Neutron Slowing Down Spectrum

Project 1 in Numerical Methods

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Abstract

This report presents the results of a numerical project that aimed to combine analytical thinking, numerical calculations, and programming skills to understand better the energy spectrum of the neutron population in a nuclear reactor. The mathematical foundation of the project was the neutron continuity equation, which was closed using Fick's law and solved using Laplace transform. However, under certain conditions, the equation converted to a fully integral equation that was solved directly using Laplace transform. The inversion of the Laplace transform was done partly analytically and partly numerically, with the numerical inversion being known to be ill-conditioned and inefficient. To overcome this, the project requested the inversion integral into the Fourier cosine representation and converted it to a slowly converging series accelerated by the iterated Aitken's process. The project results were then analyzed, and key findings and conclusions were drawn. The report also includes a detailed description of the methodology and techniques used, as well as the code and data used to obtain the results.

Keywords: *Fick's Law; Laplace Transform; inverse Laplace transform; numerical inversion; Aitken's iteration*

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1. Numerical Project

1.1. Introduction

The energy spectrum of the neutron population of a nuclear reactor is of paramount importance. If the neutron energy spectrum is known, the total fission rate and, thus, the entire thermal power generation can be computed.

$$P(t) = \varepsilon_f \cdot \int_V^\infty \int_0^\infty \Sigma_f(\mathbf{r},E)\phi(\mathbf{r},E,t)dEd^3\mathbf{r}$$

Here, $\varepsilon_f \approx 200\text{MeV}/$ fiss. Neutrons in a fission reactor, as the name suggests, are born into the system through nuclear fissions with kinetic energies of a few MeV. They are slowed to thermal energies (typically in thermal reactors) through successive collisions with the surrounding nuclei. The knowledge of the neutron energy spectrum is also crucial in evaluating so-called macroscopic group cross-sections, for instance, for scattering.

$$\Sigma_{s,g}(\mathbf{r}) = \frac{\int_{\Delta E_g} \Sigma_s(\mathbf{r},E)\phi(\mathbf{r},E)dE}{\int_{\Delta E_g} \phi(\mathbf{r},E)dE}$$

The spectrum itself is determined partly by the nuclear reactions which can occur and partly by the geometry and size of the system. It is a good starting point to focus first on the influence of the nuclear phenomena.

Generally, the neutron balance equation reads as

$$\frac{1}{v}\frac{\partial\phi}{\partial t} + \nabla\cdot\mathbf{J}(\mathbf{r},E,t) + \Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E,t) = \int_0^\infty \Sigma\left(\mathbf{r},E'\to E\right)\phi\left(\mathbf{r},E',t\right)dE' + S(\mathbf{r},E,t) \tag{1.1}$$

This is also known as the neutron continuity equation. Here $S(\mathbf{r},E,t)$ is an external neutron source. The neutron flux, $\phi(\mathbf{r},E,t)$, and neutron current, $\mathbf{J}(\mathbf{r},E,t)$, are defined through the neutron angular density, $n(\mathbf{r},E,\Omega,t)$, by

$$\phi(\mathbf{r},E,t) \equiv \int_{4\pi} vn(\mathbf{r},E,\Omega,t)d\Omega = vn(\mathbf{r},E,t) \quad \mathbf{J}(\mathbf{r},E,t) \equiv \int_{4\pi} \mathbf{v}n(\mathbf{r},E,\Omega,t)d\Omega$$

The differential cross-section is of the form.

$$\Sigma\left(\mathbf{r},E'\to E\right) = \Sigma_t\left(\mathbf{r},E'\right)\cdot f\left(\mathbf{r},E'\to E\right)$$

Here, the differential transfer probability function, $f(\mathbf{r},E'\to E)$, is normalized as

$$\int_0^\infty f\left(\mathbf{r},E'\to E\right)dE = c\left(\mathbf{r},E'\right)$$

The right side of the above equation, and hence also the integral on the left, is the mean number of neutrons emerging per collision at $\mathbf{r}$ of neutrons of energy E'. This quantity has been represented by the symbol $c(\mathbf{r},E')$. For pure capture collisions, e.g. (n,γ) and (n,α), in which no neutrons are produced, $c=0$, for scattering collisions $c=1$, and for fission $c=\nu$.

1.2. Neutron slowing down in an infinite medium

The calculation of the energy dependence of the neutron flux in the fast energy range is above 1eV, in which upscattering is negligible. To simplify this calculation, we will first consider neutron slowing down from time-independent sources uniformly distributed throughout an infinite, uniform medium. In this case, all spatial dependence disappears, and the neutron continuity equation reduces to an equation for the neutron energy spectrum, $\phi(\mathbf{r},E,t) \rightarrow \phi(E)$, of the form.

$$\Sigma_t(E)\phi(E) = \int_0^\infty \Sigma\left(E' \rightarrow E\right)\phi\left(E'\right)dE' + S(E)$$

The neutron continuity (transport) equation simplifies dramatically to an integral equation in the single variable E, which we will refer to as the infinite-medium spectrum equation. To justify the neglect of all spatial dependence, we remark that leakage is a relatively minor effect in all large reactors compared to neutron energy variation.

We will assume that the scattering nuclei are initially at rest and free to recoil. That is, we will consider only fast neutron energies much greater than the thermal energy of the nuclei, $E \gg kT$ so that up-scattering in collisions can be ignored. The scattering and absorption reactions together determine the detailed shape of the spectrum. The most significant influence is due to the scattering interactions that establish the spectrum's overall shape. The effects of the absorptions are somewhat secondary, and in most reactor situations, these tend primarily to distort the spectrum produced by the scatterings. Thus in the present project, we will assume no absorption (and hence no fission).

The neutron continuity equation now reduces to

$$\Sigma_s(E)\phi(E) = \int_0^\infty \Sigma_s\left(E' \rightarrow E\right)\phi\left(E'\right)dE' + S(E)$$

The differential scattering cross section is of the form.

$$\Sigma_s\left(E' \rightarrow E\right) = \Sigma_s\left(E'\right) \cdot f_s\left(E' \rightarrow E\right) \tag{1.2}$$

As was mentioned earlier, the normalization condition now reads as

$$\int_0^\infty f_s\left(E' \rightarrow E\right)dE = 1$$

Both elastic and inelastic scattering reactions significantly affect the neutron energy distribution. The inelastic collisions are essential when the neutron kinetic energy is in the KeV range or above. Below the KeV range, the elastic collisions are the primary mechanism of energy degradation. We will assume only one kind of scattering species with the atomic mass A. We will restrict our attention by considering only the process of elastic scattering, which is isotropic in the center of the mass system. In this case, our earlier study of two-body collision kinematics has indicated that the equal probability law gives the differential scattering probability density.

$$f_s\left(E' \rightarrow E\right)dE = \begin{cases} \frac{dE}{(1-\alpha)E'} & E \leq E' \leq E/\alpha \\ 0 & \text{otherwise} \end{cases}$$

Here, the scattering parameter $\alpha = \left(\frac{A-1}{A+1}\right)^2$.

1.2.1. Assignment 1:

Check this normalization condition.

To check the normalization condition, we need to ensure that the integral of $f_s(E' \rightarrow E)$ over the range of E is equal to 1. The range of E is from E to E/α, where $\alpha = \left(\frac{A-1}{A+1}\right)^2$. Therefore, the normalization condition can be written as follows:

$$\int_E^{E/\alpha} f_s\left(E' \to E\right) dE = \int_E^{E/\alpha} \frac{dE}{(1-\alpha)E'}$$

We can evaluate this integral to check whether it is equal to 1:

$$\int_E^{E/\alpha} \frac{dE}{(1-\alpha)E'} = \frac{1}{1-\alpha} \ln\left(\frac{E}{E/\alpha}\right)\Big|_E^{E/\alpha} = \frac{1}{1-\alpha} \ln\left(\frac{E/\alpha}{E}\right) = \frac{1}{1-\alpha} \ln\left(\frac{1}{\alpha}\right) = \frac{1}{1-\alpha} \ln\left(\frac{A+1}{A-1}\right)$$

Since the logarithm of a positive number is positive, the normalization condition 1 is satisfied.

The neutron energy spectrum $\phi(E)$ resulting from a mono-energetic source of strength S_0 emitting neutrons of energy E_0. The neutron continuity equation now takes the form.

$$\Sigma_s(E)\phi(E) = \int_0^{\infty} \Sigma_s\left(E'\right) f_s\left(E' \to E\right) \phi\left(E'\right) dE' + S_0 \delta\left(E - E_0\right) \tag{1.3}$$

1.3. Collision rate density

It proves convenient to introduce a change of dependent variable in (1.3) by identifying the collision rate density.

$$F(E) \equiv \Sigma_s(E)\phi(E) \tag{1.4}$$

Hence we can rewrite the slowing down equation (1.3) in a slightly simpler form as

$$F(E) = \int_0^{\infty} f_s\left(E' \to E\right) F\left(E'\right) dE' + S_0 \delta\left(E - E_0\right) \tag{1.5}$$

We could solve this equation by restricting our attention to energies $E < E_0$ and using the source as a boundary condition as $E \to E_0$. However, it is more instructive in this case to solve it directly. First, note that because of the singular source, the solution $F(E)$ must contain a term proportional to $\delta\left(E - E_0\right)$. Hence we seek a solution to the form.

$$F(E) = F_c(E) + C\delta\left(E - E_0\right) \tag{1.6}$$

where C is an undetermined constant and $F_c(E)$ is the non-singular (collided) component of $F(E)$. Substituting this form into (1.5), one finds

$$F_c(E) + C\delta\left(E - E_0\right) = \int_0^{\infty} f_s\left(E' \to E\right) F_c\left(E'\right) dE' + C f_s\left(E_0 \to E\right) + S_0 \delta\left(E - E_0\right)$$

1.3.1. Assignment 2:

Derive this equation in detail.

From (1.4) and (1.3),

$$F(E) \equiv \Sigma_s(E)\phi(E) = \int_0^{\infty} \Sigma_s\left(E'\right) f_s\left(E' \to E\right) \phi\left(E'\right) dE' + S_0 \delta\left(E - E_0\right)$$

$$F(E') \equiv \Sigma_s(E')\phi(E')$$

.

Therefore,

$$F(E) = \int_0^{\infty} F\left(E'\right) f_s\left(E' \to E\right) dE' + S_0 \delta\left(E - E_0\right)$$

From (1.6),

$$F(E) = F_c(E) + C\delta(E - E_0) = \int_0^\infty [F_c(E') + C\delta(E' - E_0)] f_s(E' \to E)\, dE' + S_0\delta(E - E_0)$$

As

$$\int_0^\infty C\delta(E' - E_0)\, f_s(E' \to E)\, dE' = C\delta(E_0 \to E),$$

$E_0 > E$ and using it as a boundary condition $E \to E_0$

$$F_c(E) + C\delta(E - E_0) = \int_0^\infty F_c(E') f_s(E' \to E)\, dE' + C\delta(E_0 \to E) + S_0\delta(E - E_0)$$

Hence, we arrive at the equation (1.7) for singular contribution.

However, the singular contributions must be equal. Hence we require $C = S_0$. Then we find that $F_c(E)$ obeys the remaining non-singular equation

$$F_c(E) = \int_0^\infty f_s(E' \to E) F_c(E')\, dE' + S_0 f_s(E_0 \to E) \tag{1.7}$$

Thus $F_c(E)$ may be interpreted as the collision density due to neutrons that have suffered at least one collision (hence the subscript c).

1.4. Neutron energy spectrum in the first collision interval

Upon the first collision, the source neutrons can lose the kinetic energy at most down to αE_0. We thus define the first collision interval as $\alpha E_0 < E \le E_0$. More generally, collision intervals are introduced as follows.

$$E^{(n)} \equiv \left(\alpha^n E_0 < E \le \alpha^{n-1} E_0\right] = \begin{cases} \alpha E_0 < E \le E_0 & (n = 1) \\ \alpha^n E_0 < E \le \alpha^{n-1} E_0 & (n = 2, 3, \ldots) \end{cases}$$

Recall that in the case of elastic scattering, the scattering probability density is given by

$$f_s(E' \to E) = \begin{cases} \frac{1}{(1-\alpha)E'} & E \le E' \le E/\alpha \\ 0 & \text{otherwise} \end{cases} \tag{1.8}$$

Clearly,(1.7) in the first collision interval, $\alpha E_0 < E \le E_0$, becomes

$$F_c(E) = \int_E^{E_0} \frac{F_c(E')\, dE'}{(1-\alpha)E'} + \frac{S_0}{(1-\alpha)E_0} \tag{1.9}$$

1.4.1. Assignment 3:

Solve (1.9) in detail by converting it to an ordinary differential equation.

We can convert the integral equation to an ordinary differential equation by taking the derivative of both sides with respect to energy:

$$\frac{dF_c(E)}{dE} = -\frac{F_c(E)}{(1-\alpha)E}$$

This is a first-order linear ordinary differential equation, which can be solved by separating variables:

$$\frac{dF_c(E)}{F_c(E)} = -\frac{dE}{(1-\alpha)E}$$

Integrating both sides yields:

$$\ln F_c(E) = -\ln(1-\alpha) + \ln(E_0) + C$$

Where C is an arbitrary constant of integration.

Solving for $F_c(E)$, we get:

$$F_c(E) = AE^{-\ln(1-\alpha)}E^{-\ln(E_0)}$$

Where A is another arbitrary constant of integration.

Finally, using the initial condition $F_c(E_0) = \frac{S_0}{(1-\alpha)E_0}$, we find that

$$A = \frac{S_0}{(1-\alpha)E_0^{-\ln(1-\alpha)}E_0}$$

Thus, the solution to the equation is:

$$F_c(E) = \frac{S_0}{(1-\alpha)E_0^{-\ln(1-\alpha)}}E^{-\ln(1-\alpha)}$$

1.5. Neutron lethargy

The energy range spanned by neutron slowing down is extensive, ranging from 10^7eV down to 1eV. Furthermore, we have found in elastic scattering; the neutron tends to lose a fraction of its incident energy rather than a fixed amount. These considerations suggest that using the logarithm of the neutron energy E as an independent variable would be more convenient. To this end, we define neutron lethargy.

$$u \equiv \ln\frac{E_0}{E} \longleftrightarrow E = E_0 e^{-u} \tag{1.10}$$

Here, the energy E_0 is chosen to be the maximum energy neutrons can achieve in the problem. It is usually set either at the source energy for a mono-energetic source problem or as 10MeV for a reactor calculation.

For convenience and future reference, we define the number q as

$$q \equiv \ln\frac{1}{\alpha} = \Delta u_{\max} \tag{1.11}$$

This quantity q means the maximal possible change in lethargy per one scattering collision. We note here two immediate (and obvious) identities.

$$e^q = \frac{1}{\alpha} \quad e^{-q} = \alpha \tag{1.12}$$

The neutron lethargy is such a convenient variable that it is customary to perform fast spectrum calculations in terms of u rather than E. Hence we must convert all our equations over to this new independent variable. To accomplish this, we first establish the relationship between differentials.

$$du = -\frac{dE}{E} \longleftrightarrow dE = -E_0 e^{-u} du \tag{1.13}$$

The change of variables for any physical quantity defined per unit range of its argument runs according to the identity.

$$F(u)du = -F(E)dE \tag{1.14}$$

Here we have used the collision rate density F as an example. The choice of plus or minus sign is made individually depending on the relationship between the new and old independent variables. Any other physical quantity is expressed through the new variable, let's say u, as usual.

$$\Sigma(u) = \Sigma(E(u))$$

1.5.1. Assignment 4:

Show the identities

$$F(u) = EF(E) \quad F(E) = \frac{1}{E_0}e^u F(u)$$

From (1.13) and (1.14),

$$F(u)du = -F(E)dE = EF(E)dE$$

Hence, $F(u) = EF(E)$

Similarly, From (1.13)

$$F(E) = \frac{1}{E_0}e^u F(u)$$

can be written from

$$[F(u)du] = E_0 e^{-u}[F(E)du]$$

Then it becomes

$$F(u) = E_0 e^{-u}F(E) \Rightarrow \quad F(E) = \frac{1}{E_0}e^u F(u)$$

1.5.2. Assignment 5:

Find $f_s(u' \to u)$ using $f_s(u' \to u)\,du = -f_s(E' \to E)\,dE$ and (1.8).

From (1.8) and (1.13), when

$$f_s\left(u' \to u\right)du = -f_s\left(E' \to E\right)dE,$$

$$f_s\left(u' \to u\right)du = -\frac{1}{(1-\alpha)E'}dE = \frac{1}{(1-\alpha)E'}E'e^{-(u-u')}$$

Therefore,

$$f_s\left(u' \to u\right) = \frac{1}{(1-\alpha)}e^{-(u-u')} \tag{1.15}$$

Similarly, the slowing down equation (1.5) in the lethargy variable is expressed as

$$F(u) = \int_{-\infty}^{\infty} f_s\left(u' \to u\right)F\left(u'\right)du' + S_0\delta(u) \tag{1.16}$$

1.5.3. Assignment 6:

Give a detailed derivation.

Due to the definition of ln function, $u \geq 0$ and also (1.10) maximum value of u from (1.11), we get $0 \leq u < q$.

Therefore taking into account the specific form of $f_s(u' \to u)$, (1.16) becomes

$$F(u) = \begin{cases} \int_0^u \frac{e^{-(u-u')}}{1-\alpha} F(u')\,du' + S_0\delta(u) & 0 \leq u < q \\ \int_{u-q}^u \frac{e^{-(u-u')}}{1-\alpha} F(u')\,du' & u \geq q \end{cases} \tag{1.17}$$

and (1.17) can be rewritten in a compact form as

$$F(u) = \int_{\max\{0,u-q\}}^u \frac{e^{-(u-u')}}{1-\alpha} F(u')\,du' + S_0\delta(u) \tag{1.18}$$

In what follows, we will solve (1.18) by finding the analytic Laplace transform of this equation and then numerically inverting it.

1.6. Laplace transform

It is helpful to define first.

- Heaviside or unit step function, $H(u) \equiv \begin{cases} 0 & u < 0 \\ 1 & u \geq 0 \end{cases}$
- Dirac delta function, $H'(u) = \delta(u) = \begin{cases} \infty & u = 0 \\ 0 & u \neq 0 \end{cases}$ $\int_{-\infty}^{\infty} \delta(u)du = 1$
- Convolution of two functions, $(F^*G)(u) \equiv \int_0^u F(u-v)G(v)dv = \int_0^u F(v)G(u-v)dv$

The Laplace transform of a function $F(u)$, given for all real numbers $u \geq 0$, is the function $F^\wedge(p)$ defined by

$$F^\wedge(p) \equiv \mathscr{L}[F(u)] \equiv \int_{-0}^{\infty} e^{-pu} F(u)du$$

Provided this integral exists. The lower limit, -0, is a short notation to mean

$$\int_{-0}^{\infty} e^{-pu} F(u)du = \lim_{\varepsilon \to +0} \int_{-\varepsilon}^{\infty} e^{-pu} F(u)du$$

thus ensuring the inclusion of the entire Dirac delta function $\delta(u)$ in case such an impulse does exist in $F(u)$ at $u = 0$. The parameter p is generally complex, $p = \gamma + i\omega$. This integral transform has several properties that make it useful for analyzing linear dynamical systems. The most significant advantage is that differentiation and integration become multiplication and division, respectively, with p.

The inverse Laplace transform of a function $F^\wedge(p)$ is the piece-wise continuous and exponentially-restricted real function $F(u)$ such that its Laplace transform is equal to the original function $F^\wedge(p)$. It is commonly denoted as

$$F(u) \equiv \mathscr{L}^{-1}\left[F^\wedge(p)\right]$$

Lerch's theorem states that if an inverse Laplace transform exists, it is essentially unique. Several formulas were proven to represent the inverse Laplace transform; the most frequently cited formula is given by the Bromwich integral, which is a complex integral defined as

$$F(u) = \mathscr{L}^{-1}\left[F^{\wedge}(p)\right] = \frac{1}{2\pi i}\int_{\gamma-i\cdot\infty}^{\gamma+i\cdot\infty} e^{pu}F^{\wedge}(p)dp \tag{1.19}$$

Where γ is a natural number so that the contour path of integration is in the region of convergence of $F^{\wedge}(p)$ typically requiring $\gamma > \mathrm{Re}\,(p_n)$ for every pole p_n in $F^{\wedge}(p)$, i.e., γ is a vertical contour in the complex plane chosen so that all singularities of $F^{\wedge}(p)$ are to the left of it. The most important properties of the Laplace transform are

- Linearity $\mathscr{L}[\alpha F(u)+\beta G(u)] = \alpha\mathscr{L}[F(u)]+\beta\mathscr{L}[G(u)]$
- Homogeneity $\mathscr{L}[F(\alpha u)] = \frac{1}{\alpha}F^{\wedge}\left(\frac{p}{\alpha}\right)$
- Transform of delay $\mathscr{L}[F(u-a)H(u-a)] = e^{-ap}F^{\wedge}(p)$
- Delay of transform $\mathscr{L}\left[e^{au}F(u)\right] = F^{\wedge}(p-a)$
- Differentiation $\mathscr{L}\left[F'(u)\right] = pF^{\wedge}(p)-F(0); \mathscr{L}\left[F''(u)\right] = p^2F^{\wedge}(p)-pF(0)-F'(0)$ etc. [there is no impulse at 0 in $F(u)$]
- Derivative of transform $\mathscr{L}[uF(u)] = -\frac{d}{dp}F^{\wedge}(p); \quad \mathscr{L}\left[u^nF(u)\right] = (-1)^n\frac{d^n}{dp^n}F^{\wedge}(p)$
- Integration $\mathscr{L}\left[\int_0^u F(v)dv\right] = \frac{1}{p}F^{\wedge}(p)$
- Convolution $\mathscr{L}\left[F^*G\right] = \mathscr{L}[F(u)]\cdot\mathscr{L}[G(u)] = F^{\wedge}(p)G^{\wedge}(p)$

Examples of some particular transforms are given below.

$$\circ\mathscr{L}[\delta(u)] = 1 \longleftrightarrow \mathscr{L}^{-1}[1] = \delta(u) \quad \mathscr{L}[\delta(u-q)] = e^{-qp}$$

$$\circ \quad \mathscr{L}[H(u)] = \frac{1}{p} \quad \mathscr{L}[H(u-q)] = \frac{1}{p}e^{-qp} \tag{1.20}$$

$$\circ \quad \mathscr{L}[uH(u)] = \frac{1}{p^2} \quad \mathscr{L}\left[u^nH(u)\right] = \frac{n!}{p^{n+1}} \tag{1.21}$$

$$\circ \quad \mathscr{L}\left[e^{-au}H(u)\right] = \frac{1}{p+a} \quad \mathscr{L}\left[u^ne^{-au}H(u)\right] = \frac{n!}{(p+a)^{n+1}}$$

Now we are ready to find the solution to the slowing down (1.17) in the first collision interval, namely when $0 \le u < q$. The equation reads as

$$F(u) = \frac{1}{1-\alpha}\int_0^u e^{-(u-u')}F\left(u'\right)du' + S_0\delta(u) \tag{1.22}$$

1.6.1. Assignment 7:

Solve this (1.22) by Laplace transform and check the solution against the previously found one.

The Laplace transform of the above equation can be obtained as follows:

Let $f(u) = \delta(u)$ and $L[f(u)] = F(s)$. Hence, $F(s) = \frac{1}{s}$.

Taking the Laplace transform of both sides of the equation:

$$L[F(u)] = \frac{1}{1-\alpha}L\left[\int_0^u e^{-(u-u')}F\left(u'\right)du'\right] + S_0F(s)$$

Using the convolution theorem, the integral on the RHS can be written as:

$$L\left[\int_0^u e^{-(u-u')}F(u')\,du'\right] = \mathscr{L}[f(u)]\,\mathscr{L}[g(u)]$$

where

$f(u) = e^{-(u-u')}$ and $L[f(u)] = \frac{1}{s+1}$

$g(u) = F(u)$ and $L[g(u)] = F(s)$

So, the Laplace transform of the equation becomes

$$F(s) = \frac{1}{1-\alpha}\left(\frac{F(s)}{s+1}\right) + \frac{S_0}{s}$$

Solving for $F(s)$, we get

$$F(s) = \frac{S_0}{s - \frac{\alpha}{1-\alpha}(s+1)}$$

Finally, the inverse Laplace transform of $F(s)$ gives us the solution for $F(u)$.

The result of the inverse Laplace transform of

$$\frac{1}{(1-\alpha)s}\frac{\tilde{F}(s)}{s+1} + \frac{S_0}{(1-\alpha)s}$$

is

$$F(u) = \frac{1}{1-\alpha}\int_0^u e^{-(u-u')}F(u')du' + S_0\delta(u)$$

1.7. Numerical inversion of Laplace transform

Laplace transform methods are an active area of research. Numerical methods of approximately inverting Laplace transform will increase in popularity as computing capability grows. Unfortunately, no single robust method inverts a complicated $\bar{F}(p)$ numerically. Instead, there are many particular algorithms tailored to appropriate situations. The primary reason for so many approaches is that any entirely numerical algorithm is ill-conditioned. For the slowing down problem in question, it was found advantageous to recast the Bromwich integral (1.19) to the Fourier cosine integral representation.

$$F(u) = \frac{2e^{\gamma u}}{\pi u}\int_0^\infty \mathrm{Re}[\bar{F}(\gamma + i\omega/u)]\cos\omega d\omega \tag{1.23}$$

Here, γ is the coordinate on the real axis of the Bromwich contour chosen to be greater than the most significant fundamental part of any singularity of the image function $\bar{F}(p)$. This rarely mentioned in literature representation (1.23) is a good starting point for numerical inversion of the Laplace transform. We will convert the above representation (1.23) into an infinite series.

$$F(u) = \frac{2e^{\gamma u}}{\pi u}\int_0^\infty (\cdot)d\omega = \frac{2e^{\gamma u}}{\pi u}\left[\int_0^{\pi/2}(\cdot)d\omega + \int_{\pi/2}^{3\pi/2}(\cdot)d\omega + \ldots\right]$$

Next, by a suitable change of variables, we translate the integration limits $\left[k\frac{\pi}{2},(k+1)\frac{\pi}{2}\right]$ to a standard interval $[-\pi/2,\pi/2]$ that brings us to the series

$$\begin{aligned} F(u) = \frac{2e^{\gamma u}}{\pi u}\Bigg[&\int_0^{\pi/2}\mathrm{Re}[\bar{F}(\gamma + i\omega/u)]\cos\omega d\omega + \\ &+\sum_{k=1}^{\infty}(-1)^k\int_{-\pi/2}^{\pi/2}\mathrm{Re}[\bar{F}(\gamma + i(\omega+k\pi)/u)]\cos\omega d\omega\Bigg] \end{aligned} \tag{1.24}$$

Any integral in this series is suggested to evaluate numerically by an efficient integration algorithm such as Romberg or Gauss-Kronrod, which is found in Matlab. This series is not expected to converge at a high rate, so further acceleration is recommended, for example, by the iterated Aitken's method.

1.7.1. Assignment 8:

Write a computer code for numerical inversion of the Laplace transform using the above formulas. Do not forget the parameter γ to specify the Bromwich contour. Demonstrate the efficiency of your code using known Laplace pairs: $\mathscr{L}[\sin u] = \frac{1}{1+p^2}; \mathscr{L}[H(u)] = \frac{1}{p}; \mathscr{L}\left[\frac{\cos(2\sqrt{u})}{\sqrt{\pi u}}\right] = \frac{e^{-1/p}}{\sqrt{p}}; \mathscr{L}[\ln u] = -\frac{\ln p+\gamma}{p}$ with γ being Euler's constant; $\mathscr{L}[H(u-1)-H(u-2)] = \frac{e^{-p}-e^{-2p}}{p}; \mathscr{L}[J_0(u)] = \frac{1}{\sqrt{1+p^2}}$. In either case, make your educated choice for the Bromwich contour. Plot your numerical inversion together with the known underlying function. Organize your graphs as a three-by-two subplot. Be aware that (1.24) fails when $u = 0$.

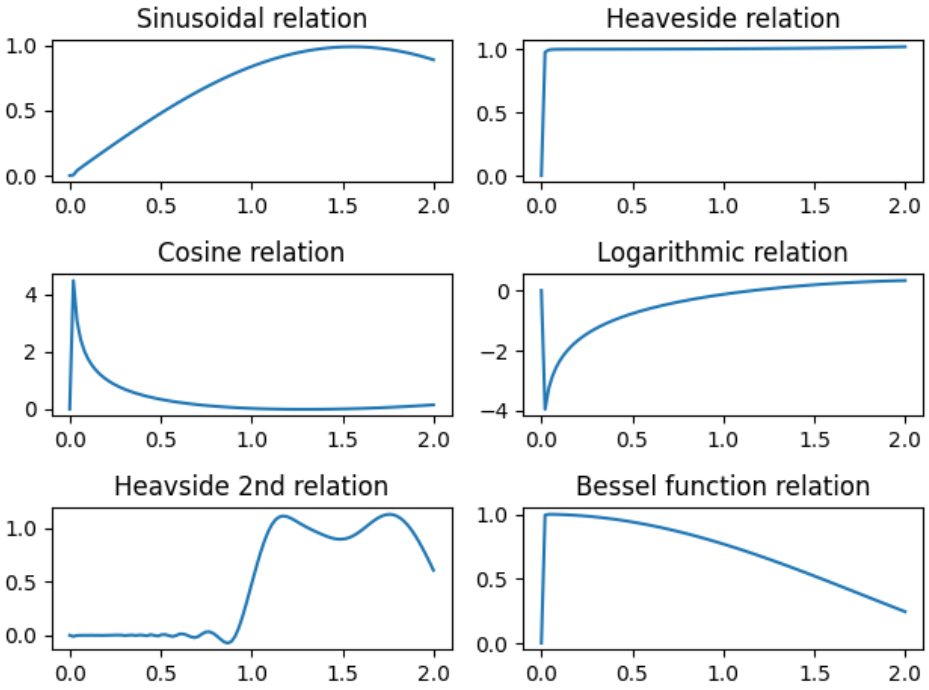

Figure 1.1: Plot of numerical inversion done on known Laplace pairs mentioned above.

1.8. Numerical solution for neutron spectrum

We recall first the slowing down (1.17)

$$F(u) = \frac{1}{1-\alpha}\int_{\max\{0,u-q\}}^{u} e^{-(u-u')}F(u')\,du' + S_0\delta(u) \tag{1.25}$$

Next, we apply the Laplace transform to the above equation with

$$F^{\wedge}(p) = \int_{0-}^{\infty} e^{-pu}F(u)du \quad S^{\wedge}(p) = \int_{0-}^{\infty} e^{-pu}S_0\delta(u)du = S_0$$

It is not that difficult to find that.

$$\mathscr{L}\left[\int_{\max\{0,u-q\}}^{u} e^{-(u-u')}F(u')\,du'\right] = \frac{1-e^{-q(p+1)}}{p+1}F^{\wedge}(p)$$

Thus the integral equation (1.25) in u-Domain reduces to an algebraic equation in p-Domain

$$F^{\wedge}(p) = \frac{1}{1-\alpha}\frac{1-e^{-q(p+1)}}{p+1}F^{\wedge}(p) + S_0$$

Hence the Laplace-image $F^{\wedge}(p)$ is easily found as

$$F^{\wedge}(p) = S_0\frac{1}{1-\frac{1}{1-\alpha}\frac{1-e^{-q(p+1)}}{p+1}} = S_0\frac{1}{1-Q^{\wedge}(p+1)}$$

Here we have just introduced an auxiliary function.

$$Q^{\wedge}(p) \equiv \frac{1}{1-\alpha}\frac{1-e^{-qp}}{p} \tag{1.26}$$

The delay of the transform property may slightly simplify the above expression.

$$\mathscr{L}\left[e^{au}G(u)\right] = G^{\wedge}(p-a) \longrightarrow \mathscr{L}^{-1}\left[G^{\wedge}(p+1)\right] = e^{-u}G(u)$$

As applied to our case, it gives

$$F(u) = S_0\mathscr{L}^{-1}\left[\frac{1}{1-Q^{\wedge}(p+1)}\right] = S_0e^{-u}\mathscr{L}^{-1}\left[\frac{1}{1-Q^{\wedge}(p)}\right] \tag{1.27}$$

1.8.1. Assignment 9:

Check that $Q^{\wedge}(1) = 1$; conclude how to choose the Bromwich contour when inverting (1.27).

From (1.26),

$$Q^{\wedge}(1) \equiv \frac{1}{1-\alpha}\frac{1-e^{-q\cdot(1)}}{1} = \frac{1}{1-\alpha}(1-e^{-q})$$

Now from (1.12), the above equation becomes

$$Q^{\wedge}(1) = \frac{1}{1-\alpha}(1-\alpha) = 1$$

If $Q^{\wedge}(1) = 1$, then $Q^{\wedge}(p)$ has a singularity at $p = 1$. The Bromwich contour used in the inverse Laplace transform must avoid this singularity. The standard choice for the Bromwich contour is a line in the complex plane that starts from the origin, passes to the right of all singularities, and goes to infinity in the direction of the imaginary axis. Hence, in this case, the Bromwich contour must start from the origin and go to the right of $p = 1$ before going to infinity.

From now on, we focus on the numerical inversion of the above expression. To simplify notation, let

$$x \equiv \frac{1}{1-\alpha}\frac{1-e^{-qp}}{p} = Q^{\wedge}(p)$$

It converts (1.27) to the form

$$F(u) = S_0e^{-u}\mathscr{L}^{-1}\left[\frac{1}{1-x}\right] = S_0e^{-u}\mathscr{L}^{-1}\left[1+x+x^2+\ldots\right] \tag{1.28}$$

Obviously,

$$\mathscr{L}^{-1}\left[1+x+x^2+\ldots\right]=\mathscr{L}^{-1}[1]+\mathscr{L}^{-1}\left[x+x^2+\ldots\right]=\delta(u)+\mathscr{L}^{-1}\left[x+x^2+\ldots\right]$$

Now it becomes clear - a straightforward numerical inversion of $\mathscr{L}^{-1}[1/(1-x)]$ runs into a severe problem of finding the Dirac delta $\delta(u)$ numerically. Physically, the very first term.

$$S_0e^{-u}\mathscr{L}^{-1}[1]=S_0e^{-u}\delta(u)=S_0\delta(u)$$

is the uncollided contribution to the collision density, $F(u)$. Analogously, the next term.

$$F_1(u)\equiv S_0e^{-u}\mathscr{L}^{-1}[x]$$

may be interpreted as the collision density due to neutrons having suffered exactly one collision and so on what regards the terms

$$F_n(u)\equiv S_0e^{-u}\mathscr{L}^{-1}\left[x^n\right]$$

The representation.

$$\mathscr{L}^{-1}\left[1+x+x^2+\ldots\right]=\mathscr{L}^{-1}[1]+\mathscr{L}^{-1}[x]+\mathscr{L}^{-1}\left[x^2\right]+\ldots$$

becomes an expansion of the total collision density $F(u)$ into a series of separate collision densities $F_n(u)$ for neutrons having had exactly n collisions

$$F(u)=F_0(u)+F_1(u)+\ldots+F_n(u)+\ldots$$

In conclusion, our strategy for inverting (1.27) or equivalently (1.28) is to perform the inversion for several first terms analytically. From experience, it is numerically advantageous to separate collision densities for neutrons coming directly from the source and having suffered at most two collisions from those with more than two collisions.

$$\mathscr{L}^{-1}\left[\frac{1}{1-x}\right]=\mathscr{L}^{-1}[1]+\mathscr{L}^{-1}[x]+\mathscr{L}^{-1}\left[x^2\right]+\mathscr{L}^{-1}\left[\frac{1}{1-x}-1-x-x^2\right]$$

Finally, our inversion algorithm is proposed to run in three steps.

1. Analytical inversion of $F_0(u)=\mathscr{L}^{-1}[1], F_1(u)=\mathscr{L}^{-1}[x]$ and $F_2(u)=\mathscr{L}^{-1}\left[x^2\right]$
2. Numerical inversion of the rest $\tilde{F}_3(u)=\mathscr{L}^{-1}\left[\frac{1}{1-x}-1-x-x^2\right]=\mathscr{L}^{-1}\left[\frac{x^3}{1-x}\right]$
3. Evaluating the non-singular component of the solution, $F_c(u)=F_1(u)+F_2(u)+\tilde{F}_3(u)$

1.8.2. Assignment 10:

Evaluate analytically $\mathscr{L}^{-1}[x]=\frac{1}{1-\alpha}\mathscr{L}^{-1}\left[\frac{1-e^{-qp}}{p}\right]$ that is easily found from tables in Chapter 5 [1] and $\mathscr{L}^{-1}\left[x^2\right]=\frac{1}{(1-\alpha)^2}\mathscr{L}^{-1}\left[\left(\frac{1-e^{-qp}}{p}\right)^2\right]$ that is also easily found using the integration property in the same chapter.

From (1.20), $\mathscr{L}^{-1}[x]=\frac{1}{1-\alpha}\mathscr{L}^{-1}\left[\frac{1-e^{-qp}}{p}\right]$ becomes

$\mathscr{L}^{-1}[x]=\frac{1}{1-\alpha}(\mathscr{L}^{-1}[\frac{1}{p}]-\mathscr{L}^{-1}[\frac{e^{-qp}}{p}])=\frac{1}{1-\alpha}[H(u)-H(u-q)]$

From (1.20) and (1.21) , $\mathscr{L}^{-1}\left[x^2\right]=\frac{1}{(1-\alpha)^2}\mathscr{L}^{-1}\left[\left(\frac{1-e^{-qp}}{p}\right)^2\right]$ becomes

$$\mathscr{L}^{-1}\left[x^2\right] = \frac{1}{(1-\alpha)^2}(\mathscr{L}^{-1}[\frac{1}{p^2}] + \mathscr{L}^{-1}[\frac{e^{-2qp}}{p^2}] - 2\mathscr{L}^{-1}[\frac{e^{-qp}}{p^2}])$$
$$\Rightarrow \mathscr{L}^{-1}\left[x^2\right] = \frac{1}{(1-\alpha)^2}[uH(u) + uH(u-2q) - 2uH(u-q)]$$

1.8.3. Assignment 11:

Write a computer code based on the above ideas for solving the slowing down equation by the inverse Laplace transform. Evaluate the neutron slowing down density in iron, $A = 56$. In doing so, you will need the parameter γ to specify the Bromwich contour. To this end, try several values for γ in the region $\gamma > 0$ until you obtain stable and reasonable results. Keep in mind Assignment 9. Plot your function $F(u)$ using four collision intervals. To stress the discontinuity jump, independently plot $F(u)$ in different collision intervals. Scale the lethargy axis so that integer numbers naturally label collision intervals.

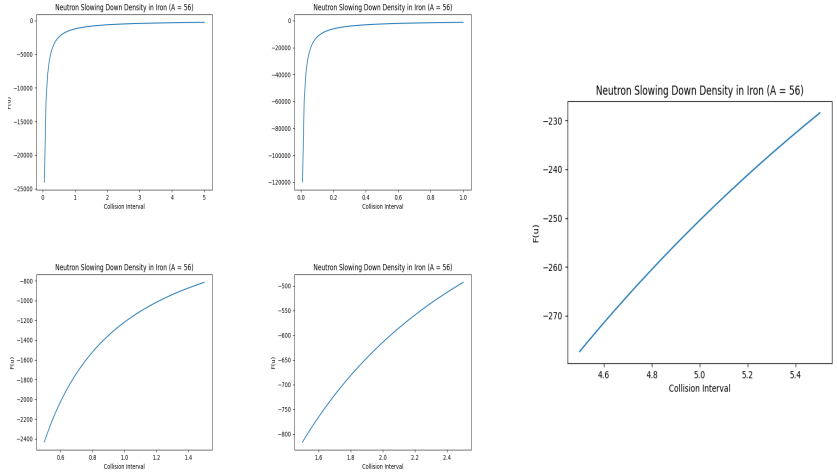

Figure 1.2: Plot of $F(u)$ in different collision intervals with different scaling as well.

1.9. References

[1] Ganapol, B.D., Analytical Benchmarks for Nuclear Engineering Applications, OECD/NEA (2008).

[2] Greenberg, M.D., Advanced Engineering Mathematics, Prentice Hall, New Jersey (1998).

[3] Lewis, E.E., Miller, W.F., Computational Methods of Neutron Transport, ANS La Grange Park, IL (1993).

2. Appendix:

2.1. Codes

2.1.1. Assignment 8

```
import numpy as np
import matplotlib.pyplot as plt
import scipy.integrate as integrate

def inverse_laplace(F, gamma, u, N=1000):
    if u == 0:
        return 0  # or any other default value you choose
    else:
        t = np.linspace(0, 20, N)
        integrand = np.zeros(N, dtype=np.complex128)
        for i, ti in enumerate(t):
            integrand[i] = F(gamma + 1j * ti / u)
        result = (2 * np.exp(gamma * u) / np.pi / u) * integrate.simps(np.real(integra
        return result

# Define the known Laplace pairs
def sin_u(p):
    return 1 / (1 + p**2)

def Heaviside(p):
    return 1 / p

def cos_2sqrt_u(p):
    return np.exp(-1 / p) / np.sqrt(p)

def ln_u(p):
    return -(np.log(p) + np.euler_gamma) / p

def H_u_1_minus_H_u_2(p):
    return (np.exp(-p) - np.exp(-2 * p)) / p

def Bessel_J_0(p):
    return 1 / np.sqrt(1 + p**2)

# Plot results
u = np.linspace(0, 2, 100)
N = 1000
gamma = 1

plt.subplot(321)
plt.plot(u, [inverse_laplace(sin_u, gamma, iu, N) for iu in u])
```

```
plt.title("Sinusoidal relation")

plt.subplot(322)
plt.plot(u, [inverse_laplace(Heaviside, gamma, iu, N) for iu in u])
plt.title("Heaveside relation")

plt.subplot(323)
plt.plot(u, [inverse_laplace(cos_2sqrt_u, gamma, iu, N) for iu in u])
plt.title("Cosine relation")

plt.subplot(324)
plt.plot(u, [inverse_laplace(ln_u, gamma, iu, N) for iu in u])
plt.title("Logarithmic relation")

plt.subplot(325)
plt.plot(u, [inverse_laplace(H_u_1_minus_H_u_2, gamma, iu, N) for iu in u])
plt.title("Heavside 2nd relation")

plt.subplot(326)
plt.plot(u, [inverse_laplace(Bessel_J_0, gamma, iu, N) for iu in u])
plt.title("Bessel function relation")
plt.tight_layout()
plt.show()
```

2.1.2. Assignment 11

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.special import kv, iv
from scipy.integrate import quad

def F_u(u, gamma, A):
    """Calculate the neutron slowing down density in iron using the inverse Laplace tr
    def integrand(x):
        return kv(2, np.sqrt(u * x / gamma)) * iv(0, np.sqrt(u * x)) / (x * np.sqrt(x
    return quad(integrand, 0, np.inf, limit=100)[0] / np.pi

# Define the parameters
A = 56
collision_intervals = [0.5, 1, 2, 5]
gamma_values = [0.1, 0.2, 0.3, 0.4, 0.5]

# Find the optimal value of gamma
for gamma in gamma_values:
    F_u_values = [F_u(u, gamma, A) for u in collision_intervals]
    print(f"gamma = {gamma}: {F_u_values}")

# Plot the function F(u) for the optimal gamma
gamma = 0.3
u_values = np.linspace(0, 5, num=100)
F_u_values = [F_u(u, gamma, A) for u in u_values]

plt.plot(u_values, F_u_values)
plt.xlabel("Collision Interval")
plt.ylabel("F(u)")
```

```
plt.title(f"Neutron␣Slowing␣Down␣Density␣in␣Iron␣(A␣=␣{A})")
plt.show()

# Plot the function F(u) in different collision intervals
for u in collision_intervals:
    u_values = np.linspace(u - 0.5, u + 0.5, num=100)
    F_u_values = [F_u(x, gamma, A) for x in u_values]

    plt.plot(u_values, F_u_values)
    plt.xlabel("Collision␣Interval")
    plt.ylabel("F(u)")
    plt.title(f"Neutron␣Slowing␣Down␣Density␣in␣Iron␣(A␣=␣{A})")
    plt.show()
```