22.51 Problem Set 8 (due Wed, Nov. 28)

1 Conservation of Probability

Question: Earlier in this class we proved $\hat{U}(t)$, and consequently $\hat{U}_I(t)$, is unitary even when $\hat{\mathcal{H}}(t)$ has explicit time-dependence, therefore any normalized initial state $|\psi(0)\rangle$ remains normalized during its time-evolution, so "the probability is conserved". This is however not immediately apparent from equations (6.25) and (6.29), and we would like to demonstrate the conservation more explicitly.

Define a generic small parameter $\lambda \in \mathbf{R}$ as,

$$\frac{1}{\hbar}\int_0^t dt'\hat{V}_I(t') \quad\sim\quad \lambda \quad\ll\quad 1,$$

then in the expansion, the first and second order amplitude coefficients are,

$$c_{nm}^{(1)}(t) \quad\sim\quad \lambda, \qquad c_{nm}^{(2)}(t) \quad\sim\quad \lambda^2.$$

(**a**). When $n \neq m$, e.g. the final state is not the initial state, what is the leading order in λ of the $|m\rangle \rightarrow |n\rangle$ *transition probability*?

(**b**). By (**a**), what can be said about the *escaping probability* from $|m\rangle$?

(**c**). When $n = m$, we are looking at the *staying probability*. There are,

$$c_{mm}^{(1)}(t) \quad\sim\quad \lambda, \qquad c_{mm}^{(2)}(t) \quad\sim\quad \lambda^2,$$

too, but the big difference between $c_{mm}(t)$ and $c_{n\neq m m}(t)$ is that $c_{mm}^{(0)}(t) = 1$, so,

$$c_{mm}(t) \;=\; 1 + a\lambda + b\lambda^2 + ..., \qquad a, b \sim 1. \tag{1}$$

Based on (1), what generally can be said about the staying probability, and the λ-order of the escaping probability assuming total probability conservation? Does there appear to be a contradiction with (**b**)'s result?

(**d**). Fortunately, this paradox can be resolved when a in (1) is *purely imaginary*. Show this.

(**e**). Work out the details to leading order and show that the staying probability is *monotonically decreasing* in quadratic order of λ.

Answer:

(**a**). λ^2.

(**b**). Again λ^2.

(**c**). If (1) is true, then,

$$|c_{mm}(t)|^2 = 1 + (a+a^*)\lambda + (b+b^*+aa^*)\lambda^2 + \mathcal{O}(\lambda^3),$$

so in general, $1-|c_{mm}(t)|^2$ is order λ, which does appear to contradict with (**b**)'s conclusion.

(**d**). Unless, of course, a is purely imaginary, so the first order coefficient $a+a^*=0$, and one has to look beyond the first order, to the second order. This is true here because,

$$a \equiv c_{mm}^{(1)}(t) = \frac{1}{i\hbar}\int_0^T e^{i\omega_{mm}t'} V_{mm}(t')dt' = \frac{1}{i\hbar}\int_0^T V_{mm}(t')dt',$$

since $\omega_{mm}=0$ and $V_{mm}(t) \equiv \langle m|\hat{V}(t)|m\rangle$ must be real as $\hat{V}(t)$ is Hermitian.

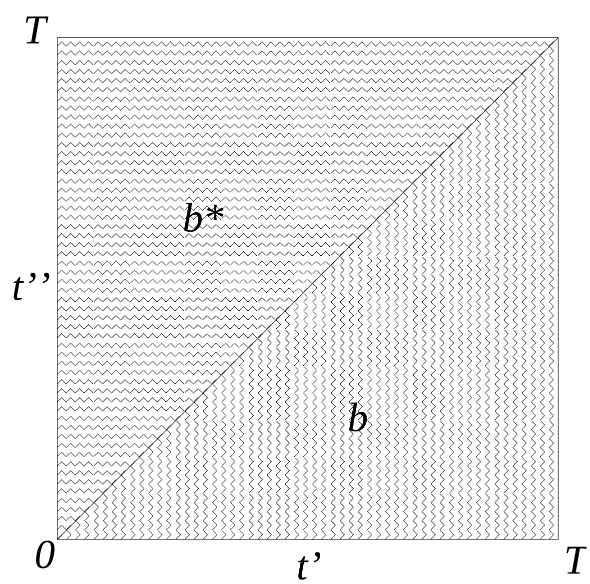

Figure 1: Double Time Integration.

(**e**).

$$b \equiv c_{mm}^{(2)}(t) = \left(\frac{1}{i\hbar}\right)^2 \sum_l \int_0^T e^{i\omega_{ml}t'} V_{ml}(t')dt' \int_0^{t'} e^{i\omega_{lm}t''} V_{lm}(t'')dt'',$$

$$b^* = \left(\frac{1}{i\hbar}\right)^2 \sum_l \int_0^T \left[e^{i\omega_{ml}t'} V_{ml}(t')\right]^* dt' \int_0^{t'} \left[e^{i\omega_{lm}t''} V_{lm}(t'')\right]^* dt''$$

$$
\begin{aligned}
&= \left(\frac{1}{i\hbar}\right)^2 \sum_l \int_0^T e^{i\omega_{lm}t'} V_{lm}(t')dt' \int_0^{t'} e^{i\omega_{ml}t''} V_{ml}(t'')dt'' \\
&= \left(\frac{1}{i\hbar}\right)^2 \sum_l \int_0^T e^{i\omega_{lm}t''} V_{lm}(t'')dt'' \int_0^{t''} e^{i\omega_{ml}t'} V_{ml}(t')dt',
\end{aligned}
$$

where there has been a change of labeling index $t' \leftrightarrow t''$ in the last step. So, from Fig. 1 we see that,

$$
\begin{aligned}
b + b^* &= \left(\frac{1}{i\hbar}\right)^2 \sum_l \int_0^T e^{i\omega_{lm}t'} V_{lm}(t')dt' \int_0^T e^{i\omega_{ml}t''} V_{ml}(t'')dt'' \\
&= \left(\frac{1}{i\hbar}\right)^2 \sum_l \left| \int_0^T e^{i\omega_{lm}t'} V_{lm}(t')dt' \right|^2 . \qquad (2)
\end{aligned}
$$

Also,

$$
aa^* = -\left(\frac{1}{i\hbar}\right)^2 \left| \int_0^T e^{i\omega_{mm}t'} V_{mm}(t')dt' \right|^2 .
$$

Thus,

$$
b + b^* + aa^* = -\frac{1}{\hbar^2} \sum_{l \neq m} \left| \int_0^T e^{i\omega_{lm}t'} V_{lm}(t')dt' \right|^2 ,
$$

which is exactly minus the *escaping probability.* So we see that the total probability is indeed conserved to the leading orders, and the *staying probability* is monotonically decreasing as λ^2.

2 Delta-Function and Density of States

Question:

(**a**). Using the residue integration technique, prove that,

$$
\lim_{\epsilon \to 0^+} \frac{\epsilon}{\pi(x^2 + \epsilon^2)} = \delta(x).
$$

(**b**). In chap 5.1 we showed how to obtain the density of states for a translationally invariant system ($\mathbf{k}$ can then be used as labeling index) assuming one knows the dispersion relation. Calculate the density of states $g(E)$ of a free electron of mass m and spin $+\frac{\hbar}{2}$ in a box (periodic boundary condition or infinite-well confinement - it doesn't matter) of volume V, when E is much larger than the minimum quantum energy.

(**c**). What is the density of states $g(E)$ of the combined system of one electron (mass m_1, spin $+\frac{\hbar}{2}$) and one photon (spin $+\hbar$) in a box V, assuming they do not interact? Here E is the total energy, and is assumed to be much larger than the minimum quantum energy.

(**d**). A more general definition of the density of states $g(E)$ which is still valid when the system loses translational symmetry (for example, electron in an amorphous solid) would be,

$$g(E) \equiv \sum_n \delta(E - E_n), \quad E \in \mathbf{R},$$

where,

$$\hat{\mathcal{H}}|n\rangle = E_n|n\rangle.$$

Let us define the *resolvent* of $\hat{\mathcal{H}}$ to be,

$$\hat{G}(z) \equiv (z - \hat{\mathcal{H}})^{-1}, \quad z \in \mathbf{C}.$$

Prove that,

$$g(E) = -\frac{1}{\pi} \lim_{\epsilon \to 0^+} \mathrm{ImTr}\left[\hat{G}(E + i\epsilon)\right], \quad E \in \mathbf{R}.$$

(**e**). The following identity is widely used (in EE for example),

$$\int_{-\infty}^{\infty} \exp(i\omega t) dt = 2\pi\delta(\omega), \tag{3}$$

which if taken literally, does not make sense because the LHS integral is not absolutely convergent. Demonstrate however that,

$$\lim_{T\to\infty} \int_{-T}^{T} \exp(i\omega t) dt = 2\pi\delta(\omega),$$

and,

$$\lim_{\epsilon\to 0^+} \int_{-\infty}^{\infty} e^{-\epsilon|t|} \exp(i\omega t) dt = 2\pi\delta(\omega).$$

Therefore, (3) should be interpreted in the context of finite T-truncation or adiabatic switching, which are both *termination schemes*. All processes in this world *are* finitely terminated.

Answer:

(**a**). Define complex function,

$$f(z) \equiv \frac{\epsilon}{\pi(z^2 + \epsilon^2)} = \frac{1}{2\pi i}\left(\frac{1}{z - i\epsilon} - \frac{1}{z + i\epsilon}\right),$$

which is analytic in $\mathbf{C}$ except at simple poles $i\epsilon$ and $-i\epsilon$. Let us do a loop integral in the upper half plane that includes only the $i\epsilon$ pole, then,

$$\left[\int_{\text{CR}} + \int_{\text{C1}}\right] f(z)dz \;=\; 2\pi i \cdot \frac{1}{2\pi i} \;=\; 1,$$

by the residue theorem. On the other hand, as $R \to \infty$,

$$|f(z)| \;\sim\; \frac{1}{R^2},$$

so,

$$\left|\int_{\text{CR}} f(z)dz\right| \;\sim\; \frac{1}{R^2}\cdot R \;=\; \frac{1}{R} \;\to\; 0,$$

and therefore,

$$\int_{\text{C1}} f(z)dz \;=\; 1 \;=\; \int_{-\infty}^{\infty} f(x)dx \;=\; \int_{-\infty}^{\infty} \frac{\epsilon}{\pi(x^2+\epsilon^2)}dx.$$

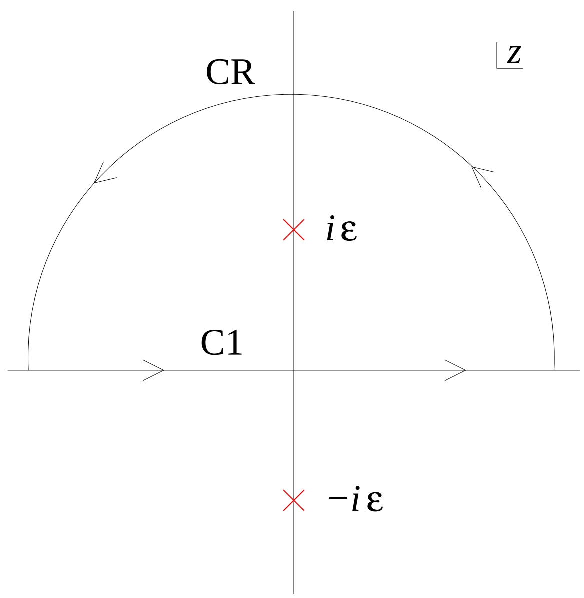

Figure 2: Residue integration for Lorentzian.

The above is true for any ϵ, but it is clear that as $\epsilon \to 0$, $f(x)$ becomes a narrower and narrower function centered around $x = 0$. Thus,

$$\lim_{\epsilon\to 0^+} \frac{\epsilon}{\pi(x^2+\epsilon^2)} \;=\; \delta(x) \;=\; -\frac{1}{\pi}\lim_{\epsilon\to 0^+} \text{Im}\frac{1}{x+i\epsilon}.$$

Addendum: I would like to prove the following identity which is very useful for physicists,

$$\lim_{\epsilon\to 0^+} \frac{1}{x \pm i\epsilon} \;=\; \mathcal{P}\left(\frac{1}{x}\right) \mp i\pi\delta(x), \tag{4}$$

where $\mathcal{P}(1/x)$ means principal value integration for $1/x$, defined as below,

$$\int_a^b \mathcal{P}\left(\frac{1}{x}\right) g(x)dx \;\equiv\; \lim_{\epsilon\to 0^+}\left[\int_a^{-\epsilon} \frac{g(x)}{x}dx + \int_\epsilon^b \frac{g(x)}{x}dx\right],$$

if $a < 0 < b$ and $g(x)$ is any 0^{th}-order continuous 1D function at $x = 0$. $\mathcal{P}(1/x)$ allows one to "overcome" x^{-1} type singularities occurring in the integration.

The imaginary part of (4) is already illustrated. For the real part, there is,

$$\text{Re}\frac{1}{x+i\epsilon} \;=\; \frac{1}{2}\left(\frac{1}{x+i\epsilon} + \frac{1}{x-i\epsilon}\right) \;=\; \frac{x}{x^2+\epsilon^2},$$

which is plotted in Fig. 3(a).

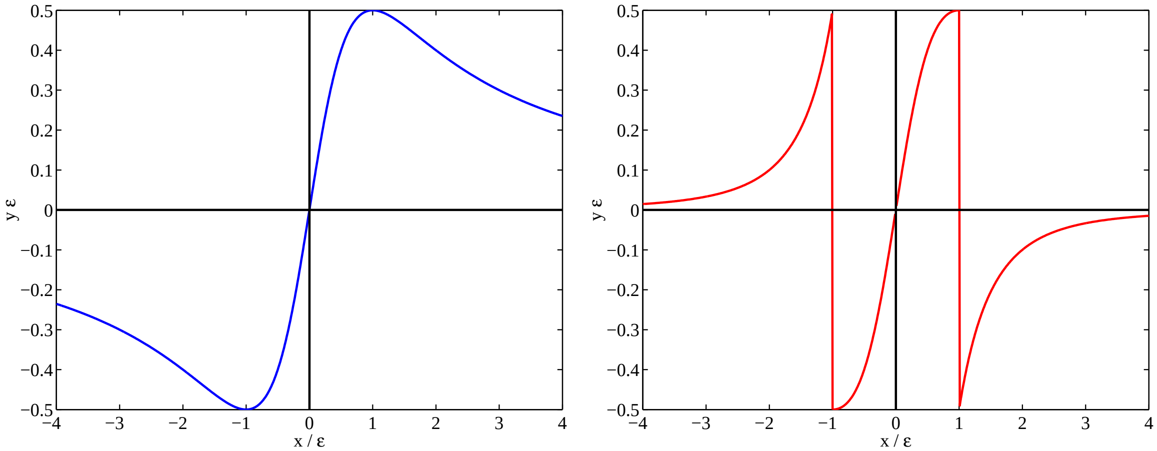

Figure 3: (a). The function $\text{Re}\frac{1}{x-i\epsilon}$. (b). The residual $\text{Re}\frac{1}{x-i\epsilon} - \frac{\theta(|x|>\epsilon)}{x}$.

What we need to show is that,

$$\lim_{\epsilon\to 0^+} I_1(\epsilon) - I_2(\epsilon) \;=\; 0,$$

where,

$$I_1(\epsilon) \;\equiv\; \left[\int_a^{-\epsilon} + \int_\epsilon^b\right] \frac{g(x)}{x}dx, \qquad I_2(\epsilon) \;\equiv\; \int_a^b \frac{x}{x^2+\epsilon^2} g(x)dx.$$

Let us break up $I_2(\epsilon)$ into,

$$I_2(\epsilon) \quad = \quad I_3(\epsilon) + I_4(\epsilon),$$

where,

$$I_3(\epsilon) \quad \equiv \quad \int_{-\epsilon}^{+\epsilon} \frac{x}{x^2+\epsilon^2} g(x)dx, \qquad I_4(\epsilon) \quad \equiv \quad \left[\int_a^{-\epsilon} + \int_\epsilon^b\right] \frac{x}{x^2+\epsilon^2} g(x)dx.$$

For $I_3(\epsilon)$, let us expand $g(x)$ as,

$$g(x) \quad = \quad g(0) + g'(0)x + \mathcal{O}(x^2).$$

Observe that,

$$\int_{-\epsilon}^{+\epsilon} \frac{x}{x^2+\epsilon^2} g(0)dx \quad = \quad 0, \qquad \int_{-\epsilon}^{+\epsilon} \frac{x}{x^2+\epsilon^2} \cdot xdx \quad = \quad \mathcal{O}(\epsilon).$$

We find,

$$\lim_{\epsilon\to 0^+} I_3(\epsilon) \quad = \quad \lim_{\epsilon\to 0^+} \mathcal{O}(\epsilon) \quad = \quad 0.$$

Notice that even if there is first-order discontinuity: $g'(0^+) \neq g'(0^-)$, this argument still holds.

For $I_4(\epsilon)$, let it be subtracted off by $I_1(\epsilon)$. Since,

$$\frac{x}{x^2+\epsilon^2} - \frac{1}{x} \quad = \quad -\frac{\epsilon^2}{x(x^2+\epsilon^2)},$$

this difference again can be shown to be vanishing in the limit of $\epsilon \longrightarrow 0$ as $\mathcal{O}(\epsilon^{-1})$ by scaling analysis similar to $I_3(\epsilon)$ (see Fig. 3(b)). Therefore,

$$\lim_{\epsilon\to 0^+} \mathrm{Re}\frac{1}{x+i\epsilon} \quad = \quad \mathcal{P}(1/x),$$

and (4) is a succinct and powerful summary of our results.

(**b**). The dispersion relation of a free electron from the non-relativistic Schrodinger's equation is,

$$E \quad = \quad \frac{\hbar^2 k^2}{2m}, \qquad k \quad = \quad \frac{\sqrt{2mE}}{\hbar}.$$

Therefore a thin spherical shell in the **k**-space has volume,

$$d^3\mathbf{k} \;=\; 4\pi k^2 dk \;=\; 4\pi \frac{2mE}{\hbar^2}\frac{\sqrt{m}dE}{\sqrt{E}\hbar},$$

which would roughly contain,

$$dN \;=\; \frac{V}{8\pi^3}\cdot d^3\mathbf{k},$$

number of **k**-points when E is much larger than the minimum quantum energy so the granularity of the quantum levels is averaged out, irrespective of whether the volume is a confinement box like a blackbody cavity, or the hypothetical world under Born - von Karman periodic boundary condition. Thus,

$$g(E) \;\equiv\; \frac{dN}{dE} \;=\; \frac{V}{8\pi^3}4\pi\frac{2mE}{\hbar^2}\frac{\sqrt{m}}{\sqrt{E}\hbar} \;=\; \frac{Vm^{3/2}}{\pi^2\hbar^3}\sqrt{E}.$$

The $\sqrt{E}$ behavior is indeed observed in many simple metals like Al and Cu even though the valence electrons are not entirely free.

(**c**). For a single photon of prescribed spin, the density of states is,

$$g(E) \;=\; \frac{V}{8\pi^3}4\pi\left(\frac{E}{\hbar c}\right)^2\frac{1}{\hbar c} \;=\; \frac{V}{2\pi^2\hbar^3c^3}E^2.$$

It is easy to show that the combined density of states of two non-interacting systems, each with density of states $g_1(E)$ and $g_2(E)$, respectively, is,

$$g(E) \;=\; \int_0^E g_1(E')g_2(E-E')dE'.$$

By Maple,

$$\int_0^E \sqrt{E'}\,(E-E')^2\,dE' \;=\; \frac{16}{105}E^{7/2},$$

therefore the total density of states is,

$$g(E) \;=\; \frac{Vm^{3/2}}{\pi^2\hbar^3}\frac{V}{2\pi^2\hbar^3c^3}\frac{16}{105}E^{7/2}.$$

(**d**). There is,

$$\mathrm{Tr}\hat{G}(z) \;\equiv\; \sum_n \langle n|(z-\hat{\mathcal{H}})^{-1}|n\rangle \;=\; \sum_n (z-E_n)^{-1}.$$

So,

$$-\frac{1}{\pi}\lim_{\epsilon\to 0^+}\mathrm{Im}\mathrm{Tr}\hat{G}(E+i\epsilon) = -\frac{1}{\pi}\sum_n \lim_{\epsilon\to 0^+}\mathrm{Im}(E+i\epsilon-E_n)^{-1} = \sum_n \delta(E-E_n) \equiv g(E).$$

The beauty of this theorem is that $\mathrm{Tr}\hat{G}(z)$ is manifestly independent of the basis used. Although here we use the energy eigenstates $\{|n\rangle\}$ to prove the theorem, we are not obliged to use them when evaluating $\mathrm{Tr}\hat{G}(z)$. This offers unique insights into the connection between *local* and *global pictures* of the system.

$\hat{G}(z)$, by the way, is the Laplace transform of the Schrodinger's equation. It is the *propagator*, or the Green's function, of the quantum dynamics in z-space, and can be probed in various ways.

(**e**). First let us consider the function,

$$f(x) \equiv \frac{2\sin x}{x},$$

and its integral,

$$I \equiv \int_{-\infty}^{+\infty} f(x)dx,$$

which is actually *absolutely convergent* since the $\sin x$ factor is oscillatory and henceforth regularize the $1/x$ long tail in the integration. When $x\sim 0$, $f(x)\sim 2$ is also well behaved, so we could make use of the following construction,

$$I = \lim_{\epsilon\to 0^+} 2\int_{\epsilon}^{+\infty} f(x)dx,$$

by the fact that $f(x)$ is even and regular. However,

$$\int_{\epsilon}^{+\infty} f(x)dx = \int_{\epsilon}^{+\infty}\frac{e^{ix}-e^{-ix}}{ix}dx = \left[\int_{-\infty}^{-\epsilon}+\int_{\epsilon}^{+\infty}\right]\frac{e^{ix}}{ix}dx.$$

Now let us define a complex function,

$$g(z) \equiv \frac{e^{iz}}{iz}, \quad z\in\mathbf{C},$$

which is analytic everywhere except for the simple pole at $z=0$. Therefore the contour integral shown in Fig. 4,

$$\left[\int_{\mathrm{C1}}+\int_{\mathrm{CR}}+\int_{\mathrm{C}\epsilon}\right] g(z)dz = 0.$$

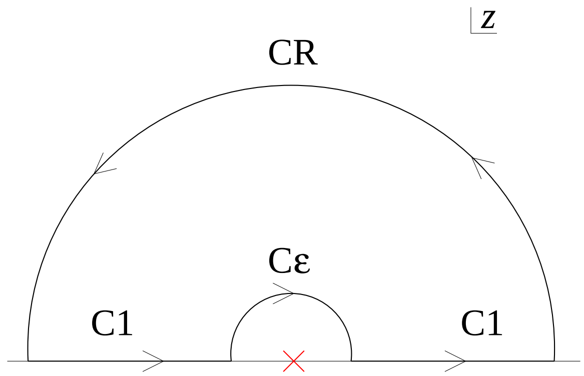

Figure 4: Residue integration for sinc().

But, the CR integral vanishes as $R \to \infty$, since e^{iz} vanishes in the upper half plane:

$$\int_{\mathrm{CR}} \frac{e^{iRe^{i\theta}}}{iRe^{i\theta}} dRe^{i\theta} = \int_0^\pi e^{iRe^{i\theta}} d\theta,$$

and there is only θ range $\sim \mathcal{O}(1/R)$ that gives significant contribution. On the other hand, for Cϵ integral,

$$e^{i\epsilon e^{i\theta}} \approx 1, \qquad \int_{\mathrm{C}\epsilon} \frac{e^{i\epsilon e^{i\theta}}}{i\epsilon e^{i\theta}} d\epsilon e^{i\theta} \approx \int_\pi^0 d\theta = -\pi.$$

Therefore,

$$\int_{\mathrm{C1}} g(z)dz = \pi, \quad \int_\epsilon^{+\infty} f(x)dx = \pi, \quad \int_{-\infty}^{\infty} \frac{2\sin x}{x} = 2\pi.$$

Let us define,

$$f_T(\omega) \equiv \int_{-T}^{T} \exp(i\omega t)dt = \frac{\exp(i\omega T) - \exp(-i\omega T)}{i\omega} = \frac{2\sin(\omega T)}{\omega},$$

and observe that,

$$\int_{-\infty}^{+\infty} f_T(\omega)d\omega = \int_{-\infty}^{+\infty} \frac{2\sin(\omega T)}{\omega T} d(\omega T) = \int_{-\infty}^{\infty} \frac{2\sin x}{x} = 2\pi,$$

which is independent of T. Therefore, as $T \to \infty$, $f_T(\omega) \to 2\pi\delta(\omega)$, and so,

$$\lim_{T\to\infty} \int_{-T}^{T} \exp(i\omega t)dt = 2\pi\delta(\omega).$$

Also note that under finite translation a,

$$\lim_{T\to\infty}\int_{-T+a}^{T+a}\exp(i\omega t)dt \;=\; \lim_{T\to\infty} e^{i\omega a}\int_{-T}^{T}\exp(i\omega t)dt \;=\; e^{i\omega a}2\pi\delta(\omega) \;=\; 2\pi\delta(\omega),$$

so this abrupt truncation-style termination scheme is in fact robust.

If one prefers a smoother termination scheme, then adiabatic switching is a good idea, where one multiplies any function to be Fourier transformed by $e^{-|\epsilon|t}$ and then take the stabilized result to the $\epsilon \to 0^+$ limit. Suppose $f(x) = 1$, then its stabilized Fourier transform is,

$$\int_{-\infty}^{\infty} e^{-\epsilon|t|}\exp(i\omega t)dt \;=\; \frac{1}{\epsilon - i\omega} + \frac{1}{\epsilon + i\omega} \;=\; \frac{2\epsilon}{\epsilon^2+\omega^2} \;=\; 2\pi\cdot\frac{\epsilon}{\pi(x^2+\epsilon^2)},$$

which we know from (**a**) behaves like $2\pi\delta(\omega)$ as $\epsilon \to 0^+$.

We thus have illustrated in several contexts the *abstract idea* of,

$$\int_{-\infty}^{\infty}\exp(i\omega t)dt \;=\; 2\pi\delta(\omega),$$

which is *independent* of the details of the termination schemes, although a termination scheme *is* necessary. Analogy with this arises repeatedly in physics when mathematical difficulties seem to be insurmountable, quite often due to the inapplicability of the physical laws developed for the present scale to other scales. For example, laws developed for 100 MeV physics may be entirely unfit for 200 GeV physics, so in fact the actual 200 GeV physics may stabilize a divergent integral for the 100 MeV physics problem. On the other hand, it is illustrated by the above example that one *does not have to know* the details of the 200 GeV physics to reach useful conclusions for the 100 MeV physics problem, and the technique allowing one to do this is called *renormalization*.