' &\left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)}\right]\\
&\times \left[-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)})\Psi^{(1)}(x')\right], && (0.73)
\end{aligned}$$

we obtain

$$\begin{aligned}
\Psi^{(2)}(x) = \int_a^b dx' &\left[\sum_j \frac{\Phi_j(x)\Phi_j^*(x')}{(\lambda_n - \lambda_j)}\right]\\
\times &\left[-\Delta\lambda^{(2)}\Phi_n(x') + (h(x') - \Delta\lambda^{(1)}) \sum_{k\neq n} \frac{\Phi_k(x')\ h_{kn}}{(\lambda_n - \lambda_k)}\right], && (0.74)
\end{aligned}$$

which also becomes

$$\Psi^{(2)}(x)=\sum_{j}\frac{\Phi_j(x)}{(\lambda_n-\lambda_j)}\left[\int_a^b dx'\Phi_j^*(x')(-\Delta\lambda^{(2)})\Phi_n(x')\right.$$
$$\left.+\int_a^b dx'\Phi_j^*(x')\left[h(x')-\Delta\lambda^{(1)}\right]\sum_{k\neq n}\frac{\Phi_k(x')h_{kn}}{(\lambda_n-\lambda_k)}\right], \tag{0.75}$$

where

$$h_{kn}=\int_a^b dx''\Phi_k^*(x'')h(x'')\Phi_n(x''). \tag{0.76}$$

For $j=n$, we again set the numerator to zero:

$$\int_a^b dx'\Phi_n^*(x')\Delta\lambda^{(2)}\Phi_n(x')=\int_a^b dx'\Phi_n^*(x')\left[h(x')-\Delta\lambda^{(1)}\right]\sum_{k\neq n}\frac{\Phi_k(x')h_{kn}}{(\lambda_n-\lambda_k)}, \tag{0.77}$$

$$\Delta\lambda^{(2)}\int_a^b dx'\Phi_n^*(x')\Phi_n(x')=\sum_{k\neq n}\left[\frac{\left[\int_a^b dx'\Phi_n^*(x')h(x')\Phi_k(x')\right]h_{kn}}{(\lambda_n-\lambda_k)}\right.$$
$$\left.-\Delta\lambda^{(1)}\frac{\left[\int_a^b dx'\Phi_n^*(x')\Phi_k(x')\right]h_{kn}}{(\lambda_n-\lambda_k)}\right]. \tag{0.78}$$

Using the orthogonality relation [Eq. (0.67)] we obtain

$$\Delta\lambda^{(2)}=\sum_{k\neq n}\frac{h_{nk}h_{kn}}{(\lambda_n-\lambda_k)}. \tag{0.79}$$

Substituting this in equation (0.63) we obtain $\Psi^{(2)}(x)$ as

$$\Psi^{(2)}(x)=\sum_{j\neq n}\frac{\Phi_j(x)}{(\lambda_n-\lambda_j)}\left[(-\Delta\lambda^{(2)})\int_a^b dx'\Phi_j^*(x')\ \Phi_n(x')\right.$$
$$+\sum_{k\neq n}\frac{\left[\int_a^b dx'\Phi_j^*(x')h(x')\Phi_k(x')\right]\ h_{kn}}{(\lambda_n-\lambda_k)}$$
$$\left.-\left(\Delta\lambda^{(1)}\right)\int_a^b dx'\Phi_j^*(x')\Phi_k(x')\sum_{k\neq n}\frac{h_{kn}}{(\lambda_n-\lambda_k)}\right]. \tag{0.80}$$

Using the orthogonality relation [Eq. (0.67)] this also becomes

$$\Psi^{(2)}(x) = \sum_{j\neq n} \frac{\Phi_j(x)}{(\lambda_n - \lambda_j)} \Bigg[(-\Delta\lambda^{(2)})\delta_{jn} + \sum_{k\neq n} \frac{h_{jk}\ h_{kn}}{(\lambda_n - \lambda_k)} - \left(\Delta\lambda^{(1)}\right) \delta_{jk} \sum_{k\neq n} \frac{h_{kn}}{(\lambda_n - \lambda_k)} \Bigg]. \tag{0.81}$$

Finally, using $\Delta\lambda^{(1)} = h_{nn}$ we obtain

$$\Psi^{(2)}(x) = \sum_{j\neq n} \Phi_j(x) \quad \left[\sum_{k\neq n} \frac{[h_{jk} - \delta_{jk}h_{nn}]\, h_{kn}}{(\lambda_n - \lambda_j)(\lambda_n - \lambda_k)} \right]. \tag{0.82}$$

Example (0.1): Slightly anharmonic oscillator in one dimension:
We now consider the slightly anharmonic oscillator problem in quantum mechanics with the potential

$$V(x) = \frac{1}{2}k_2x^2 - k_3x^3, \tag{0.83}$$

where k_2 and k_3 are constants such that $k_3 \ll k_1$. We have already solved the Schrödinger equation for the harmonic oscillator potential, $V(x) = \frac{1}{2}k_2x^2$, in Chapter 4 that leads to the following eigenvalue equation:

$$\frac{d^2\Psi_n}{dx^2} - x^2\Psi_n + \epsilon\Psi_n(x) = 0, \tag{0.84}$$

where

$$x = \frac{x_{\text{physical}}}{\sqrt{\hbar/m\omega}},\ \epsilon = \frac{E}{\hbar\omega/2}. \tag{0.85}$$

We rewrite the exactly solvable case as

$$\pounds_0\Phi_n + \epsilon_n\Phi_n(x) = 0, \tag{0.86}$$

$$\pounds_0 = \frac{d^2}{dx^2} - x^2, \tag{0.87}$$

where the solution is given in terms of the Hermite polynomials [Eq. (4.47)]:

$$\Phi_n(x) = \frac{e^{-x^2/2}H_n(x)}{\sqrt{2^n n!\sqrt{\pi}}},\ n = 0, 1, \ldots\ . \tag{0.88}$$

We are now looking for the solution of the slightly anharmonic oscillator that satisfies the equation

$$(\pounds_0 + \lambda)\Psi(x) = \alpha x^3\Psi, \tag{0.89}$$

where $\alpha \ll 1$. The perturbed energy eigenvalues are written as

$$\lambda = \epsilon_n + \alpha\Delta\lambda^{(1)} + \alpha^2\Delta\lambda^{(2)} + \cdots \ , \tag{0.90}$$

where

$$\epsilon_n = 2n + 1 \tag{0.91}$$

are the exact eigenvalues. We can easily verify that

$$\Delta\lambda^{(1)} = h_{nn} = \int_{-\infty}^{\infty} dx' \Phi_n^2(x') x'^3 = 0. \tag{0.92}$$

For $\Psi^{(1)}(x)$ we need to evaluate the integral

$$h_{kn} = \int_{-\infty}^{\infty} dx' \frac{e^{-x'^2} H_n(x') x'^3 H_k(x')}{\sqrt{2^n n!}\sqrt{2^k k!}\sqrt{\pi}}. \tag{0.93}$$

Using the recursion relation [Eq. (4.40)]

$$xH_n = \frac{1}{2}H_{n+1} + nH_{n-1}, \tag{0.94}$$

we write

$$x^2 H_n = \frac{1}{2}\left(\frac{1}{2}H_{n+2} + (n+1)H_n\right) + n\left(\frac{1}{2}H_n + (n-1)H_{n-2}\right), \tag{0.95}$$

$$= \frac{1}{4}H_{n+2} + \frac{2n+1}{2}H_n + n(n-1)H_{n-2}. \tag{0.96}$$

Similarly,

$$x^3 H_n = \frac{1}{8}H_{n+3} + \frac{3}{4}(n+1)H_{n+1} + \frac{3}{2}n^2 H_{n-1} + n(n-1)(n-2)H_{n-3}. \tag{0.97}$$

Using Equation (0.97) in (0.93), along with the orthogonality relation

$$\int_{-\infty}^{\infty} dx e^{-x^2/2} H_n(x) H_k(x) = 0, \ n \neq k, \tag{0.98}$$

we obtain

$$h_{kn} = 0, \tag{0.99}$$

unless

$$k = (n+3), \ (n+1), \ (n-1), \ (n-3). \tag{0.100}$$

We evaluate the component $h_{n(n+3)}$ as

$$h_{n(n+3)} = h_{(n+3)n} = \frac{1}{8}\int_{-\infty}^{\infty} dx' e^{-x'^2/2}\frac{H_{n+3}(x')}{\sqrt{2^n n!}}\frac{H_{n+3}(x')}{\sqrt{2^{n+3}(n+3)!\sqrt{\pi}}} \tag{0.101}$$

$$= \frac{1}{8}\frac{\sqrt{2^{n+3}(n+3)!}}{\sqrt{2^n n!}}\left\{\int_{-\infty}^{\infty} dx' \frac{e^{-x'^2}H_{n+3}^2(x')}{\left[\sqrt{2^{n+3}(n+1)!\sqrt{\pi}}\right]^2}\right\} \tag{0.102}$$

$$= \frac{1}{8}\sqrt{8}\sqrt{\frac{(n+3)!}{n!}} \tag{0.103}$$

$$= \sqrt{\frac{(n+3)(n+2)(n+1)}{8}}. \tag{0.104}$$

Similarly, we evaluate the other nonzero components:

$$h_{(n-3)n} = \sqrt{\frac{n(n-1)(n-2)}{8}}, \tag{0.105}$$

$$h_{n(n+1)} = 3(n+1)\sqrt{\frac{n+1}{8}}, \tag{0.106}$$

$$h_{n(n-1)} = 3n\sqrt{\frac{n}{8}}. \tag{0.107}$$

Using these results we now write

$$\Delta\lambda^{(2)} = \sum_k \frac{h_{nk}h_{kn}}{2(n-k)} \tag{0.108}$$

$$= \frac{\frac{1}{8}(n+3)(n+2)(n+1)}{-6} \tag{0.109}$$

$$+ \frac{\frac{1}{8}n(n-1)(n-2)}{6} + \frac{9(n+1)^2(n+1)}{-2(8)} + \frac{9n^2 n}{2(8)},$$

hence obtain

$$\epsilon = (2n+1) - \alpha^2\frac{[30n^2+30n+11]}{16} + 0(\alpha^3). \tag{0.110}$$

Similarly, we evaluate the first nonzero term of the perturbed wave function as

$$\Psi(x) = \Phi_n(x) + \alpha\left[\frac{\sqrt{n(n-1)(n-2)}}{12\sqrt{2}}\Phi_{n-3}(x)\right.$$

$$- \frac{\sqrt{(n+3)(n+2)(n+1)}}{12\sqrt{2}}\Phi_{n+3}(x)$$

$$\left. + \frac{3n\sqrt{n}}{4\sqrt{2}}\Phi_{n-1}(x) - \frac{3(n+1)\sqrt{n+1}}{4\sqrt{2}}\Phi_{n+1}(x)\right] + 0(\alpha^2). \tag{0.111}$$

Degenerate Perturbation Theory:

The preceding formalism works fine as long as the eigenvalues are distinct, that is, $\lambda_i \neq \lambda_j$, when $i \neq j$. In the event that multiple eigenvalues turn out to be equal, the method can still be rescued with a simple procedure. We first remember that the first-order correction to $\Psi(x)$ [Eq. (0.72)], that is, $\Psi^{(1)}(x)$, is written as

$$\Psi^{(1)}(x) = \sum_{k \neq n} \Phi_k(x) \, \left[\frac{h_{kn}(x)}{(\lambda_n - \lambda_k)} \right]. \tag{0.112}$$

In the above series the expansion coefficients,

$$\left[\frac{h_{kn}}{(\lambda_n - \lambda_k)} \right], \tag{0.113}$$

diverge for the degenerate eigenvalues, where $\lambda_n = \lambda_k$ for $n \neq k$. This would be okay, if somehow the corresponding matrix elements, h_{kn}, $k \neq n$, also vanished. In other words, if the submatrix, h_{kn}, corresponding to the degenerate eigenvalues are diagonal. From Sturm-Liouville theory we know that for hermitian operators for distinct eigenvalues the corresponding eigenfunctions are mutually orthogonal. However, for the degenerate eigenvalues there is an ambiguity. All the vectors that are perpendicular to the remaining eigenvectors corresponding to the distinct eigenvalues are legitimate eigenvectors for the degenerate eigenvalues. For example, if $\lambda_1 = \lambda_2 \neq \lambda_3$, all the vectors that lie on a plane perpendicular to the third eigenvector for λ_3 are good eigenvectors for λ_1 and λ_2. Normally, we would pick any two perpendicular vectors on this plane as the eigenvectors of λ_1 and λ_2, thus obtaining a mutually orthogonal eigenvector set for $\lambda_1, \lambda_2, \lambda_3$. In the presence of a perturbation we use this freedom to find an appropriate orientation for the eigenvectors of λ_1 and λ_2, such that the 2×2 submatrix, h_{kn},

$$\int_a^b dx' \Phi_k^*(x') h(x') \Phi_n(x') = h_{kn}, \tag{0.114}$$

corresponding to the degenerate eigenvalues is diagonal. In other words, the perturbation removes the degeneracy and picks a particular orientation for the orthogonal eigenvectors of λ_1 and λ_2 on the plane perpendicular to the third eigenvector corresponding to the distinct eigenvalue. This procedure is called diagonalization. For an l-fold degenerate eigenvalue, the corresponding submatrix to be diagonalized is an $l \times l$ square matrix. This procedure, albeit being cumbersome, can be extended to higher order terms in the perturbation expansion and to any number of multiply degenerate eigenvalues. A short example for this process can be found in Mathews and Walker (Bayin, 2006). For a review of the eigenvalue problems and the diagonalization of matrices see Bayin (2008).

Exercise (0.1): Find the solution of the following eigenvalue problem:

$$\frac{d^2\Psi}{d\theta^2} + \cot\theta \frac{d\Psi}{d\theta} + \lambda\Psi = \alpha \cos^2\theta \Psi,$$

where $\Psi = \Psi(\theta)$ is defined over the interval $0 \le \theta \le \pi$ and must be square-integrable with the weight function $\sin\theta$. The parameter α is $\ll 1$, hence the solution can be expanded in terms of the positive powers of α. Find the solution which in the limit as $\alpha \to 0$, has the eigenvalue

$$\lambda^{(0)} = l(l+2)$$

with $l = 2$. Also, for this eigenvalue find the eigenvalue correct to order α^2 and the solution $\Psi(\theta)$ correct to order α.

II. Constructing the Green's function:

(Problems 19.4, 19.5 and 19.6)

Let us start with the most general second-order differential equation:

$$\pounds y(x) = f(x, y(x)), \ \ x \in [a, b], \tag{0.115}$$

$$\pounds = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x), \tag{0.116}$$

where for self-adjoint operators

$$p_1(x) = p_0'(x). \tag{0.117}$$

Green's function, $G(x, x')$, allows us to convert the differential equation [Eq. (0.115)] into an integral equation:

$$y(x) = \int_a^b dx' G(x, x') f(x', y(x')), \tag{0.118}$$

where the Green's function satisfies the differential equation

$$\pounds G(x, x') = \delta(x - x') \tag{0.119}$$

with the same boundary conditions that $y(x)$ is required to satisfy. These boundary conditions are usually one of the following two types:

I. Single point boundary condition:

$$G(a, x') = 0, \tag{0.120}$$

$$\frac{\partial G(a, x')}{\partial x} = 0. \tag{0.121}$$

II. Two point boundary condition:

$$G(a, x') = 0, \tag{0.122}$$

$$G(b, x') = 0. \tag{0.123}$$

From the differential equation that the Green's function satisfies:

$$p_0(x)\frac{d^2G(x,x')}{dx^2} + p_1(x)\frac{dG(x,x')}{dx} + p_2(x)G(x,x') = \delta(x-x'), \qquad (0.124)$$

we can deduce that $G(x,x')$ must be continuous at $x = x'$. Otherwise, $G(x,x')$ would be proportional to the unit step function and since the derivative of the unit step function is a Dirac-delta function, the first term on the left would be proportional to the derivative of the Dirac-delta function, which would make it incompatible with the Dirac-delta function on the right-hand side. Let us now integrate the differential equation between $x' \in (x'-\epsilon, x'+\epsilon)$ and take the limit $\epsilon \to 0$:

$$\begin{aligned}\int_{x'-\epsilon}^{x'+\epsilon} dx'\ p_0(x')\frac{d^2G(x,x')}{dx'^2} + \int_{x'-\epsilon}^{x'+\epsilon} dx'\ p_1(x')\frac{dG(x,x')}{dx'} \\ + \int_{x'-\epsilon}^{x'+\epsilon} dx'\ p_2(x')G(x,x') = \int_{x'-\epsilon}^{x'+\epsilon} dx'\ \delta(x-x'). \qquad (0.125)\end{aligned}$$

We now analyze this equation term by term. From the definition of the dirac-delta function the first term on the right is 1 :

$$\int_{x'-\epsilon}^{x'+\epsilon} dx'\ \delta(x-x') = 1. \qquad (0.126)$$

In the integrals on the right-han side, since p_0, p_1, p_2 are continuous functions, in the limit as $\epsilon \to 0$, we can replace them with their values at $x = x'$:

$$\begin{aligned}p_0(x')\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dx'\frac{d^2G(x,x')}{dx'^2} + p_1(x')\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dx'\frac{dG(x,x')}{dx'} \\ +p_2(x')\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dx' G(x,x') = 1. \qquad (0.127)\end{aligned}$$

Since $G(x,x')$ is continuous at $x = x'$, in the limit as $\epsilon \to 0$, the last term on the left-hand side vanishes:

$$\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dx' G(x,x') = 0, \qquad (0.128)$$

thus leaving

$$p_0(x')\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dx'\frac{d^2G(x,x')}{dx'^2} + p_1(x')\lim_{\epsilon\to 0}\int_{x'-\epsilon}^{x'+\epsilon} dG(x,x') = 1 \qquad (0.129)$$

or

$$\begin{aligned}p_0(x')\lim_{\epsilon\to 0}\left[\frac{dG(x,x'+\epsilon)}{dx'} - \frac{dG(x,x'-\epsilon)}{dx'}\right] \\ +p_1(x')\lim_{\epsilon\to 0}\left[G(x,x'+\epsilon) - G(x,x'-\epsilon)\right] = 1. \qquad (0.130)\end{aligned}$$

From the continuity of $G(x,x')$, in the limit as $\epsilon \to 0$, the second term on the left-hand side vanishes, thus leaving us with the fact that the derivative of $G(x,x')$ has a finite discontinuity by the amount $1/p_0(x')$ at $x = x'$.

Using these results, we now construct the Green's function under more general conditions than used in Sections 19.1-19.4. Let the general solution of $\pounds y(x) = 0$ be given as

$$y(x) = ay_1(x) + by_2(x), \tag{0.131}$$

where $\pounds y_1(x) = 0$ and $\pounds y_2(x) = 0$. We write the general form of the Green's function as

$$\begin{aligned} G(x,x') &= Ay_1(x) + By_2(x), \quad x - x' > 0, \\ G(x,x') &= Cy_1(x) + Dy_2(x), \quad x - x' < 0. \end{aligned} \tag{0.132}$$

At $x = x'$ the two functions must match and their derivatives differ by $1/p_0(x)$:

$$Ay_1(x') + By_2(x') = Cy_1(x') + Dy_2(x'), \tag{0.133}$$

$$Ay_1'(x') + By_2'(x') = Cy_1'(x') + Dy_2'(x') + \frac{1}{p_0(x')}. \tag{0.134}$$

We first write these equations as

$$(A - C)y_1(x') + (B - D)y_2(x') = 0, \tag{0.135}$$

$$(A - C)y_1'(x') + (B - D)y_2'(x') = \frac{1}{p_0(x')}, \tag{0.136}$$

so that

$$(A - C) = \frac{\begin{vmatrix} 0 & y_2(x') \\ 1/p_0(x') & y_2'(x') \end{vmatrix}}{\begin{vmatrix} y_1(x') & y_2(x') \\ y_1'(x') & y_2'(x') \end{vmatrix}} \tag{0.137}$$

$$= -\frac{y_2(x')}{p_0(x')W(x')}, \tag{0.138}$$

where the Wronskian, $W(y_1, y_2)$, is defined as

$$W(x') = y_1(x')y_2'(x') - y_2(x')y_1'(x'). \tag{0.139}$$

Similarly,

$$(B - D) = \frac{y_1(x')}{p_0(x')W(x')}. \tag{0.140}$$

We can now write the Green's function as

$$G(x',x) = Cy_1(x) + Dy_2(x) - \frac{[y_1(x)y_2(x') - y_2(x)y_1(x')]}{p_0(x')W(x')}, \; x - x' > 0, \tag{0.141}$$

and

$$G(x - x') = Cy_1(x) + Dy_2(x),\ \ x - x' < 0. \tag{0.142}$$

Let us now impose the boundary conditions.

Type 1: Using

$$G(a, x') = 0, \tag{0.143}$$

$$\frac{\partial G(a, x')}{\partial x'} = 0, \tag{0.144}$$

we write

$$Cy_1(a) + Dy_2(a) = 0, \tag{0.145}$$

$$Cy_1'(a) + Dy_2'(a) = 0. \tag{0.146}$$

Since $W(x') \neq 0$, we get

$$C = D = 0, \tag{0.147}$$

thus the Green's function becomes

$$G(x', x) = \Theta(x - x')\frac{[y_1(x)y_2(x') - y_2(x)y_1(x')]}{p_0(x')W(x')}, \tag{0.148}$$

where $\Theta(x - x')$ is the unit step function.

As an example [Prob. (19.5)], consider

$$\frac{d^2y}{dx^2} + k_0^2 y(x) = f(x),\ \ y(0) = y'(0) = 0. \tag{0.149}$$

The two linearly independent solutions satisfying the boundary conditions are

$$y_1(x) = \cos(k_0 x), \tag{0.150}$$

$$y_2(x) = \sin(k_0 x). \tag{0.151}$$

With the Wronskian determined as $W(x) = k_0$, Equation (0.148) allows us to write the Green's function as

$$G(x', x) = \Theta(x - x')\frac{\sin[k_0(x - x')]}{k_0}, \tag{0.152}$$

which agrees with our earlier result [Eq. (19.143)].

Type II: We now use the two point boundary condition:

$$G(a, x') = 0, \tag{0.153}$$

$$G(b, x') = 0 \tag{0.154}$$

to write

$$Cy_1(a) + Dy_2(a) = 0, \tag{0.155}$$

$$Cy_1(b) + Dy_2(b) - \frac{[y_1(b)y_2(x') - y_2(b)y_1(x')]}{p_0(x')W(x')} = 0. \tag{0.156}$$

Simultaneous solution of these yield the Green's function

$$G(x,x') = \frac{[y_1(x')y_2(a) - y_1(a)y_2(x')]\,[y_1(b)y_2(x) - y_2(b)y_1(x)]}{[y_1(b)y_2(a) - y_1(a)y_2(b)]\,p_0(x')W(x')},\ x - x' > 0, \tag{0.157}$$

$$G(x,x') = \frac{[y_1(x)y_2(a) - y_1(a)y_2(x)]\,[y_1(b)y_2(x') - y_2(b)y_1(x')]}{[y_1(b)y_2(a) - y_1(a)y_2(b)]\,p_0(x')W(x')},\ x - x' < 0. \tag{0.158}$$

The second solution:

In constructing Green's functions by using the above formulas we naturally need two linearly independent solutions and also the Wronskian of the solutions. The nice thing about the Wronskian in this case is that it can be obtained from the differential operator:

$$\pounds = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x),\ x \in [a,b]. \tag{0.159}$$

Let us now write the derivative of the Wronskian

$$\frac{dW(x)}{dx} = \frac{d}{dx}\left[y_1(x)y_2'(x) - y_2(x)y_1'(x)\right], \tag{0.160}$$

$$= y_1(x)y_2''(x) - y_1''(x)y_2(x). \tag{0.161}$$

where

$$\left[p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)\right] y_i(x) = 0,\ i = 1 \text{ or } 2. \tag{0.162}$$

We rewrite the differential equation, $\pounds y(x) = 0$, as

$$\frac{d^2y_i}{dx^2} + P(x)\frac{dy_i}{dx} + Q(x)y_i(x) =\ \ i = 1 \text{ or } 2, \tag{0.163}$$

to get

$$y_1y_2'' - y_1''y_2 = -P(x)[y_1y_2' - y_2y_1'], \tag{0.164}$$

$$= -P(x)W(x), \tag{0.165}$$

thus

$$\frac{dW}{dx} = -P(x)W(x). \tag{0.166}$$

Hence the Wronskian can be obtained from the differential operator, $\pounds$, by the integral

$$W(x) = e^{-\int_a^x dx' P(x')}. \tag{0.167}$$

Furthermore, by using the Wronskian and a special solution, we can also obtain a second solution. If we write $W(x)$ as

$$W(x) = y_1 y_2' - y_2 y_1' \tag{0.168}$$

$$= y_1^2 \frac{d}{dx}\left(\frac{y_2}{y_1}\right), \tag{0.169}$$

we obtain

$$y_2(x) = y_1(x) \int_a^x \frac{W(x')}{y_1^2(x')} dx'. \tag{0.170}$$

In other words, a second solution, y_2, can be obtained from a given solution, y_1, and the Wronskian, W.

Example (0.2): Green's function for the Helmholtz equation in spherical coordinates:

We consider the open problem for the Helmholtz equation in spherical coordinates with an inhomogeneous term, $F(r)$:

$$\overrightarrow{\nabla}^2 \Psi(r,\theta,\phi) + k^2 \Psi(r,\theta,\phi) = F(r), \ r \in [0,\infty]. \tag{0.171}$$

In terms of the spherical harmonics the general solution can be written as

$$\Psi(r,\theta,\phi) = \sum_{lm} R_l(kr) Y_{lm}(\theta,\phi). \tag{0.172}$$

Substituting this into the Helmholtz equation [Eq. (0.171)] we obtain the differential equation that $R_l(kr)$ satisfies as

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R_l(kr) = 0. \tag{0.173}$$

Substituting

$$R_l(kr) = \frac{y_l(kr)}{kr}, \tag{0.174}$$

we also obtain

$$y_l''(x) + \left[1 - \frac{l(l+1)}{x^2}\right] y_l(x) = 0, \tag{0.175}$$

where

$$x = kr. \tag{0.176}$$

The two linearly independent solutions can be written in terms of Bessel functions, J_n, N_n, as

$$R_l(kr) = \frac{y_l(kr)}{kr} = \begin{cases} j_l(kr) = \sqrt{\dfrac{\pi}{2}}\dfrac{J_{l+1/2}(kr)}{\sqrt{kr}}, \\ \\ n_l(kr) = \sqrt{\dfrac{\pi}{2}}\dfrac{N_{l+1/2}(kr)}{\sqrt{kr}}. \end{cases} \tag{0.177}$$

For large r these solutions behave as

$$R_l(kr) = \lim_{r\to\infty} \begin{cases} j_l(kr) \overset{r\to\infty}{\to} \dfrac{\cos(kr-(l+1)\frac{\pi}{2})}{kr}, \\ \\ n_l(kr) \overset{r\to\infty}{\to} \dfrac{\sin(kr-(l+1)\frac{\pi}{2})}{kr}. \end{cases} \tag{0.178}$$

Using Equations (0.141) and (0.142) we can now construct the Green's function as

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{p_0(r)W(r')}, \ r - r' > 0, \tag{0.179}$$

$$g_l(r,r') = Cj_l(kr) + Dn_l(kr), \ r - r' < 0. \tag{0.180}$$

For a regular solution at the origin we set $D = 0$. We evaluate the Wronskian, $W(r)$, by using Equation (0.167) as

$$\frac{dW}{W} = -P(r)dr \tag{0.181}$$

$$= -\frac{2}{r}dr, \tag{0.182}$$

which yields

$$W(r) = \frac{\text{constant}}{r^2}. \tag{0.183}$$

To evaluate the constant we use the asymptotic forms of the Bessel functions as

$$\lim_{r\to\infty} W(kr) = \lim_{r\to\infty} \begin{vmatrix} j_l(kr) & n_l(kr) \\ j_l'(kr) & n_l'(kr) \end{vmatrix} \tag{0.184}$$

$$= \begin{vmatrix} \dfrac{\cos(kr-(l+1)\frac{\pi}{2})}{kr} & \dfrac{\sin(kr-(l+1)\frac{\pi}{2})}{kr} \\ \dfrac{-k\sin(kr-(l+1)\frac{\pi}{2})}{kr} & \dfrac{k\cos(kr-(l+1)\frac{\pi}{2})}{kr} \end{vmatrix} \tag{0.185}$$

$$= \frac{k}{(kr)^2} \tag{0.186}$$

$$= \frac{1}{kr^2}, \tag{0.187}$$

thus

$$W(r) = \frac{1}{kr^2}. \tag{0.188}$$

Since $p_0(x) = 1$ [Eq. (0.162)], we write

$$g_l(r, r') = Cj_l(kr) + Dn_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{(1/kr'^2)}, \ r - r' > 0, \tag{0.189}$$

$$g_l(r, r') = Cj_l(kr) + Dn_l(kr), \ r - r' < 0. \tag{0.190}$$

For a solution regular at the origin we set $D = 0$:

$$g_l(r, r') = Cj_l(kr) - \frac{j_l(kr)n_l(kr') - n_l(kr)j_l(kr')}{(1/kr'^2)}, \ r - r' > 0, \tag{0.191}$$

$$g_l(r, r') = Cj_l(kr), \ r - r' < 0. \tag{0.192}$$

To determine the remaining constant we demand that as $r \to \infty$ we have a spherically outgoing wave, that is,

$$\lim_{r \to \infty} g_l(r, r') \to \frac{e^{ikr}}{r}. \tag{0.193}$$

This implies the relation

$$\frac{kr'^2 j_l(kr')}{[C - kr'^2 n_l(kr')]} = i, \tag{0.194}$$

which gives

$$C = -ikr'^2 h^{(1)}(kr'). \tag{0.195}$$

Substituting this into the expression for the Green's function [Eqs. (0.191) and (0.192)] we obtain, after some algebra,

$$g_l(r, r') = -ikr'^2 h_l^{(1)}(kr)j_l(kr'), \ r - r' > 0, \tag{0.196}$$

$$g_l(r, r') = -ikr'^2 h_l^{(1)}(kr')j_l(kr), \ r - r' < 0. \tag{0.197}$$

We usually write this as

$$g_l(r, r') = -ikr'^2 h_l^{(1)}(kr_>)j_l(kr_<). \tag{0.198}$$

Exercise (0.2): Find the Green's function for the Helmholtz equation outside a spherical boundary with the radius a and satisfying the boundary conditions

$$R(a) = \text{finite}, \tag{0.199}$$

$$R(r) \overset{r \to \infty}{\to} \frac{e^{ikr}}{kr}. \tag{0.200}$$

Example (0.3): In Section 19.1.15 using the Fourier transforms we have solved the Helmholtz equation

$$\overrightarrow{\nabla}^2\Psi(\overrightarrow{r}) + k^2\Psi(\overrightarrow{r}) = F(\overrightarrow{r}),\ r \in [0,\infty], \tag{0.201}$$

as

$$\Psi(\overrightarrow{r}) = \xi(\overrightarrow{r}) + \int d\overrightarrow{r} G(\overrightarrow{r},\overrightarrow{r}')F(\overrightarrow{r}'), \tag{0.202}$$

where $\xi(\overrightarrow{r})$ is the solution of the homogeneous equation:

$$\overrightarrow{\nabla}^2\Psi(\overrightarrow{r}) + k^2\Psi(\overrightarrow{r}) = 0, \tag{0.203}$$

and the Green's function, $G(\overrightarrow{r},\overrightarrow{r}')$, is given as

$$G(\overrightarrow{r},\overrightarrow{r}') = -\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}. \tag{0.204}$$

We expand $F(\overrightarrow{r}')$ as

$$F(\overrightarrow{r}') = \sum_{l,m} F_l(r')Y_{lm}(\theta',\phi'), \tag{0.205}$$

where the angular part is separated and then expanded in term of spherical harmonics. Since $G(\overrightarrow{r},\overrightarrow{r}')$ depends only on $\left|\overrightarrow{r}-\overrightarrow{r}'\right|$, we can write its expansion as

$$G(\overrightarrow{r},\overrightarrow{r}') = \sum_{l''=0}^{\infty} C_{l''}(r,r')P_{l''}(\cos\theta_{12}), \tag{0.206}$$

where θ_{12} is the angle between $\overrightarrow{r}$ and $\overrightarrow{r}'$. Using the addition theorem of spherical harmonics [Eq. (11.325)] we can write this as

$$G(\overrightarrow{r},\overrightarrow{r}') = \sum_{l''=0}^{\infty} C_{l''}(r,r') \sum_{m''=-l''}^{l''} \frac{4\pi}{(2l''+1)} Y^*_{l''m''}(\theta',\phi')Y_{l''m''}(\theta,\phi), \tag{0.207}$$

which allows us to write the solution as

$$\begin{aligned}\Psi(\overrightarrow{r}) &= \xi(\overrightarrow{r}) \\ &+ \left[\int_0^{2\pi}\int_0^{\pi} d\Omega' \int_0^{\infty} dr'\ r'^2\right. \\ &\times \left.\sum_{l'',m'',l,m} \frac{4\pi}{(2l''+1)} C_{l''}(r,r')Y^*_{l''m''}(\theta',\phi')F_l(r')Y_{lm}(\theta',\phi')\right] Y_{l''m''}(\theta,\phi).\end{aligned} \tag{0.208}$$

We can also expand the solution, $\Psi(\overrightarrow{r})$, and $\xi(\overrightarrow{r})$ to write

$$\sum_{l,m} R_l(kr) Y_{lm}(\theta,\phi) = \sum_{l,m} \xi(r) Y_{lm}(\theta,\phi) + \sum_{l,m} \left[\frac{4\pi}{(2l+1)} \int_0^\infty dr'\ r'^2 C_l(r,r') F_l(r') \right] Y_{lm}(\theta,\phi), \tag{0.209}$$

where we have used the orthogonality relation [Eq. (2.179)] of the spherical harmonics. Comparing both sides of Equation (0.209) gives

$$R_l(kr) = \xi(r) + \frac{4\pi}{(2l+1)} \int_0^\infty dr'\ r'^2 C_l(r,r') F_l(r'). \tag{0.210}$$

We now compare Equation (0.210) with Example 0.2, where

$$R_l(kr) = \xi(r) + \int_0^\infty dr' g_l(r,r') F_l(r'), \tag{0.211}$$

to get the relation between $C_l(r,r')$ and $g_l(r,r')$ as

$$\frac{4\pi}{(2l+1)} r'^2 C_l(r,r') = g_l(r,r'). \tag{0.212}$$

Using Equation (0.198) this becomes

$$\frac{4\pi}{(2l+1)} r'^2 C_l(r,r') = -ikr'^2 h_l^{(1)}(kr_>) j_l(kr_<). \tag{0.213}$$

Finally, substituting this into Equation (0.207) and with Equation (0.204) gives us

$$-\frac{1}{4\pi} \frac{e^{ik|\overrightarrow{r}-\overrightarrow{r}'|}}{|\overrightarrow{r}-\overrightarrow{r}'|} = -ik \sum_{l=0}^{\infty} h_l^{(1)}(kr_>) j_l(kr_<) \sum_{m=-l}^{l} Y^*_{lm}(\theta',\phi') Y_{lm}(\theta,\phi), \tag{0.214}$$

a formula extremely useful in applications.

Example (0.3): Diffraction from a circular aperture:

In the previous problems we have considered the entire space. If there are some black surfaces that restrict the region available to us, we use the formula [Eq. (19.238)]

$$\Psi(\overrightarrow{r}) = \int_V d\overrightarrow{r}' G(\overrightarrow{r},\overrightarrow{r}') F(\overrightarrow{r}') + \sum_{i=1}^{k} \int ds'_i\ \widehat{\mathbf{n}}'_i \cdot \left[\Psi(\overrightarrow{r}') \overrightarrow{\nabla}' G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}') \overrightarrow{\nabla}' \Psi(\overrightarrow{r}') \right]. \tag{0.215}$$

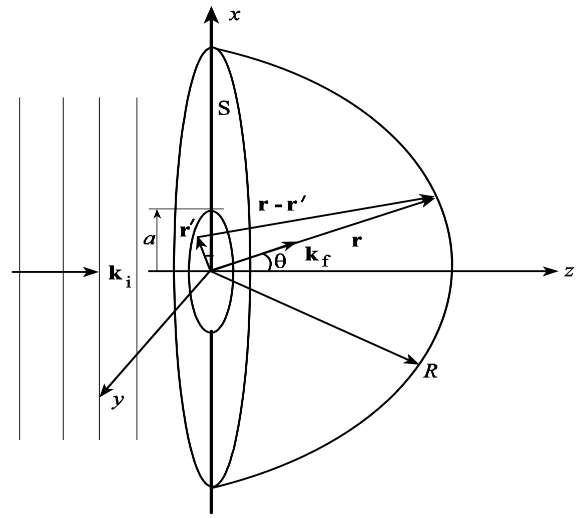

Fig. 0.1 Diffraction from a spherical aperture.

Let us now apply this formula to diffraction from a circular aperture, where a plane wave,

$$\Psi(\overrightarrow{r}) = Ae^{ikz}, \tag{0.216}$$

moving in the z-direction is incident upon a screen lying in the xy-plane with a circular aperture. Our region of integration is the inside of the hemisphere as the radius R goes to infinity (Fig. 0.1). The surfaces that bound our region are the screen, S, which lies in the xy-plane and which has a circular aperture of radius a, and the surface of the hemisphere as $R \to \infty$. Inside the hemisphere there are no sources: $F(\overrightarrow{r}') = 0$, hence the Green's function in this region is

$$G(\overrightarrow{r}, \overrightarrow{r'}) = -\frac{1}{4\pi} \frac{e^{ik\left|\overrightarrow{r} - \overrightarrow{r}'\right|}}{|\overrightarrow{r} - \overrightarrow{r}'|}. \tag{0.217}$$

The solution is now written entirely in terms of surface integrals as

$$\begin{aligned}\Psi(\overrightarrow{r}) = &\int_{xy\text{-plane}} ds'\, \widehat{\mathbf{e}}_z \cdot \left[\Psi(\overrightarrow{r}')\overrightarrow{\nabla}' G(\overrightarrow{r}, \overrightarrow{r}') - G(\overrightarrow{r}, \overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')\right] \\ &+ \int_{R\to\infty} ds'\, \widehat{\mathbf{e}}_r \cdot \left[\Psi(\overrightarrow{r}')\overrightarrow{\nabla}' G(\overrightarrow{r}, \overrightarrow{r}') - G(\overrightarrow{r}, \overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')\right],\end{aligned} \tag{0.218}$$

where $\overrightarrow{r}'$ is a vector on the aperture. We use $\overrightarrow{k}_i$ to denote wave vector of the incident plane wave moving in the direction of $\overrightarrow{\mathbf{e}}_z$, and use $\overrightarrow{k}_f$ for the diffracted wave propagating in the direction of $\overrightarrow{r}$. Both vectors have the same magnitude: $\left|\overrightarrow{k}_i\right| = \left|\overrightarrow{k}_f\right| = k$. We impose the following boundary conditions: On the hemisphere and in the limit as the radius, R, goes to infinity, we have an outgoing spherical wave:

$$\Psi(\overrightarrow{r}) \overset{r\to\infty}{\to} f(\theta,\phi)\frac{e^{ikr}}{r}, \tag{0.219}$$

On the screen:

$$\Psi(\overrightarrow{r})\big|_{z=0} = 0, \tag{0.220}$$

$$\overrightarrow{\nabla}\Psi(\overrightarrow{r})\Big|_{z=0} = 0 \tag{0.221}$$

and on the aperture:

$$\Psi = Ae^{ikz'}\Big|_{z'=0} = A, \tag{0.222}$$

$$\frac{d\Psi}{dz'} = Aike^{ikz'}\Big|_{z'=0} = Aik. \tag{0.223}$$

Let us first look at the integral over the hemisphere, which we can write as

$$\int\int_{R\to\infty} r'^2 d\Omega' f(\theta',\phi')\left[\frac{e^{ikr'}}{r'}\frac{\partial}{\partial r'}\left(-\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}\right)\right.$$
$$\left.+\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}\frac{\partial}{\partial r'}\left(\frac{e^{ikr'}}{r'}\right)\right]. \tag{0.224}$$

In the limit as $R \to \infty$, the quantity inside the square brackets goes to zero as $1/r'^3$, hence the above integral goes to zero as $1/r'$. This leaves us with the first term in Equation (0.218):

$$\Psi(\overrightarrow{r}) = \int_{xy\text{-plane}} ds'\ \widehat{\mathbf{e}}_n \cdot \left[\Psi(\overrightarrow{r}')\overrightarrow{\nabla}'G(\overrightarrow{r},\overrightarrow{r}') - G(\overrightarrow{r},\overrightarrow{r}')\overrightarrow{\nabla}'\Psi(\overrightarrow{r}')\right]. \tag{0.225}$$

From the boundary conditions on the screen [Eqs. (0.220) and (0.221)], we see that the only contribution to this integral comes from the aperture, where the boundary conditions are given by Equations (0.222) and (0.223), hence we write

$$\Psi(\overrightarrow{r}) = -\int_{\text{Aperture}} ds'\ A\left[\frac{\partial}{\partial z'}\left(-\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}\right)\right.$$
$$\left.-ik\left(-\frac{1}{4\pi}\frac{e^{ik\left|\overrightarrow{r}-\overrightarrow{r}'\right|}}{\left|\overrightarrow{r}-\overrightarrow{r}'\right|}\right)\right]. \tag{0.226}$$

The extra minus sign in front of the integral comes from the fact that the outward normal to the aperture is in the negative z direction. Let

$$\overrightarrow{R} = \overrightarrow{r} - \overrightarrow{r}' = (X, Y, Z), \tag{0.227}$$

$$X = x - x', Y = y - y', Z = z - z', \tag{0.228}$$

thus

$$\Psi(\overrightarrow{r}) = -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\frac{\partial}{\partial z'}\left(\frac{e^{ikR}}{R}\right) + ik\frac{e^{ikR}}{R}\right] \tag{0.229}$$

$$= -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\frac{d}{dR}\left(\frac{e^{ikR}}{R}\right)\frac{\partial R}{\partial z'} + ik\frac{e^{ikR}}{R}\right] \tag{0.230}$$

$$= -\frac{A}{4\pi}\int_{\text{Aperture}} ds' \left[-\left(\frac{ike^{ikR}}{R} - \frac{e^{ikR}}{R^2}\right)\left(-\frac{Z}{R}\right) + ik\frac{e^{ikR}}{R}\right]. \tag{0.231}$$

We now write $|\overrightarrow{r} - \overrightarrow{r}'|$ as

$$|\overrightarrow{r} - \overrightarrow{r}'|^2 = (\overrightarrow{r} - \overrightarrow{r}') \cdot (\overrightarrow{r} - \overrightarrow{r}') \tag{0.232}$$

$$= r^2 + r'^2 + 2\overrightarrow{r} \cdot \overrightarrow{r}' \tag{0.233}$$

$$= r^2\left(1 + 2\frac{\overrightarrow{r}}{r} \cdot \frac{\overrightarrow{r}'}{r} + \frac{r'^2}{r^2}\right), \tag{0.234}$$

hence

$$|\overrightarrow{r} - \overrightarrow{r}'| = r\left(1 + 2\frac{\overrightarrow{r}}{r} \cdot \frac{\overrightarrow{r}'}{r} + \frac{r'^2}{r^2}\right)^{1/2}. \tag{0.235}$$

For $\dfrac{r'}{r} \ll 1$, we use the approximation

$$|\overrightarrow{r} - \overrightarrow{r}'| \simeq 1 + \overrightarrow{\mathbf{n}} \cdot \frac{\overrightarrow{r}'}{r} + 0\left(\frac{1}{r^2}\right), \tag{0.236}$$

where $\overrightarrow{\mathbf{n}}$ is a unit vector in the direction of $\overrightarrow{r}$. For large r, we also use the approximation

$$\frac{Z}{R} \simeq \frac{z}{R} = \cos\theta,$$

to write the solution as

$$\Psi(\overrightarrow{r}) \simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr(1-\overrightarrow{\mathbf{n}}\cdot\frac{\overrightarrow{r}'}{r})}}{r} + 0\left(\frac{1}{r^2}\right)\right] \tag{0.237}$$

$$\simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr}}{r}e^{-ik\overrightarrow{\mathbf{n}}\cdot\overrightarrow{r}'}\right] \tag{0.238}$$

$$\simeq -\frac{Aik}{4\pi}\int_{\text{Aperture}} ds' \left[(\cos\theta + 1)\frac{e^{ikr}}{r}e^{-i\overrightarrow{k}_f\cdot\overrightarrow{r}'}\right], \tag{0.239}$$

where $\overrightarrow{k}_f$ is in the direction of $\overrightarrow{r}$. For a circular aperture we can write this integral as

$$\Psi(\overrightarrow{r}) \simeq -\frac{ikA}{4\pi}(\cos\theta + 1)\frac{e^{ikr}}{r}\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r' e^{-i\overrightarrow{k}_f\cdot\overrightarrow{r}'}\right]. \tag{0.240}$$

To evaluate this integral we have to find the cosine of the angle between $\overrightarrow{k}_f$ and $\overrightarrow{r}'$. The angular coordinates of $\overrightarrow{r}$ and $\overrightarrow{r}'$ are given by (θ, ϕ) and (θ', ϕ'), respectively. Using the trigonometric relation

$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi'), \tag{0.241}$$

where γ is the angle between the two vectors, $\overrightarrow{r}$ and $\overrightarrow{r}'$, and since $\overrightarrow{r}'$ is a vector on the aperture, hence $\theta' = \pi/2$, we get

$$\cos\gamma = \sin\theta\cos(\phi - \phi'). \tag{0.242}$$

Equation (0.240) now becomes

$$\Psi(\overrightarrow{r}) \simeq -\frac{ikA}{4\pi}\frac{e^{ikr}}{r}(\cos\theta + 1)\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r' e^{-ikr'\cos\gamma}\right] \tag{0.243}$$

$$\simeq -\frac{ikA}{4\pi}\frac{e^{ikr}}{r}(\cos\theta + 1)\left[\int_0^{2\pi} d\phi' \int_0^a dr'\ r' e^{-ikr'\sin\theta\cos(\phi-\phi')}\right]. \tag{0.244}$$

We define two new variables:

$$x = kr'\sin\theta \tag{0.245}$$

and

$$\beta = \phi - \phi', \tag{0.246}$$

to write the above integrals as

$$\Psi(\overrightarrow{r}) \simeq -\frac{ikA}{2}\left(\frac{e^{ikr}}{r}\right)\frac{(\cos\theta + 1)}{k^2\sin^2\theta}\left[\frac{1}{2\pi}\int_0^{ka\sin\theta} dx\ x \int_0^{2\pi} d\beta\ e^{-ix\cos\beta}\right]. \tag{0.247}$$

We now concentrate on the integral:

$$I = \int_0^{ka\sin\theta} dx\ x\left[\frac{1}{2\pi}\int_0^{2\pi} d\beta\ e^{-ix\cos\beta}\right]. \tag{0.248}$$

Using the integral definition of Bessel functions [Eq. (6.49)] we can show that the expression inside the square brackets is nothing but $J_0(x)$, hence

$$I = \int_0^{ka\sin\theta} dx\ xJ_0(x). \tag{0.249}$$

We also use the recursion relation [Eq. (6.50)]

$$xJ_0(x) = \frac{d}{dx}[xJ_1(x)], \tag{0.250}$$

to evaluate the final integral in I as

$$I = ka \sin\theta J_1(ka \sin\theta). \tag{0.251}$$

Substituting this into Equation (0.247) gives us the solution as

$$\Psi(\overrightarrow{r}) \simeq -\frac{iAa}{2}\left(\frac{e^{ikr}}{r}\right)\frac{(\cos\theta + 1)}{\sin\theta} J_1(ka \sin\theta). \tag{0.252}$$

Since the intensity is $|\Psi(r)|^2 r^2$, we obtain

$$\text{Intensity} = \frac{A^2 a^2 (\cos\theta + 1)^2}{4r^2 \sin^2\theta} J_1^2(ka \sin\theta). \tag{0.253}$$

Problems in diffraction theory are usually very difficult and exact solutions are quite rare. For a detailed treatment of the subject we refer the reader to *Classical Electrodynamics* by Jackson (Bayin, 2006).

III. Useful Sites

Additional references and other useful information about the perturbation theory and diffraction can be found in the following sites:

`http://en.wikipedia.org/wiki/Perturbation_theory_(quantum_mechanics)`,
`http://en.wikipedia.org/wiki/Diffraction`,
`http://scienceworld.wolfram.com/physics/Diffraction.html`.

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