1 basic equations

What we are trying to solve: the operator equation

$$\mathcal{H} - \sigma\mathcal{I}|\phi\rangle = |\psi\rangle \,;\, \sigma = \sigma_R + i\sigma_i \,;$$

the result (lit transform) is given by $\mathcal{L} = \langle\phi|\phi\rangle$.We now decompose $|\phi\rangle$ and $|\psi\rangle$ in the same nonorthogonal basis $|i\rangle$. Define

$$N_{\mathrm{ij}} = \langle i|j\rangle,\, H_{\mathrm{ij}} = \langle i|\mathcal{H}|j\rangle,\, \psi_i = \langle i|\psi\rangle,\;\; |\phi\rangle = \phi_i|\, i\rangle \;,$$

i.e.,

$$\phi_i = N^{-1}_{ij}\langle j|\phi\rangle.$$

Now solve the equation for ϕ,

$$(H_{\mathrm{ij}} - \sigma N_{\mathrm{ij}})\,\phi_i = \psi_i,$$

and calculate

$$\mathcal{L} = \langle\phi|\phi\rangle = \phi_i N_{\mathrm{ij}}\phi_j \,.$$

2 reducing the basis

Here we tackle the full matrix. Disadvantage of that can be a separate inverse for each σ; no communality between the truncations at different σ. This relies on a pseudo inverse.

Use $M_{ij} = H_{ij} - \sigma N_{ij}$. Write the SVD $M = SUA^\dagger$, with S diagonal, and $U = U^T$ and $A = A^T$ (both orthogonal as M is square). We have

$$S_{ii} = \sqrt{\mathrm{ev}_i(M^T M)}.$$

We can now define a pseudo inverse by

$$M^{-1} = APS^{-1}PU^\dagger \,,$$

where P projects on sensible values of S (greater than a threshold t). This can deal with overcomplete bases, but suffers from some annoying problems, such as the number fo states involved in the iversion changing as we change σ_R.

There is a better alternative: Start again from the basic equation

$$(H_{ij} - \sigma N_{ij})\,\phi_j = \psi_i \,. \tag{1}$$

Again, a subset of indices b is defined by a truncation to those eigenvectors with $\mu^{(n)} > t$. The LIT transform is now

$$\mathcal{L} = \langle \phi | \phi \rangle = \tilde{\phi}_l \tilde{\phi}_l \, .$$

After ignoring the outer orthogonal transformations, that hide the basis reduction, this becomes even simpler in terms of the eigenvalues of

$$\tilde{H}_{ab} = \mu_a^{-1/2} O_{ai} H_{ij} O_{bj} \mu_b^{-1/2} ; \tag{2}$$

Writing

$$\tilde{H}_{ab} e_b^{(m)} = \lambda^m e_a^{(m)} \, ,$$

and

$$\tilde{\psi}^{(m)} = \sum_a \frac{1}{\sqrt{\mu_a}} O_{\mathrm{ai}} \psi_i e_a^{(m)} \, ,$$

we have

$$\mathcal{L} = \langle \phi | \phi \rangle = \sum_m \frac{\left| \tilde{\psi}^{(m)} \right|^2}{\left| \lambda^m - \sigma \right|^2} \, . \tag{3}$$

3 The inverse LIT

Since the LIT transform of any function $S(y)$ with support $[E_0, \infty]$ is defined by the following integral

$$\mathcal{L}[S](\sigma) = \int_{E_0}^{\infty} \frac{S(y)}{(y - \sigma_R)^2 + \sigma_i^2} \, dy \, , \tag{4}$$

we see that the result for the LIT transform (3) shows that the original strength function S for any discrete basis is

$$S(E) = \sum_m \left| \tilde{\psi}^{(m)} \right|^2 \delta(E - \lambda^{(m)}) \, , \tag{5}$$

a sum of discrete peaks.

That raises the question how this has discretised the continuous response $S(E)$ we are looking for. There are two options

1. This gives the value of the strength function S at the discrete energies $\lambda^{(m)}$.

2. This gives an estimate of strength in a region around the energy $\lambda^{(m)}$, weighted in an as yet unknown way.

The feeling is that the second of these is more likely correct: for fixed width σ_I, the LIT converges as we add more an more basis functions; as we increase the number of basis states and the spectrum gets denser, we thus have a concomitant reduction in strength $\left|\tilde{\psi}^{(m)}\right|^2$, otherwise there is no convergent result. Thus case 1 above must be wrong.

So is there anything we can learn from the convergence of the result? What we normally do is squint at the function, i.e., smear the function by working at fixed σ_I, rather than at all σ_I as required to do the exact inversion above. In other words, can we find a smooth function, that depends on σ_I that has the same LIT transform as the discrete sum (5) at every value of σ_I? What we would argue is that such a function becomes more-and-more smooth as we increase σ_I.

Thus we need to find a smooth function $f(y, \sigma_I)$ such that, to sufficient approximation,

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{f(y-E,\sigma_I)}{(y-\sigma_R)^2+\sigma_I^2}\mathrm{d}y &= \int \frac{f(y,\sigma_I)}{(y+E-\sigma_R)^2+\sigma_I^2}\mathrm{d}y \\ &= \frac{1}{(E-\sigma_R)^2+\sigma_I^2}\,. \end{aligned} \tag{6}$$

Does such a function exist? I am not convinced.

So let us see whether we can answer the question slightly differently: We are trying to perform an approximate inversion of the LIT equation (4), with the condition that the underlying $S(y)$ is smooth. Since we have an exact non-smooth answer, either the problem is ill-posed (more than one solution), or there is no strict solution. Since the LIT transform is a convolution, it may make sense to look this at using a Fourier transformation. Use

$$\int_{-\infty}^{\infty} \frac{e^{ik\sigma_R}}{(y-\sigma_R)^2+\sigma_I^2}\, d\sigma_R = \frac{\pi}{\sigma_I} e^{iky-\sigma_I|k|}\,, \tag{7}$$

to derive that

$$\widetilde{\mathcal{L}[S]}(k) = \frac{\pi}{\sigma_I} e^{-\sigma_I|k|} \int_{-\infty}^{\infty} S(y) e^{iky}\,\mathrm{d}y. \tag{8}$$

Here for simplicity we have defined the range of S to be infinite.

We thus see that

$$S(y) = \frac{1}{2\pi}\frac{\sigma_I}{\pi} \int_{-\infty}^{\infty} \widetilde{\mathcal{L}[S]}(k) e^{\sigma_I|k|} e^{-iky}\mathrm{d}k. \tag{9}$$

Since we want to exclude high frequency structure in S, which means short wavelength wiggles, we cut this integral off at a reciprocal scale proportional to $1/\sigma_I$. Let us choose this as α/σ_I with $\alpha = \mathcal{O}(1)$,

$$S_\sigma(y) = \frac{1}{2\sigma_I^2} \int_{-\alpha}^{\alpha} \widetilde{\mathcal{L}[S]}(q/\sigma_I) e^{|q|} e^{-iqy/\sigma} \mathrm{d}q. \tag{10}$$

A simple calculation shows that this corresponds to using a regularised δ function in (5),

$$\delta_c(y) = \frac{1}{y} \sin cy \,, \tag{11}$$

with $c = \alpha/\sigma_R$. Clearly a disadvantage of the approach is that we miss some of the strength in the LIT in the back-transform, but the positive is that we miss the low frequency wiggles. Even for $\alpha = 2$, the loss of strength is hardly important.

4 Interpretation

We have now reverted to a calculation that doesn't need the LIT, since its only remaining role is to introduce a smoothing scale to a discrete approximation of the operation

$$\mathcal{H} \left|\phi^{(n)}\right\rangle = \lambda^{(n)} \left|\phi^{(n)}\right\rangle \,, \tag{12}$$

$$S(E) = \sum_n \delta_{\sigma_I}(E - \lambda^{(n)}) \left|\langle \phi^n | \psi \rangle\right|^2 \,, \tag{13}$$

where σ_I provides the smoothing of the δ function. It may be of interest to (for instance) complex scale the Hamiltonian. It seems likely that we can write something like (needs a detailed derivation)

$$\mathcal{H} \left|\phi^{(n)}\right\rangle = (\lambda_R^{(n)} - i\lambda_I^{(n)}) \left|\phi^{(n)}\right\rangle \,, \tag{14}$$

$$S(E) = \sum_n \frac{\pi}{\lambda_I^{N)}} \frac{1}{(\lambda_R^{(n)} - E)^2 + \lambda_I^{(n)2}} \left|\langle \phi^n | \psi \rangle\right|^2 \,, \tag{15}$$

where for non-resonant states $\lambda_I \approx \tan 3\theta/2\, \lambda_R$, so that the result is automatically smooth, apart from near the threshold. I see a lot of benefits to such a form over what the LIT provides.