Last time:

- accelerated translational operators.
  - paint and shade
  - rotate
  - translate
  - rotate back

- express diagonal plane wave representation.

\[
\frac{1}{\| \mathbf{x} - \mathbf{x}' \|} = \sum_{j,k}^\infty w_{jk} e^{i \mathbf{\chi} \cdot \mathbf{x}'}
\]

"Translating" means re-centering about a box. \( \rightarrow \) only need to scale \( w_{jk} \) by exponentials.

Point to exponentials is not the common operator.

MP to exponentials is:

Recall:

\[
\frac{\gamma_m(\theta, \phi)}{\gamma_{m+1}} = A_m \left( \frac{d}{dx} + \frac{i \phi}{2} \right)^m \left( \frac{d}{d\gamma} \right)^{\ell-m} \frac{1}{\mathbf{x} \cdot \mathbf{\chi}}
\]
Usually we will not map from points to exponentials, but from multiple expansion to exponentials:

Recall: since

\[ Y_l^m(\theta, \phi) = A_{lm}(\frac{d}{dx} + i\frac{d}{dy})^m (\frac{d}{dz})^{l-m} \frac{1}{r^{l+1}} \]

for \( m \geq 0 \)

we have that in terms of plane waves: (for \( \rho > 0 \))

\[ Y_l^m(\theta, \phi) = A_{lm} \left( \sum (-i)^{l-m} \frac{(-i)^{l-m}}{2\pi} \int_0^\infty \int_0^{2\pi} e^{i\lambda(x\cos \alpha + y\sin \alpha)} \, dx \, d\lambda \right) \]

\[ = A_{lm} \frac{1}{2\pi} \int_0^{\infty} \left( -i \right)^{l-m} \lambda^{-l} e^{i\lambda} \int_0^{2\pi} e^{i\lambda \left( \cos \alpha \pm i \sin \alpha \right)} \, d\lambda \]

\[ = A_{lm} \frac{1}{2\pi} (-i)^{l-m} \int_0^{\infty} \lambda^{-l} \left( i \lambda \right)^m e^{i\lambda (x\cos \alpha + y\sin \alpha)} \, d\lambda \]

So if \( \phi(x) = \sum \sum M_{lm}^* C_{lm}(\theta, \phi) \), then

\[ \phi(x) = \sum_{m=-l}^{l} \sum_{l=0}^{\infty} V_{l,k} e^{-\lambda_k x} e^{i\lambda_k (x\cos \alpha_j + y\sin \alpha_j)} \]

with

\[ V_{l,k} = W_{l,k} \sum_{m=-l}^{l} \left( \sum (-i)^{l-m} \frac{(-i)^{l-m}}{2\pi} \int_0^\infty \int_0^{2\pi} e^{i\lambda \left( \cos \alpha_j \pm i \sin \alpha_j \right)} \, d\lambda \right) \]

\[ \Rightarrow O(p^2) \text{ compute numerically...} \]
For a $p$th order expansion, interchange the sums sinu

$$\sum_{l=0}^{p} \sum_{m=-l}^{l} \sum_{l'=1}^{l} \sum_{l''=1}^{l}$$

we have:

$$V_{jk} = \sum_{m=-p}^{p} \frac{(-1)^m}{2\pi i} \sum_{l=1}^{l} \sum_{l'=1}^{l} \sum_{l''=1}^{l} x_j^m$$

$$\exp(2\pi i\alpha)$$

$$\exp(2\pi i\beta)$$

$$\Rightarrow 0(p^3)$$

For each $m$, 2$p+1$ of them, do a sum with $\leq p$ terms.

$$\Rightarrow 0(p^3)$$

do a sum with $2p+1$ terms of $x_j$ for each $x_j$.

For each $x_j$, $0(p^2)$.

and likewise, the $\exp(2\pi i\alpha)$ operator is given by a similar expression.

so we can factorize $T_{M2L}$ as

$$T_{M2L} = \text{C}_{x2L} \text{D}_{o2L} \text{C}_{M2L}.$$
Quadrature and discretization

We need to accurately evaluate the integral

$$\int_0^\infty e^{-\lambda(z-z')} \int_0^{2\pi} e^{i\lambda((x-x')\cos \alpha + (y-y')\sin \alpha)} \, d\alpha \, dz$$

For translation up in $z$ dimension:

We know for a unit box: that

for some $x'$ and target $x$

$z - z' \in (-1, 1)$

$|x-x'| \in (-1, 1)$

$y-y' \in (-1, 1)$

We want the most efficient and accurate quadrature rule for all the range of these parameters:

$x$ integral: trapezoidal rule

$\lambda$ integral: For each $\alpha_j$ in, design a generalized Gaussian rule.
Quadrature rules for Diagonal Forms:

For $z \in (1,4)$

$x \in (-4,4)$

$y \in (-4,4)$

\[
\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{i\alpha (x \cos \alpha + y \sin \alpha)} \, d\alpha \, d\beta
\]

periodic, trapezoid, $|h| \leq \frac{\pi}{4}$

For $z = 1$, $\alpha = 30 \rightarrow |I| = 10^{-13}$ \text{ (Worst case)} \text{ slowest decay.}

$z = 4$, $\alpha = \phi \rightarrow |I| = 10^{-15}$

Goal: \text{ Find } \phi \text{ for } \text{ all } n \text{ and find } \frac{N}{\delta} \text{ number of nodes and}

\text{ to integrate } e^{i\phi (\cos \phi + \sin \phi)}.

Example: \text{ Discretize on } x \in (0,30)

\text{ and } x \in (0,2\pi)

\text{ Up to } x = 10.
In summary:

Use multiple expansion for L2L, M2M,
Expansional expansion for M2L

Moves on The Helmholtz equation.

\[(\Delta + k^2) \ u = 0\]

The important take-home message: For "k x size of domain" small,
the physics of the problem is very close to
the Laplace case. For "k x size" large,
it is very different.

Separation of variables solution:

\[u = \rho(r) \phi(\theta) \tilde{\phi}(\phi)\]

\[\Rightarrow u = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[ a_{lm} j_l(kr) + b_{lm} h_l(kr) \right] Y_l^m(\theta, \phi)\]

spherical Bessel functions.
These functions satisfy the radial ODE:

\[ \left( r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} + \left( r^2 - n(n + 1) \right) \right) \phi_n(r) = 0 \]

\[ \phi_n(r) = \sqrt{\frac{\pi}{2n+1}} J_n \left( \frac{1}{2} \right) \]

\[ h_0(r) = \frac{e^{i\phi}}{i\phi} = \text{Green's Function for the Helmholtz equation} \]

\[ (\Delta + k^2) h_0(kr)e^{i\phi} = \delta(r) \quad g_0(r) = \frac{e^{ikr}}{4\pi r} \]

**Multipole Expansions** \(\Rightarrow\) **Partial Wave Expansions**:

\[ \sum_{l,m} \frac{M_{lm}}{r^{l+1}} Y^m_l(\theta, \phi) \Rightarrow \sum_{l,m} a_{lm} Y^m_l(\theta, \phi) \]

**Local Expansions** \(\Rightarrow\)

\[ \sum_{l,m} \beta_{lm} Y^m_l(\theta, \phi) \]

**Main Addition Theorem**:

\[ g_{lm}(r) = \frac{e^{ikr}}{4\pi r} = \frac{e^{i k \|x-x'||}}{4\pi \|x-x'||} \quad \text{for } r > r' \]

\[ = \sum_{\ell=0}^{\infty} \sum_{m=\ell-\ell}^{\ell} (-1)^\ell \hat{a}_\ell(kr) \hat{a}_{m,\ell}(kr) Y^\ell_m(\theta, \phi) Y^\ell_m(\theta, \phi) \]

(Up to signs,)

\[ \text{and } \pm i \phi \]
Diagonal Plane-Wave Representation

Similar to Laplace \( \frac{1}{r} \):

\[
\frac{e^{ikr}}{r} = \frac{1}{2\pi} \int_{0}^{\infty} e^{-\frac{\sqrt{x^2 - k^2}}{2}} \int_{0}^{2\pi} e^{i\lambda(x\cos\alpha + y\sin\alpha)} \lambda \, d\alpha \, dx
\]

Cannot discretize directly along \( \lambda = 0 \Rightarrow 30 \ldots \)

The integrand in (x) has two qualitatively different behaviors: \( \lambda < k \), \( \lambda > k \). (assume \( \text{Im}(k) \geq 0 \)).

If \( \lambda < k \), then \( \sqrt{x^2 - k^2} = i \Re \ldots \Rightarrow \text{"Propagating"} \)

If \( \lambda > k \), then \( k\sqrt{x^2 - k^2} > 0 \Rightarrow \text{"Evanescent"} \)

Possible Options: Contour deformation / change of variable.

Assume Singularity at \( \lambda = k \).

The physically meaningful side, \( \text{Im}(k) \leq 0 \), has to correspond to decreasing waves.

The original wave equation:

\[
\frac{e^{ikr}}{r} = e^{i\frac{\pi}{2}} e^{-\frac{k}{r}} \to 0 \text{ as } r \to \infty.
\]
So any contour must not cross \( k \):

\[ y^2 - k^2 = -k^2 \cos^2 \theta \]

\[ y = k \cos \theta \]

\[ x = k \sin \theta \]

\[ x^2 = y^2 + k^2 \]

Ex: Deform to: \( \int_0^\infty \rightarrow \int_0^{\pi/2} \)

\[ \int_0^\infty \rightarrow \int_0^{\pi/2} \]

\[ \rightarrow \int_0^{\pi/2} e^{-ik \cos \theta} \int_0^{\pi/2} \frac{1}{x \sin \theta} \sin \theta d\theta \]

\[ + \int_0^\infty e^{-i\pi \alpha} J_0 \left( \sqrt{x^2 + k^2} \right) d\alpha \]

Similar to Laplace quadratures.

For \( \theta \): Gauss-Legendre

\( \alpha \): Trapezoidal

Infinitely many contour deformation exists.

Quadratic scaling is more sensitive to bar size, size of \( k \), etc.
To recap where the diagonal forms enter:

\[ 199p^2 \] (symmetry can reduce this to \( 40p^2 \))

This box can wait to receive all the translates, then perform \( \frac{1}{X2L} \) (which is \( \frac{1}{L_3} \) (or \( \frac{1}{p^3} \))

Maxwell

\[ \nabla \times \mathbf{E} = \frac{\varepsilon_0}{\mu_0} \frac{\partial \mathbf{H}}{\partial t} \]
\[ \nabla \cdot \mathbf{E} = 0 \]
\[ \nabla \times \mathbf{H} = -\frac{\varepsilon_0}{\mu_0} \frac{\partial \mathbf{E}}{\partial t} \]
\[ \nabla \cdot \mathbf{H} = 0 \]

\[ \Rightarrow \mathbf{H} = \nabla \times \mathbf{S} \]
\[ \mathbf{E} = \varepsilon_0 \mathbf{S} \]
\[ \int_{S'} \mathbf{E} \cdot d\mathbf{s} = \Phi \]

Vector wave equation.

This has or gave the Green's Function:

\[ G_k = (I + \frac{i}{k} \nabla \nabla) \frac{e^{ikr}}{4\pi r} \]

In either case, an integral with the Green's function is merely some sort of derivative of \( e^{ikr} \).