Review Topics & Formulas for Unit 4

Dirac-delta representation of differential operators

$$\int_{y=a}^{y=b} dy \langle x|h(x)\mathbf{1}|y\rangle \psi(y) = \int_{y=a}^{y=b} dy\, h(x)\delta(y,x)\psi(y) = h(x)\psi(x) \qquad (11.2.14a)$$

$$\int_{y=a}^{y=b} dy \langle x|g(x)\mathbf{D}|y\rangle \psi(y) = \int_{y=a}^{y=b} dy\, g(x)\frac{d\delta(y,x)}{dy}\psi(y) = g(x)\frac{d\psi(x)}{dx} \qquad (11.2.14b)$$

$$\int_{y=a}^{y=b} dy \langle x|f(x)\mathbf{D}^2|y\rangle \psi(y) = \int_{y=a}^{y=b} dy\, f(x)\frac{d^2\delta(y,x)}{dy^2}\psi(y) = f(x)\frac{d^2\psi(x)}{dx^2} \qquad (11.2.14c)$$

Adjoint operator
$$\langle x|\mathbf{L}^\dagger|y\rangle = f^*(y)\frac{d^2\delta(x,y)}{dx^2} + g^*(y)\frac{d\delta(x,y)}{dx} + h^*(y)\delta(x,y) \qquad (11.2.18)$$

$$L^\dagger \cdot \psi(x) = \frac{d^2\left(f^*(x)\psi(x)\right)}{dx^2} - \frac{d\left(g^*(x)\psi(x)\right)}{dx} + h^*(x)\psi(x) \qquad (11.2.20a)$$

Fourier transform of $\psi(x)$ $\langle k|\psi\rangle = \int_{-\infty}^{+\infty} dx \langle k|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{+\infty} dx \frac{e^{-ikx}}{\sqrt{2\pi}}\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dx\, e^{-ikx}\,\psi(x)$

Momentum p-op. in x-basis $\langle x|\mathbf{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)$ Coordinate x-op. in k-basis $\langle k|\mathbf{x}|\psi\rangle = i\frac{\partial}{\partial k}\psi(k)$

Schrodinger's time-dependent $\Psi(x,t) = \langle x|\Psi(t)\rangle$ *wave equation*.

$$i\hbar\langle x|\frac{\partial}{\partial t}|\Psi\rangle = \langle x|\frac{\mathbf{p}^2}{2M} + V(\mathbf{x})|\Psi\rangle, \quad \text{or:} \quad i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2M}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \qquad (11.4.5c)$$

Schrodinger's time-independent $\psi_\varepsilon(x) = \langle x|\varepsilon\rangle$ *wave eigenequation*.

$$\langle x|\mathbf{H}|\varepsilon\rangle = \varepsilon\langle x|\varepsilon\rangle, \quad \text{or:} \quad \frac{-\hbar^2}{2M}\frac{\partial^2\psi_\varepsilon(x)}{\partial x^2} + V(x)\psi_\varepsilon(x) = \varepsilon\psi_\varepsilon(x) \qquad (11.4.5d)$$

Bilateral B-type hyper-Schrodinger equations have even derivatives.

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = d_0\Psi(x,t) + d_2\frac{\partial^2\Psi(x,t)}{\partial x^2} + d_4\frac{\partial^4\Psi(x,t)}{\partial x^4} + d_6\frac{\partial^6\Psi(x,t)}{\partial x^6} + \cdots \qquad (11.5.10c)$$

Circulating or *Complex C*-type hyper-Schrodinger equations. (The *odd-k* d_k are imaginary.)

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = d_0\Psi(x,t) + d_1\frac{\partial\Psi(x,t)}{\partial x} + d_2\frac{\partial^2\Psi(x,t)}{\partial x^2} + d_3\frac{\partial^3\Psi(x,t)}{\partial x^3} + d_4\frac{\partial^4\Psi(x,t)}{\partial x^4} + \cdots \qquad (11.5.13)$$

Asymmetric or *A*-type Schrodinger equations have *q*-dependent connectivity terms $d_{k,l,..}(q_m)$.

$$i\hbar\frac{\partial\Psi(q_m,t)}{\partial t} = \sum_{k,l} d_{k,l,\cdots}(q_m)\frac{\partial^{k+l..}\Psi(q_m,t)}{\partial q_1^k\partial q_2^l\cdots} \qquad (11.5.15)$$

Infinite square well eigensolutions $\langle x|\varepsilon_n\rangle = \psi_n(x) = A\sin(k_n x) = A\sin\left(\frac{n\pi x}{W}\right) \quad (n=1,2,3,...\infty) \qquad (12.1.1c)$

$$\varepsilon_n = \frac{\hbar^2}{2M}k^2 = \frac{\hbar^2 n^2\pi^2}{2MW^2} = \left(1^2, 2^2, 3^2, ...\text{or } n^2\right)\frac{h^2}{8MW^2} \qquad (12.1.1d)$$

Dipole expectation $\langle x\rangle_\Psi = \langle\Psi|\mathbf{x}|\Psi\rangle = \Sigma_{m=1}^\infty\ \Sigma_{n=1}^\infty\ \langle\Psi|\varepsilon_m\rangle\langle\varepsilon_m|\mathbf{x}|\varepsilon_n\rangle\langle\varepsilon_n|\Psi\rangle \qquad (12.1.11)$

$$\langle\Psi|\mathbf{x}|\Psi\rangle = \left(|\alpha|^2+|\beta|^2\right)\frac{W}{2} + \langle\varepsilon_1|\mathbf{x}|\varepsilon_2\rangle\left(\alpha^*\beta+\beta^*\alpha\right)$$
$$= \frac{W}{2} + \frac{8W\cdot 1\cdot 2}{\pi^2\left(1^2-2^2\right)^2}\, 2|\alpha(0)\beta(0)|\cos\left(\omega_1-\omega_2\right)t \xrightarrow[\alpha=\beta]{} \frac{W}{2} + 0.18W\ \cos\left(\omega_1-\omega_2\right)t \qquad (12.1.15b)$$

Delta function: $\delta(x-a)=\langle x|a\rangle=\Sigma_{n=1}^{\infty}\langle x|\varepsilon_n\rangle\langle\varepsilon_n|a\rangle=\Sigma_{n=1}^{\infty}a_n\sin k_n x$, $a_n = (2/W)\sin k_n a$ (12.2.1a)

Approximate delta: $\Psi(x)\cong\frac{2}{\pi}\int_0^{K_{\max}}dk\sin ka\sin kx\cong\frac{\sin K_{\max}(x\text{-}a)}{\pi(x\text{-}a)}$ for: $x\approx a$ (12.2.3)

Heisenberg uncertainty relation $\Delta x\cdot|K_{\max}| = \Delta x\cdot\Delta k = \pi$ or: $\Delta x\cdot\Delta p = \pi\hbar = h/2$ (12.2.5)

Schrodinger's integral eigen-equation. $\frac{\hbar^2}{2M}k^2\langle k|\varepsilon\rangle+\int dk' V(k-k')\langle k'|\varepsilon\rangle=\varepsilon\langle k|\varepsilon\rangle$ (11.4.13a)

where $V(k-k')=\langle k|V|k'\rangle=\frac{1}{2\pi}\int dx\, e^{-i(k-k')x}V(x)$ (11.4.13b)

Square potential boundary relations

$$\begin{pmatrix}\Psi\\ D\Psi\end{pmatrix}=\begin{pmatrix}e^{ikx} & e^{-ikx}\\ ike^{ikx} & -ike^{-ikx}\end{pmatrix}\begin{pmatrix}R\\ L\end{pmatrix},\qquad \begin{pmatrix}R\\ L\end{pmatrix}=\frac{i}{2k}\begin{pmatrix}-ike^{-ikx} & -e^{-ikx}\\ -ike^{ikx} & e^{ikx}\end{pmatrix}\begin{pmatrix}\Psi\\ D\Psi\end{pmatrix} \qquad (13.1.8a)$$

ELementary *crossing matrix relation* for a single boundary point (x=a).

$$\begin{pmatrix}R'\\ L'\end{pmatrix}=\begin{pmatrix}\left(1+\frac{k}{k'}\right)\frac{e^{i(k-k')a}}{2} & \left(1-\frac{k}{k'}\right)\frac{e^{-i(k+k')a}}{2}\\ \left(1-\frac{k}{k'}\right)\frac{e^{i(k+k')a}}{2} & \left(1+\frac{k}{k'}\right)\frac{e^{i(k'-k)a}}{2}\end{pmatrix}\begin{pmatrix}R\\ L\end{pmatrix} \qquad (13.1.10b)$$

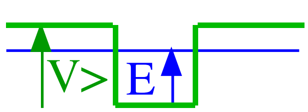
Standing wave ratio(SWR) due to single boundary $SWR=\frac{L'+R'}{L'-R'}=\frac{\frac{2k'R'}{k+k'}}{\frac{2kR'}{k+k'}}=\frac{k'}{k}=\frac{\sqrt{E}}{\sqrt{E-V}}$ (13.1.10f)

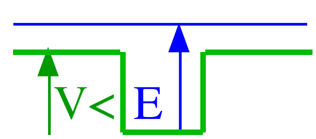
Double step boundary $L''=\frac{1}{2}e^{ika}\left[\left(1-\frac{k}{k''}\right)\cos k'a+i\left(\frac{k'}{k''}-\frac{k}{k'}\right)\sin k'a\right]R$ (13.1.25b)

$(1-{}^{k}/_{k''})=0$ or $k=k''$, with $\sin k'a=0$ (3.4.25c) $k'=\sqrt{(kk'')}$with: $\cos k'a=0$ (3.4.25d)

The Bound Case: E<V (13.2.5a) *The Free Case: E>V* (13.2.5b)

$$\frac{1}{T}=\left|\cos\sqrt{2\varepsilon}a-\frac{(2\varepsilon-\upsilon)}{2\sqrt{\varepsilon(\upsilon-\varepsilon)}}\sin\sqrt{2\varepsilon}a\right|^2, \qquad \frac{1}{T}=1+\frac{(\upsilon)^2}{4(\varepsilon-\upsilon)\varepsilon}\sin^2\sqrt{2\varepsilon}a,$$





Bound case: Sine-line square well solution

$k\,a+\delta = n\,\pi - \delta$, or: $k\,a/2 = n\,\pi/2 - \delta$ $(n = 1, 2, 3, ...)$ (13.2.9d)

$k\,a/2 = a/2\sqrt{(2V)}\sin\delta$ (13.2.9d)

C-matrix and S-matrix for single boundary and General C-to-S relations

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} \frac{\Sigma}{\Pi} e^{-i\Delta a} & \frac{\Delta}{\Pi} e^{-i\Sigma a} \\ \frac{\Delta}{\Pi} e^{i\Sigma a} & \frac{\Sigma}{\Pi} e^{i\Delta a} \end{pmatrix}, \text{ where: } \begin{array}{l} \Sigma = k_2 + k_1 \\ \Delta = k_2 - k_1 \\ \Pi = 2\sqrt{k_2 \, k_1} \end{array},$$

$$\Sigma^2 = \Delta^2 + \Pi^2$$

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} \frac{-\Delta}{\Sigma} e^{-i(\Sigma-\Delta)a} & \frac{\Pi}{\Sigma} e^{i\Delta a} \\ \frac{\Pi}{\Sigma} e^{i\Delta a} & \frac{\Delta}{\Sigma} e^{i(\Sigma+\Delta)a} \end{pmatrix} = e^{i\Delta a} \begin{pmatrix} \frac{-\Delta}{\Sigma} e^{-i\Sigma a} & \frac{\Pi}{\Sigma} \\ \frac{\Pi}{\Sigma} & \frac{\Delta}{\Sigma} e^{i\Sigma a} \end{pmatrix}$$

$$\begin{pmatrix} S_{11} = -\frac{C_{12}}{C_{11}} & S_{12} = \frac{1}{C_{11}} \\ S_{21} = \frac{1}{C_{11}} & S_{22} = \frac{C_{21}}{C_{11}} \end{pmatrix}, \quad \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}^{-1} = \begin{pmatrix} S^\dagger_{11} = -\frac{C_{21}}{C_{22}} & S^\dagger_{12} = \frac{1}{C_{22}} \\ S^\dagger_{21} = \frac{1}{C_{22}} & S^\dagger_{22} = \frac{C_{12}}{C_{22}} \end{pmatrix} = \begin{pmatrix} S^*_{11} & S^*_{21} \\ S^*_{12} & S^*_{22} \end{pmatrix} \quad (13.3.5)$$

$$\begin{pmatrix} C_{11} = \frac{1}{S_{12}} & C_{12} = \frac{-S_{11}}{S_{12}} \\ C_{21} = \frac{S_{22}}{S_{12}} & C_{22} = \frac{1}{S^*_{12}} \end{pmatrix}, \quad \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}^{-1} = \begin{pmatrix} C_{22} = \frac{1}{S^*_{12}} & -C_{12} = \frac{S_{11}}{S_{12}} \\ -C_{21} = \frac{-S_{22}}{S_{12}} & C_{11} = \frac{1}{S_{12}} \end{pmatrix} = \begin{pmatrix} \frac{1}{S^*_{21}} & -\frac{S^*_{22}}{S^*_{12}} \\ \frac{S^*_{11}}{S^*_{12}} & \frac{1}{S_{21}} \end{pmatrix}$$

Pauli-Hamilton expansion of S-Matrix (Single boundary)

$$S = ie^{i\Delta a}\left[\mathbf{1}\left(\frac{\Delta}{\Sigma}\sin\Sigma a\right) - i\left(\sigma_X \frac{\Pi}{\Sigma} - \sigma_Z \frac{\Delta}{\Sigma}\cos\Sigma a\right)\right]$$

Kinematic parameters Σ, Δ, and Π tand rotation axis polar angle ϑ and angle Θ of rotation.

$$\frac{\Delta}{\Sigma}\sin\Sigma a = \cos\frac{\Theta}{2}, \quad \frac{\Pi}{\Sigma} = \hat{\Theta}_X \sin\frac{\Theta}{2} = \sin\vartheta\sin\frac{\Theta}{2}, \quad \frac{-\Delta}{\Sigma}\cos\Sigma a = \hat{\Theta}_Z \sin\frac{\Theta}{2} = \cos\vartheta\sin\frac{\Theta}{2}. \quad (13.3.9)$$

Eigenvector:	*Eigenvalue of* $\mathbf{R}[0\vartheta\Theta]$:	*Eigenvalue of* S:
$\begin{pmatrix} \cos\vartheta/2 \\ \sin\vartheta/2 \end{pmatrix}$	$e^{-i\frac{\Theta}{2}}$	$e^{i\mu_1} = e^{i\left(\frac{-\Theta}{2}+\Delta a+\frac{\pi}{2}\right)}$
$\begin{pmatrix} \sin\vartheta/2 \\ -\cos\vartheta/2 \end{pmatrix}$	$e^{+i\frac{\Theta}{2}}$	$e^{i\mu_2} = e^{i\left(\frac{\Theta}{2}+\Delta a+\frac{\pi}{2}\right)}$

(13.3.11b)

Eigenchannel waves Ψ^ν each with an individual *eigenchannel phase shift* $\mu_\nu/2$.

$$\begin{aligned} \Psi^\nu_{(LEFT)} &= \left(e^{i\mu_\nu} I^R_{2\nu}\, e^{-ik_2x} + I^R_{2\nu}\, e^{ik_2x}\right)/\sqrt{k_2}, & \Psi^\nu_{(RIGHT)} &= \left(I^L_{1\nu}\, e^{-ik_1x} + e^{i\mu_\nu} I^L_{1\nu}\, e^{ik_1x}\right)/\sqrt{k_1} \\ &= I^R_{2\nu}\left(e^{-i(k_2x-\mu_\nu)} + e^{ik_2x}\right)/\sqrt{k_2} & &= I^L_{1\nu}\left(e^{-ik_1x} + e^{i(k_1x+\mu_\nu)}\right)/\sqrt{k_1} \\ &= I^R_{2\nu} e^{i\mu_\nu/2}\, 2\cos\left(k_2x - \mu_\nu/2\right)/\sqrt{k_2} & &= I^L_{1\nu}\, e^{i\mu_\nu/2}\, 2\cos\left(k_1x + \mu_\nu/2\right)/\sqrt{k_1} \end{aligned}$$

Eigenchannel	*Eigenchannel Amplitudes*	*Eigenchannel Phase Shifts*
$v=1$	$\begin{pmatrix} I^L_{1v}/\sqrt{k_1} \\ I^R_{2v}/\sqrt{k_2} \end{pmatrix} = \begin{pmatrix} \left(1/\sqrt{k_1}\right)\cos\vartheta/2 \\ \left(1/\sqrt{k_2}\right)\sin\vartheta/2 \end{pmatrix}$	$\mu_1 = \frac{-\Theta}{2} + \Delta a + \frac{\pi}{2}$
$v=2$	$\begin{pmatrix} I^L_{1v}/\sqrt{k_1} \\ I^R_{2v}/\sqrt{k_2} \end{pmatrix} = \begin{pmatrix} \left(1/\sqrt{k_1}\right)\sin\vartheta/2 \\ -\left(1/\sqrt{k_2}\right)\cos\vartheta/2 \end{pmatrix}$	$\mu_2 = \frac{\Theta}{2} + \Delta a + \frac{\pi}{2}$

(13.3.15c)

The angles are found using (3.4.45) with (3.4.38c).

$$\Theta = 2\cos^{-1}\left(\frac{\Delta\sin\Sigma a}{\Sigma}\right), \quad \sin\vartheta = \frac{\Pi}{\Sigma\sin\frac{\Theta}{2}}, \quad \cos\vartheta = \frac{-\Delta\cos\Sigma a}{\Sigma\sin\frac{\Theta}{2}}. \qquad (13.3.15d)$$

$$\cos\frac{\vartheta}{2} = \sqrt{\frac{1+\cos\vartheta}{2}} = \sqrt{\frac{\Sigma\sin\frac{\Theta}{2} - \Delta\cos\Sigma a}{2\Sigma\sin\frac{\Theta}{2}}}, \quad \sin\frac{\vartheta}{2} = \sqrt{\frac{1-\cos\vartheta}{2}} = \sqrt{\frac{\Sigma\sin\frac{\Theta}{2} + \Delta\cos\Sigma a}{2\Sigma\sin\frac{\Theta}{2}}} \qquad (13.3.15e)$$

The C-matrix for a square well from $x=b$ and to $x=a$ as sketched in Fig. 13.3.6(a) is as follows.

$$C = \begin{pmatrix} e^{ikL}\left[\cos\ell L - i\cosh 2\alpha\,\sin\ell L\right] & -ie^{-ik(a+b)}\sinh 2\alpha\,\sin\ell L \\ ie^{ik(a+b)}\sinh 2\alpha\,\sin\ell L & e^{-ikL}\left[\cos\ell L + i\cosh 2\alpha\,\sin\ell L\right] \end{pmatrix}$$

(13.3.33a)

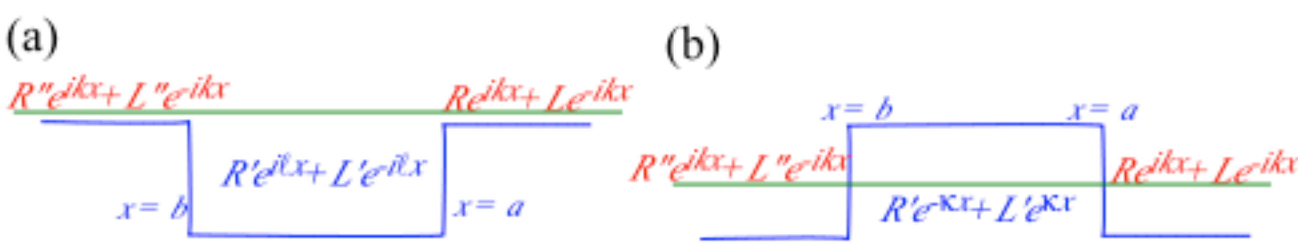
$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \ell = \sqrt{\frac{2m(E-V)}{\hbar^2}} \qquad \left(= \sqrt{\frac{2m\left(E+|V|\right)}{\hbar^2}} \; for: V<0 \right) \qquad (13.3.33)$$

A notation using hyperbolic functions

$$\cosh 2\alpha = \frac{1}{2}\left(\frac{\ell}{k}+\frac{k}{\ell}\right) = \frac{\ell^2+k^2}{2k\ell}, \quad \sinh 2\alpha = \frac{1}{2}\left(\frac{\ell}{k}-\frac{k}{\ell}\right) = \frac{\ell^2-k^2}{2k\ell}, \qquad (13.3.33c)$$

$$\cosh\alpha = \frac{k+\ell}{2\sqrt{k\ell}} = \frac{\Sigma}{\Pi}, \quad \sinh\alpha = \frac{\ell-k}{2\sqrt{k\ell}} = \frac{\Delta}{\Pi} \qquad (13.3.33d)$$

$$\cosh 4\alpha = \frac{1}{2}\left(\frac{\ell^2}{k^2}+\frac{k^2}{\ell^2}\right), \quad \sinh 4\alpha = \frac{1}{2}\left(\frac{\ell^2}{k^2}-\frac{k^2}{\ell^2}\right) \qquad (13.3.33e)$$



If E is below a square barrier V: $C=\begin{pmatrix} e^{ikL}\left[\cosh\kappa L+i\sinh 2\beta\sinh\kappa L\right] & ie^{-ik(a+b)}\cosh 2\beta\sinh\kappa L \\ -ie^{ik(a+b)}\cosh 2\beta\sinh\kappa L & e^{-ikL}\left[\cosh\kappa L-i\sinh 2\beta\sinh\kappa L\right]\end{pmatrix}$

(13.3.34a)

where: $k=\sqrt{\frac{2mE}{\hbar^2}}$, $\quad$ -i$\ell=\kappa=\sqrt{\frac{2m(V-E)}{\hbar^2}}$ $\quad\left(for: V>E>0\right)$ (13.3.34b)

Again, $L=a-b$ and a convenient notation uses hyperbolic functions.

$$\cosh 2\beta=\frac{1}{2}\left(\frac{\kappa}{k}+\frac{k}{\kappa}\right)=\frac{\kappa^2+k^2}{2k\kappa},\qquad \sinh 2\beta=\frac{1}{2}\left(\frac{\kappa}{k}-\frac{k}{\kappa}\right)=\frac{\kappa^2-k^2}{2k\kappa}\qquad(13.3.34c)$$

$$\cosh\beta=\frac{k+\kappa}{2\sqrt{k\kappa}}\equiv\frac{\sigma}{\rho},\qquad \sin\mathrm{h}\beta=\frac{\kappa-k}{2\sqrt{k\kappa}}\equiv\frac{\delta}{\rho}\qquad(13.3.34d)$$

$$\cosh 4\beta=\frac{1}{2}\left(\frac{\kappa^2}{k^2}+\frac{k^2}{\kappa^2}\right),\qquad \sinh 4\beta=\frac{1}{2}\left(\frac{\kappa^2}{k^2}-\frac{k^2}{\kappa^2}\right)\qquad(13.3.34e)$$

S-matrix: $\mathbf{S}=e^{i\mu_0}\frac{\left[\mathbf{1}\cos k\left(a+b\right)\sinh 2\alpha\sin\ell L-i\left[\sigma_X+\sigma_Z\sin k\left(a+b\right)\sinh 2\alpha\sin\ell L\right]\right]}{\sqrt{1+\sinh^2 2\alpha\sin^2\ell L}}$

$$e^{i\mu_0}=\frac{ie^{-ikL}\left[\cos\ell L+i\cosh 2\alpha\sin\ell L\right]}{\sqrt{1+\sinh^2 2\alpha\sin^2\ell L}}$$

$$\frac{\cos k\left(a+b\right)\sinh 2\alpha\sin\ell L}{\sqrt{1+\sinh^2 2\alpha\sin^2\ell L}},\qquad \frac{1}{\sqrt{1+\sinh^2 2\alpha\sin^2\ell L}},\qquad \frac{\sin k\left(a+b\right)\sinh 2\alpha\sin\ell L}{\sqrt{1+\sinh^2 2\alpha\sin^2\ell L}}$$

$$=\cos\frac{\Theta}{2},\qquad =\sin\vartheta\sin\frac{\Theta}{2},\qquad =\cos\vartheta\sin\frac{\Theta}{2}.$$