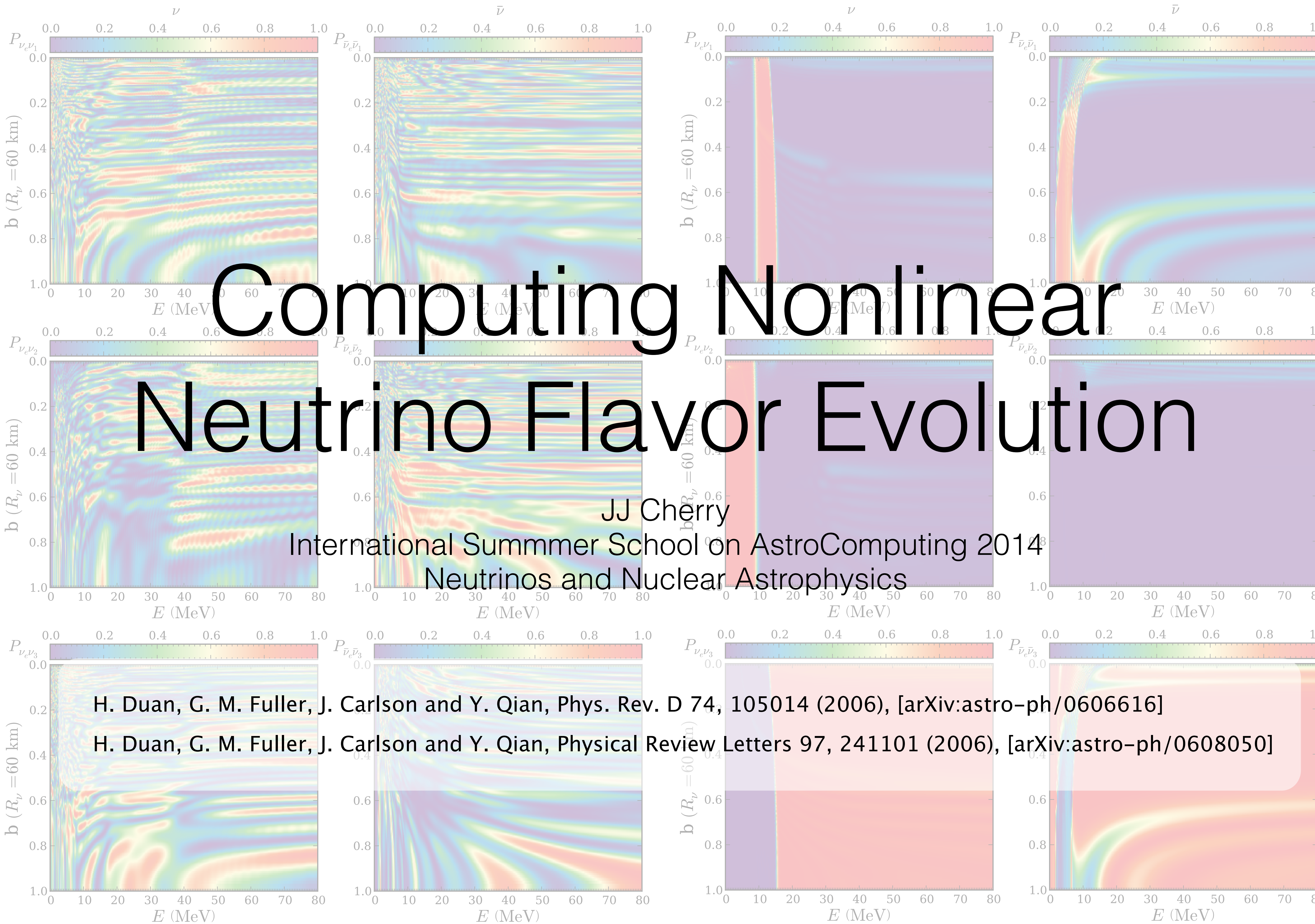


Computing Nonlinear Neutrino Flavor Evolution

JJ Cherry

International Summmer School on AstroComputing 2014
Neutrinos and Nuclear Astrophysics

H. Duan, G. M. Fuller, J. Carlson and Y. Qian, Phys. Rev. D 74, 105014 (2006), [arXiv:astro-ph/0606616]

H. Duan, G. M. Fuller, J. Carlson and Y. Qian, Physical Review Letters 97, 241101 (2006), [arXiv:astro-ph/0608050]

What do we want to learn today?

- Sooner or later, you will be working on a project and someone will point out that there is a miserably complicated problem that you need to solve *BEFORE* you get to the result you are interested in.

- “Some times a project is fun to work on because nobody knows anything about it, and then the experimentalists catch up with you and ask you what is going on.” -G.M. Fuller

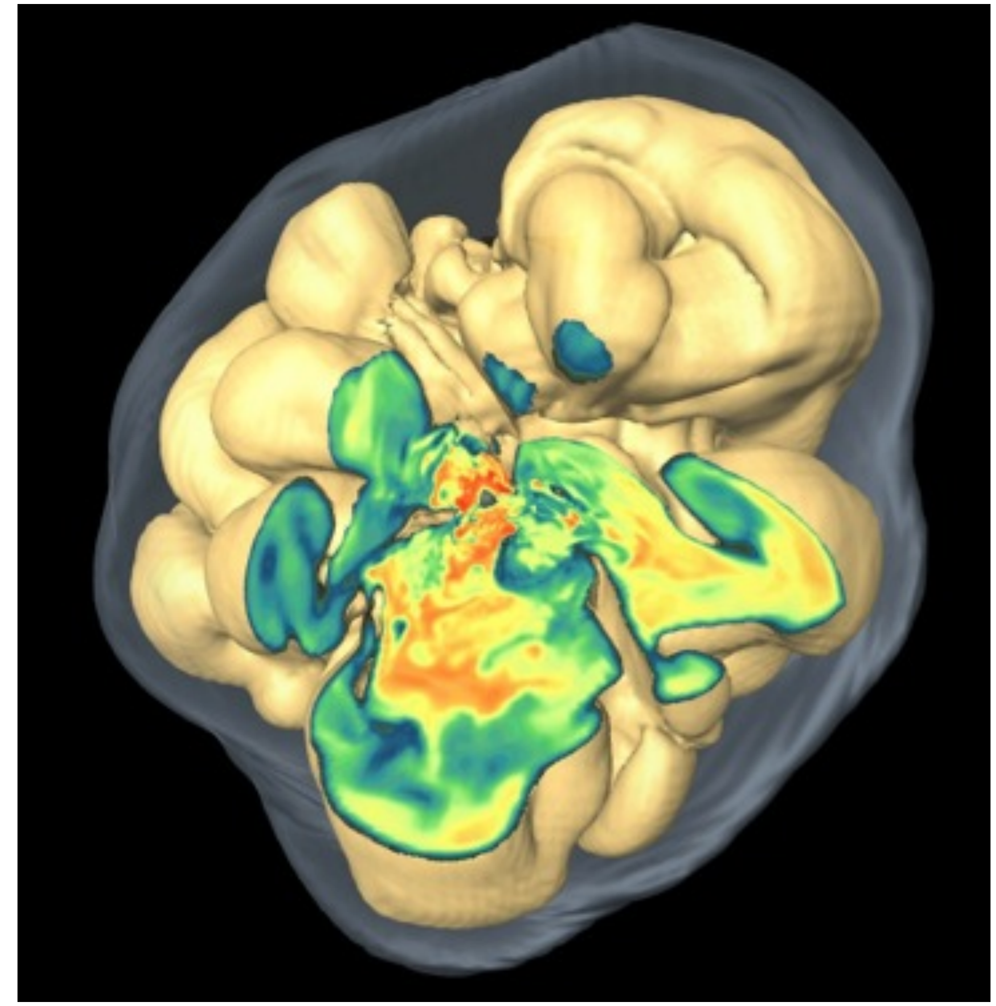
- Today, we’ll start with a very tough problem and break down the thought process of how develop a parallel computing approach to solving it.

Why we want to solve nonlinear neutrino flavor evolution

In the supernova environment, neutrino flavor states directly effect heating efficiency and nucleo-synthesis.

$$\nu_e + n \rightarrow p^+ + e^-$$

$$\bar{\nu}_e + p^+ \rightarrow n + e^+$$



F. Hanke, A. Marek, B. Müller & H. Th. Janka (arXiv:1108.4355)

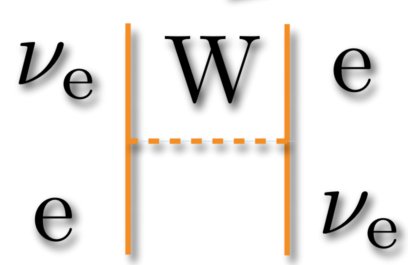
For a baryon to be ejected for the supernova, it must absorb ~10 neutrinos to gain enough energy to escape the region around the PNS.

Coherent Forward Scattering: Neutrino Flavor Evolution

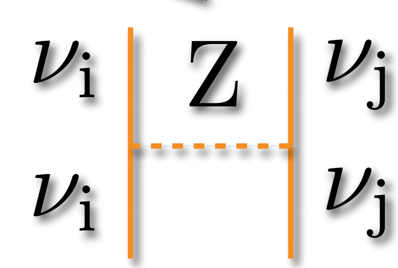
$$\psi_{\nu,\mathrm{i}} = \begin{bmatrix} \text{amplitude to be } \nu_\mathrm{e} \\ \text{amplitude to be } \nu_\mu \\ \text{amplitude to be } \nu_\tau \end{bmatrix}$$

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

neutrino-electron
charged current
forward exchange
scattering



neutrino-neutrino
neutral current
forward scattering



Neutrino Mixing: How do we associate flavor states to mass states?

$$\begin{pmatrix} |\nu_e\rangle \\ |\nu_\mu\rangle \\ |\nu_\tau\rangle \end{pmatrix} = U_m \begin{pmatrix} |\nu_1\rangle \\ |\nu_2\rangle \\ |\nu_3\rangle \end{pmatrix}$$

4 mixing parameters

$$\theta_{12},\ \theta_{23},\ \theta_{13},\ \delta$$

$$U_m = U_{23}U_{13}U_{12} =$$

$$\begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{13}s_{13}e^{i\delta} & c_{12}c_{23} - s_{12}s_{13}s_{13}e^{i\delta} & c_{13}s_{12} \\ s_{12}s_{23} - c_{12}s_{13}c_{13}e^{i\delta} & c_{12}s_{23} - s_{12}s_{13}c_{13}e^{i\delta} & c_{13}c_{23} \end{pmatrix}$$

$$\sin^2 2\theta_{23} \approx 1.0$$

$$\tan^2\theta_{12} \approx 0.42 - 0.45$$

$$\sin^2 2\theta_{13} = 0.09 \pm .021$$

F. P. An, et. al., Observation of electron-antineutrino disappearance at Daya Bay, (arXiv:

Neutrino Mass: how oscillation happens

We know the mass-squared differences:

$$\begin{cases} \Delta m_{\odot}^2 \approx 7.6 \times 10^{-5}\, \mathrm{eV}^2 \\ \Delta m_{\mathrm{atm}}^2 \approx 2.4 \times 10^{-3}\, \mathrm{eV}^2 \end{cases}$$

$$\text{e.g., } \Delta m_{12}^2 = m_2^2 - m_1^2$$

$$i\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle \rightarrow \ \hat{H} = \left(\hat{p}^2 + \hat{m}^2\right)^{(1/2)} \approx \hat{p} + \hat{m}^2/2\hat{p}$$

Neutrino Mass: how oscillation happens

We know the mass-squared differences:
$$\begin{cases} \Delta m^2_\odot \approx 7.6\times 10^{-5}\,\mathrm{eV}^2 \\ \Delta m^2_{\mathrm{atm}} \approx 2.4\times 10^{-3}\,\mathrm{eV}^2 \end{cases}$$

$$\text{e.g., } \Delta m^2_{12} = m^2_2 - m^2_1$$

$$i\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle \rightarrow \hat{H} = \left(\hat{p}^2 + \hat{m}^2\right)^{(1/2)} \approx \hat{p} + \hat{m}^2/2\hat{p}$$

$$i\frac{\partial|\Psi_\mathrm{m}\rangle}{\partial t} = \left[\left(p + \frac{m_1^2+m_2^2+m_3^2}{4p}\right)\hat{I} + \frac{1}{2p}\begin{pmatrix} -\frac{\Delta m^2_{21}+\Delta m^2_{31}}{3} & 0 & 0 \\ 0 & \frac{2\Delta m^2_{21}-\Delta m^2_{31}}{3} & 0 \\ 0 & 0 & \frac{2\Delta m^2_{31}-\Delta m^2_{21}}{3} \end{pmatrix}\right]|\Psi_\mathrm{m}\rangle$$

Neutrino Mass: how oscillation happens

We know the mass-squared differences:

$$\begin{cases} \Delta m^2_\odot \approx 7.6 \times 10^{-5}\,\mathrm{eV}^2 \\ \Delta m^2_{\mathrm{atm}} \approx 2.4 \times 10^{-3}\,\mathrm{eV}^2 \end{cases}$$

$$\text{e.g., } \Delta m^2_{12} = m^2_2 - m^2_1$$

$$i\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle \rightarrow \hat{H} = \left(\hat{p}^2 + \hat{m}^2\right)^{(1/2)} \approx \hat{p} + \hat{m}^2/2\hat{p}$$

$$i\frac{\partial|\Psi_{\mathrm{m}}\rangle}{\partial t} = \left[\left(p + \frac{m_1^2 + m_2^2 + m_3^2}{4p}\right)\hat{I} + \frac{1}{2p}\begin{pmatrix} -\frac{\Delta m^2_{21}+\Delta m^2_{31}}{3} & 0 & 0 \\ 0 & \frac{2\Delta m^2_{21}-\Delta m^2_{31}}{3} & 0 \\ 0 & 0 & \frac{2\Delta m^2_{31}-\Delta m^2_{21}}{3} \end{pmatrix}\right]|\Psi_{\mathrm{m}}\rangle$$

In the Flavor Basis:

$$H_{\mathrm{vac}} = \frac{1}{2E_\nu} \times U_m \begin{pmatrix} -\frac{\Delta m^2_{21}+\Delta m^2_{31}}{3} & 0 & 0 \\ 0 & \frac{2\Delta m^2_{21}-\Delta m^2_{31}}{3} & 0 \\ 0 & 0 & \frac{2\Delta m^2_{31}-\Delta m^2_{21}}{3} \end{pmatrix} U_m^\dagger$$

The Matter Potential

$$H_{\mathrm{mat}} = \begin{pmatrix} \sqrt{2} G_{\mathrm{F}} n_{\mathrm{e}}\left(r, \theta, \phi\right) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

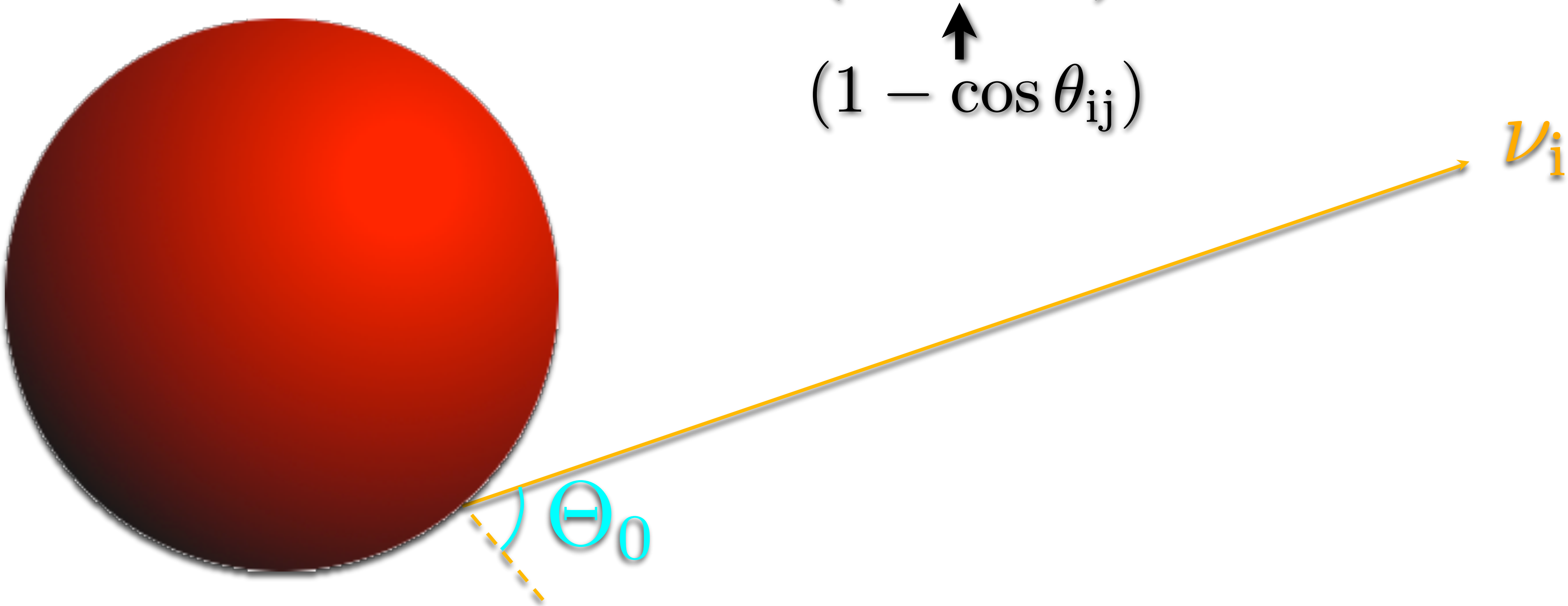
Again, only the traceless piece contributes.

$$H_e = \begin{pmatrix} -\frac{2\sqrt{2} G_{\mathrm{F}} n_{\mathrm{e}}(r,\theta,\phi)}{3} & 0 & 0 \\ 0 & \frac{\sqrt{2} G_{\mathrm{F}} n_{\mathrm{e}}(r,\theta,\phi)}{3} & 0 \\ 0 & 0 & \frac{\sqrt{2} G_{\mathrm{F}} n_{\mathrm{e}}(r,\theta,\phi)}{3} \end{pmatrix}$$

Neutrino Self-Coupling: Flavor States and Geometry

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^{\dagger}_{\nu,\mathrm{j}} \\ &- \sqrt{2} G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^{\dagger}_{\bar{\nu},\mathrm{j}} \end{aligned}$$

$$(1 - \cos\theta_{\mathrm{ij}})$$

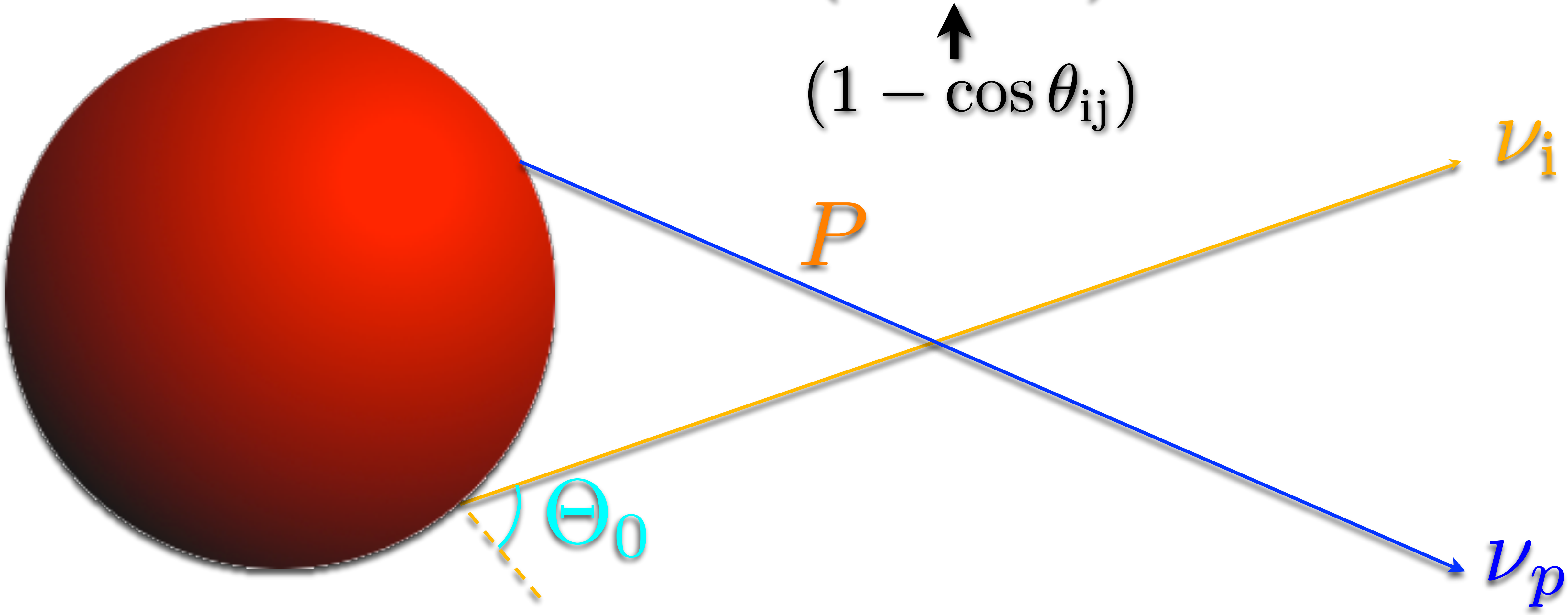


All together, we solve about $10^6 - 10^7$ non-linearly coupled differential equations at each radial step.

Neutrino Self-Coupling: Flavor States and Geometry

$$H_{\nu\nu,\mathrm{i}} = \sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^{\dagger}_{\nu,\mathrm{j}} - \sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^{\dagger}_{\bar{\nu},\mathrm{j}}$$

$(1-\cos\theta_{\mathrm{ij}})$

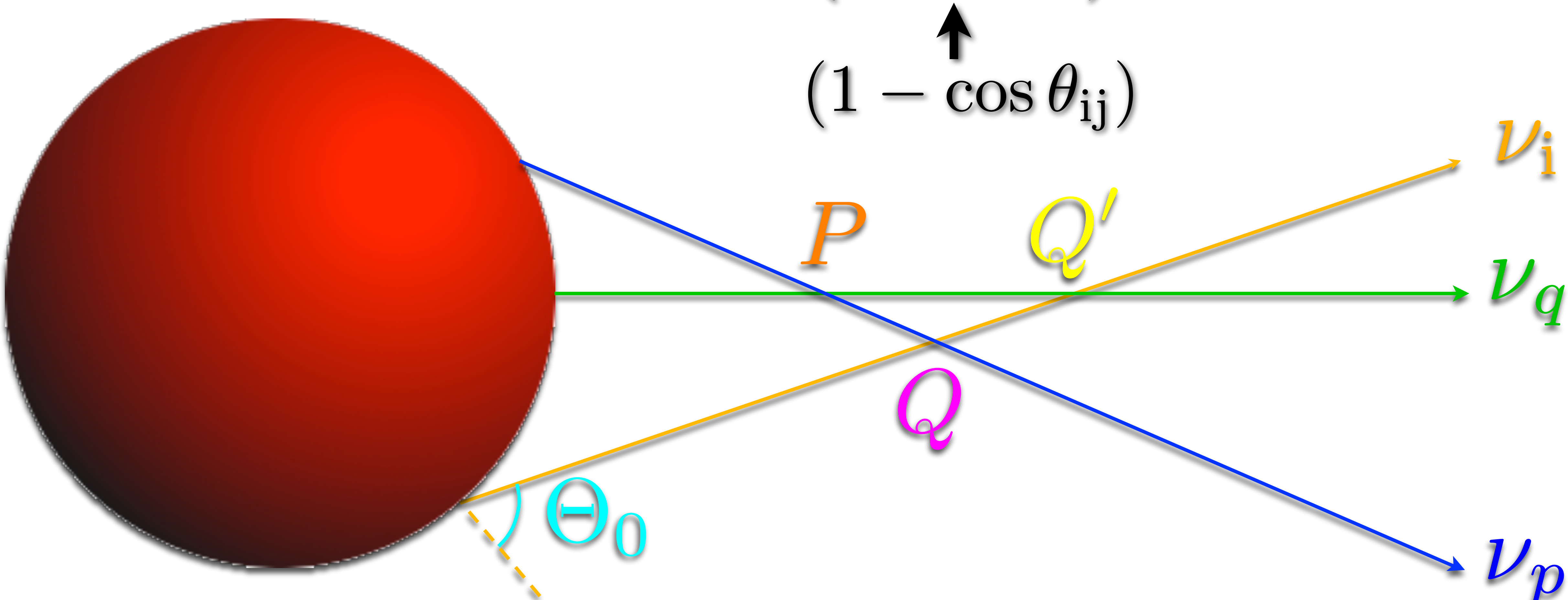


All together, we solve about $10^6 - 10^7$ non-linearly coupled differential equations at each radial step.

Neutrino Self-Coupling: Flavor States and Geometry

$$H_{\nu\nu,\mathrm{i}} = \sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^\dagger_{\nu,\mathrm{j}} - \sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^\dagger_{\bar{\nu},\mathrm{j}}$$

$$(1-\cos\theta_{\mathrm{ij}})$$



All together, we solve about $10^6 - 10^7$ non-linearly coupled differential equations at each radial step.

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

$$H_{\nu\nu,i}(r,\ \theta_i,\ \phi_i,\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\left[r,\ E_j,\ \theta_j,\ \phi_j\right])$$

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

$$H_{\nu\nu,i}(r,\ \theta_i,\ \phi_i,\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\left[r,\ E_j,\ \theta_j,\ \phi_j\right])$$

Taking Stock

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

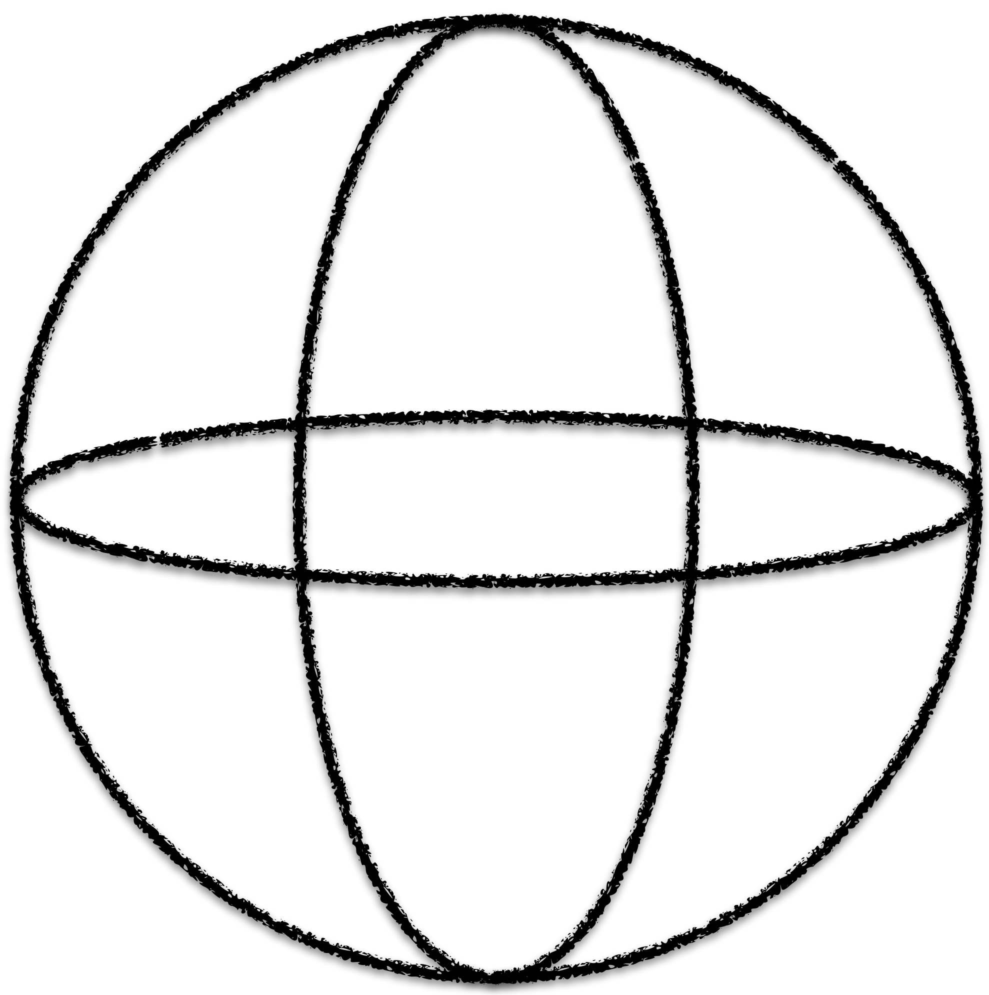
$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

$$H_{\nu\nu,i}(r,\ \theta_i,\ \phi_i,\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\left[r,\ E_j,\ \theta_j,\ \phi_j\right])$$

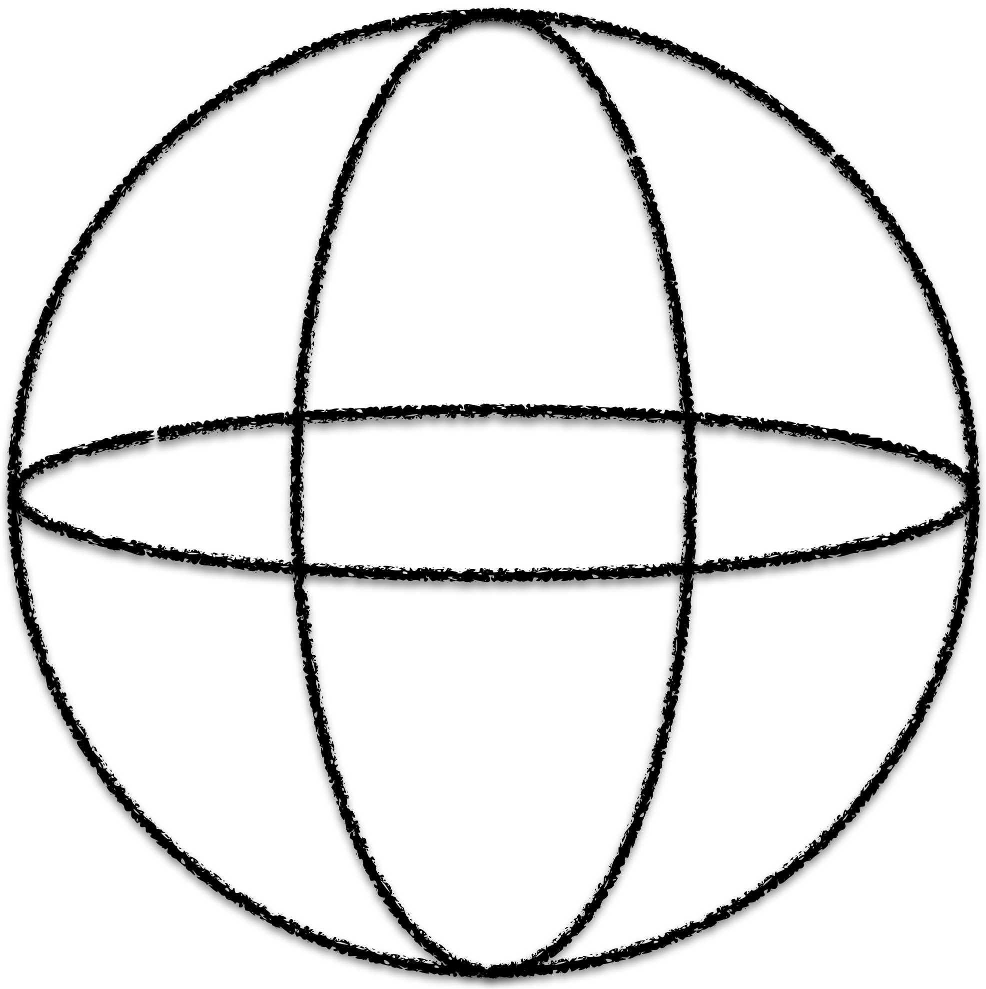
Nature only helps a bit, we still have 6 dimensions to deal with!

Spherical Symmetry is our Friend



$$H_{e,i}(n_e\,[r,\ \theta_i,\ \phi_i])$$

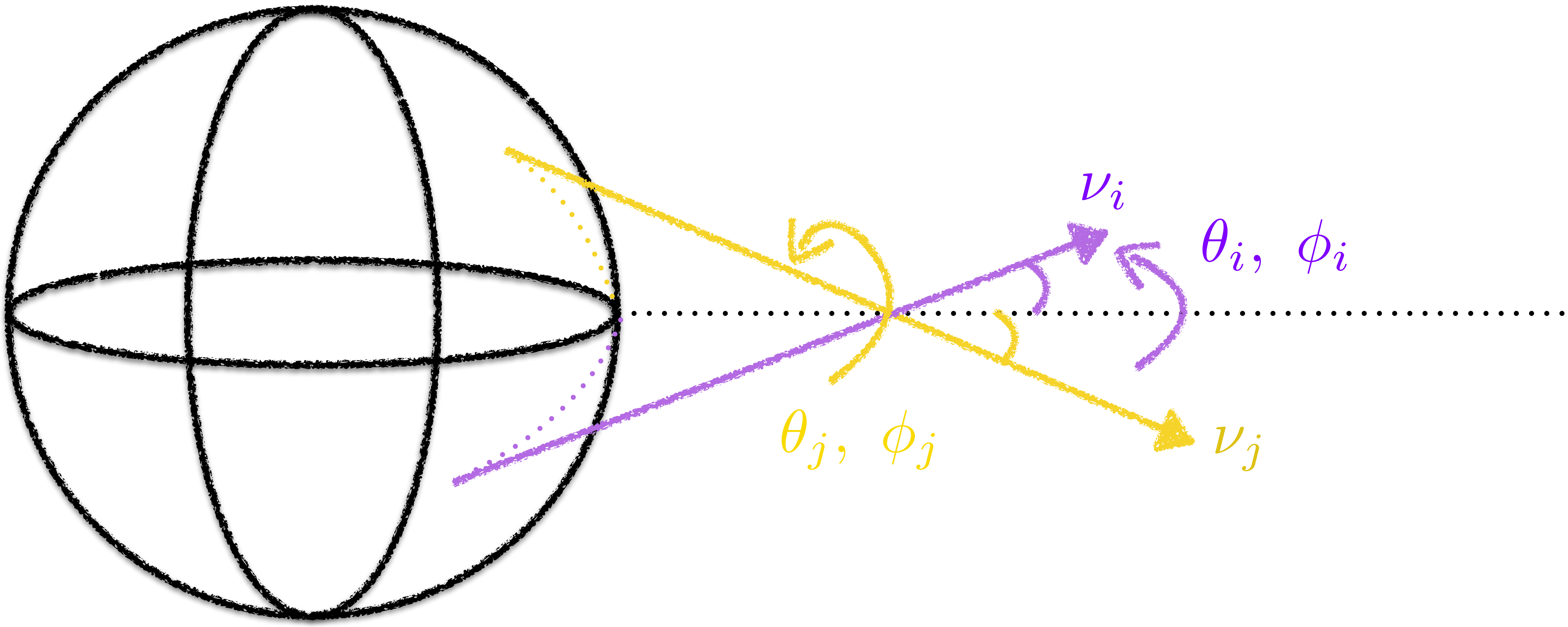
Spherical Symmetry is our Friend



$$H_{e,i}(n_e\left[r, \not{\theta_i}, \not{\phi_i}\right])$$

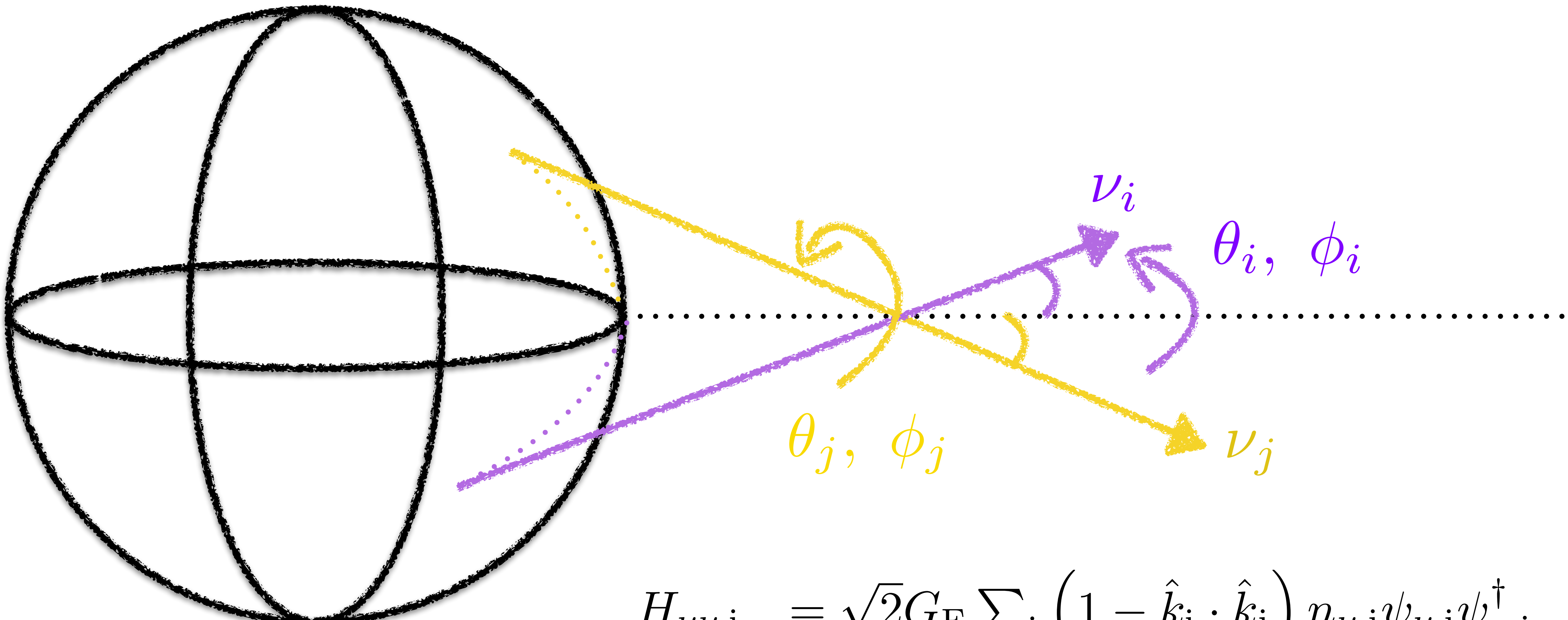
Spherical Symmetry is our Friend

$$H_{e,i}(n_e\,[r,\,\theta_i,\,\phi_i])$$



Spherical Symmetry is our Friend

$$H_{e,i}(n_e\,[r,\,\cancel{\theta_i},\,\cancel{\phi_i}])$$

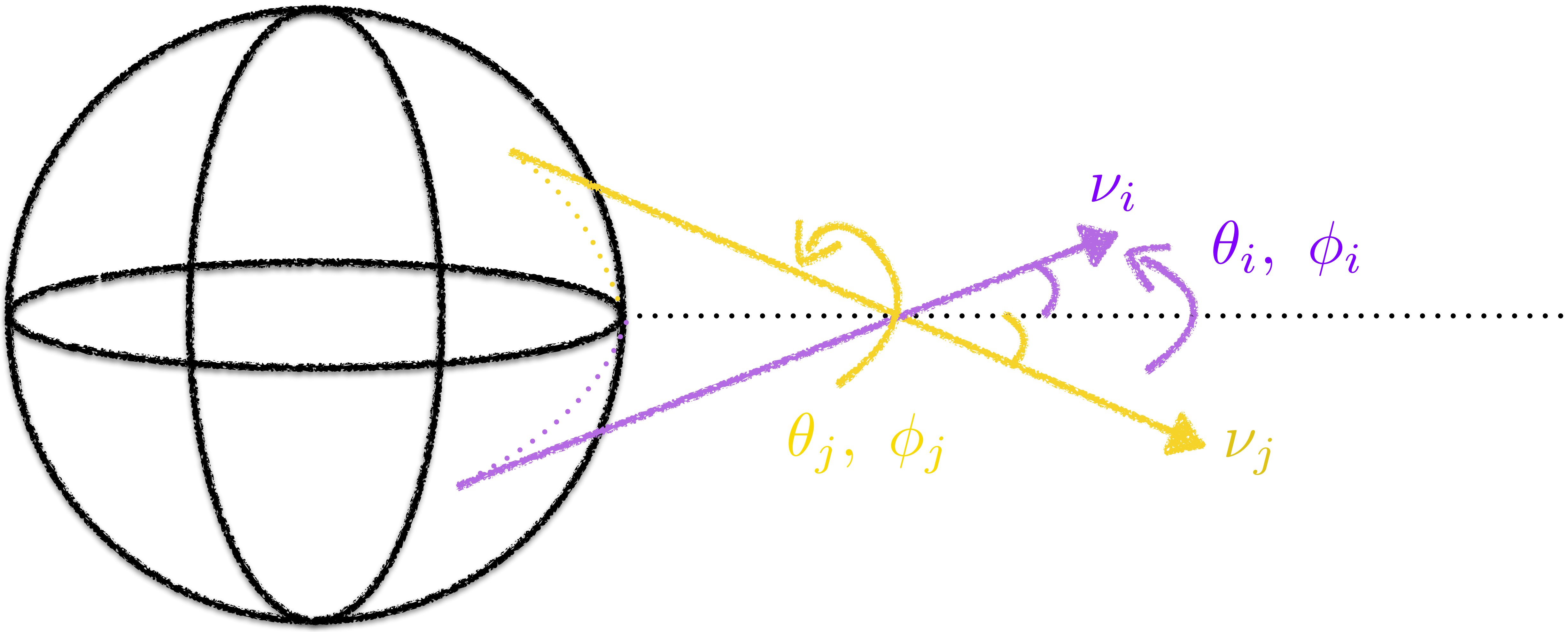


$$
\begin{aligned}
H_{\nu\nu,\mathrm{i}} \quad &= \sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^{\dagger}_{\nu,\mathrm{j}} \\
&-\sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^{\dagger}_{\bar{\nu},\mathrm{j}}
\end{aligned}
$$

$(1-\cos\theta_{\mathrm{ij}})$

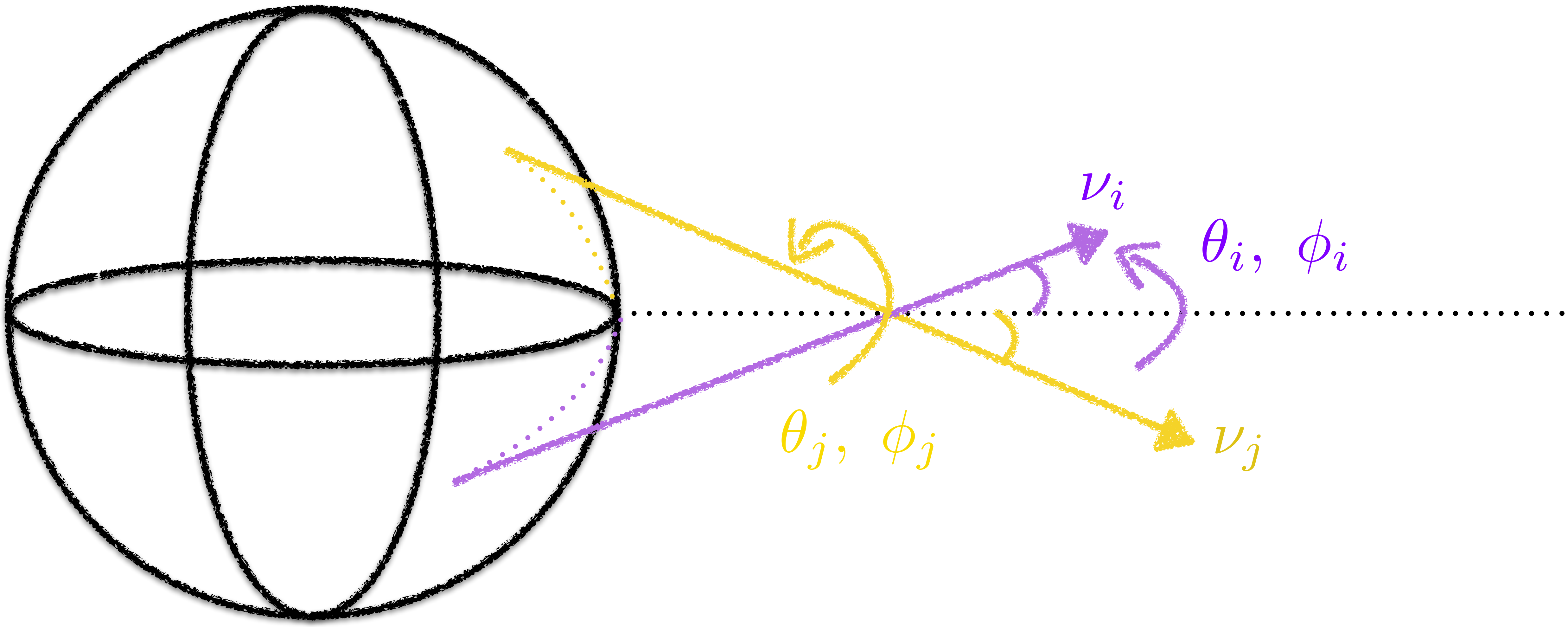
Spherical Symmetry is our Friend

$$H_{e,i}(n_e\,[r,\ \cancel{\theta_i},\ \cancel{\phi_i}])$$



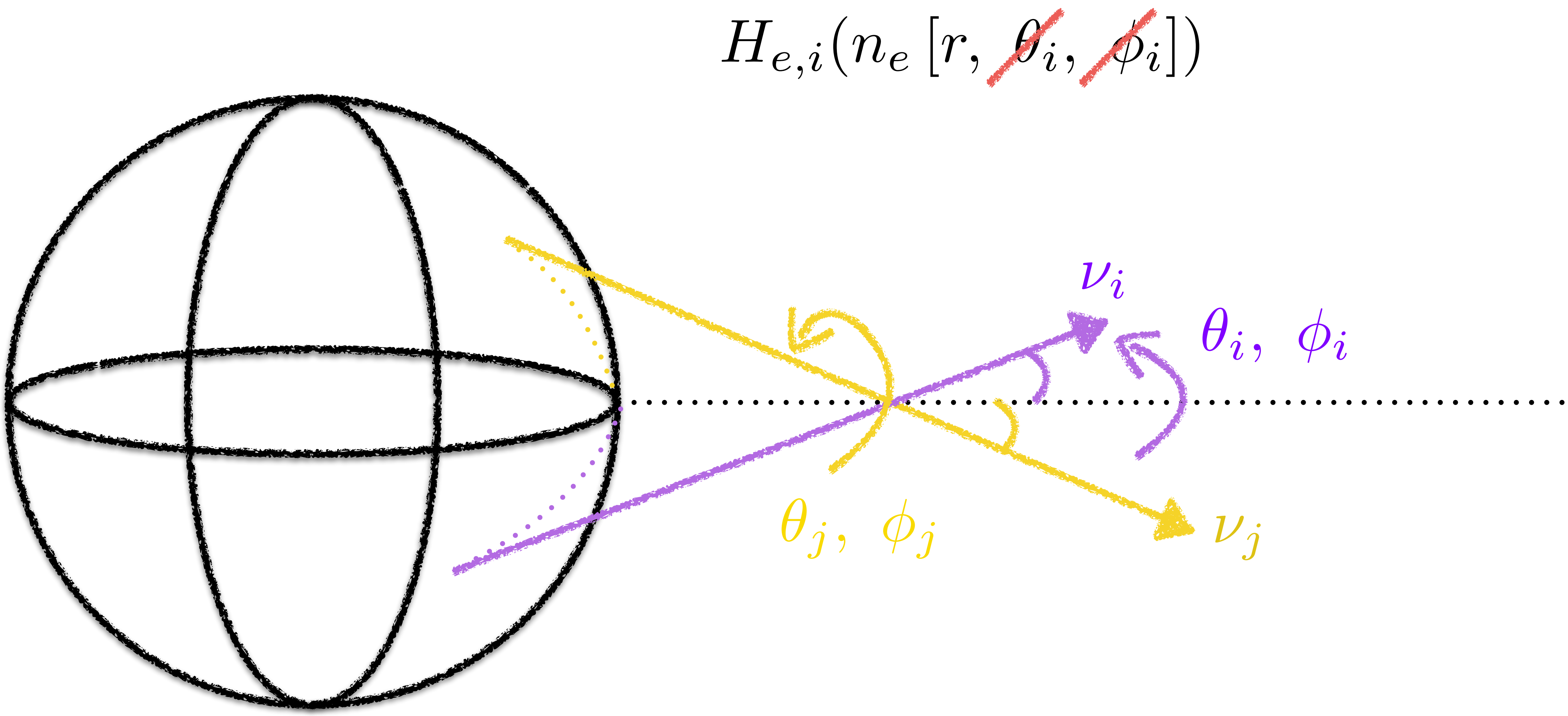
Spherical Symmetry is our Friend

$H_{e,i}(n_e\,[r,\, \cancel{\theta_i},\, \cancel{\phi_i}])$



$$\hat{k}_i \cdot \hat{k}_j = \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \left(\cos\phi_i \cos\phi_j + \sin\phi_i \sin\phi_j\right)$$

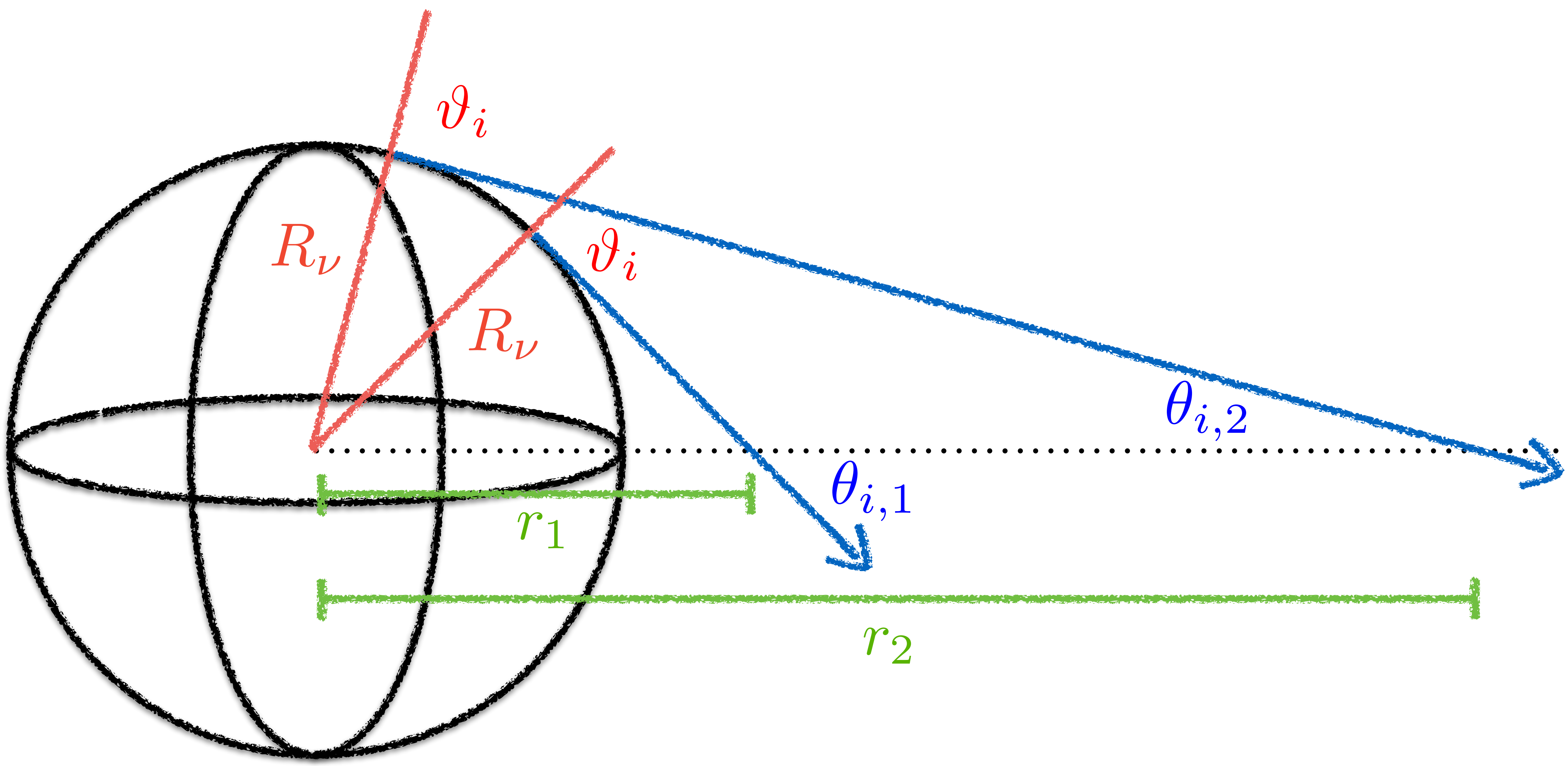
Spherical Symmetry is our Friend



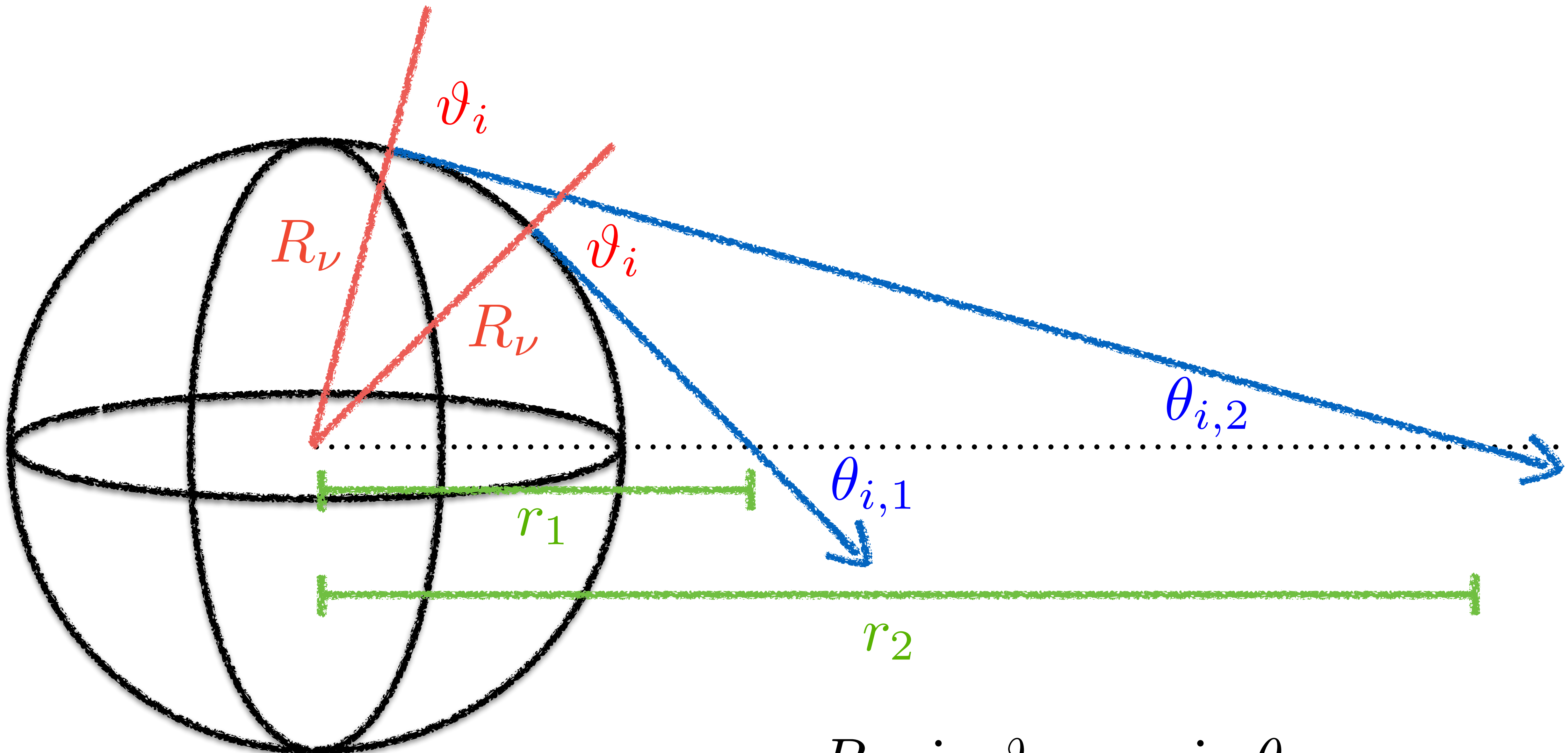
$$\hat{k}_i \cdot \hat{k}_j = \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \left(\cos\phi_i \cos\phi_j + \sin\phi_i \sin\phi_j\right)$$

$$\frac{1}{2\pi}\int_0^{2\pi} \hat{k}_i \cdot \hat{k}_j d\phi_j = \cos\theta_i \cos\theta_j$$

Basic Trigonometry is our Friend, as well

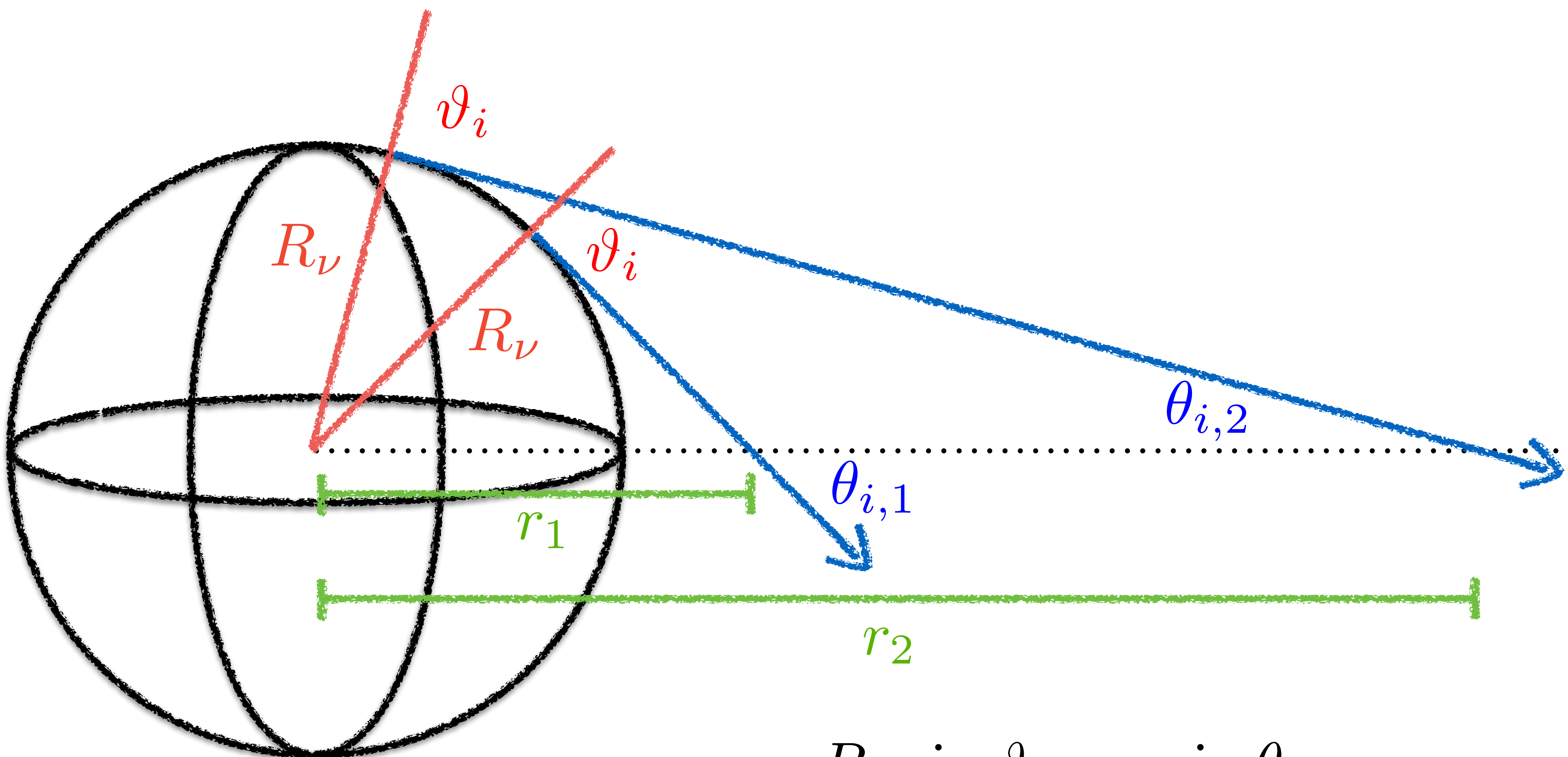


Basic Trigonometry is our Friend, as well



$$R_\nu \sin\vartheta_i = r \sin\theta_i$$

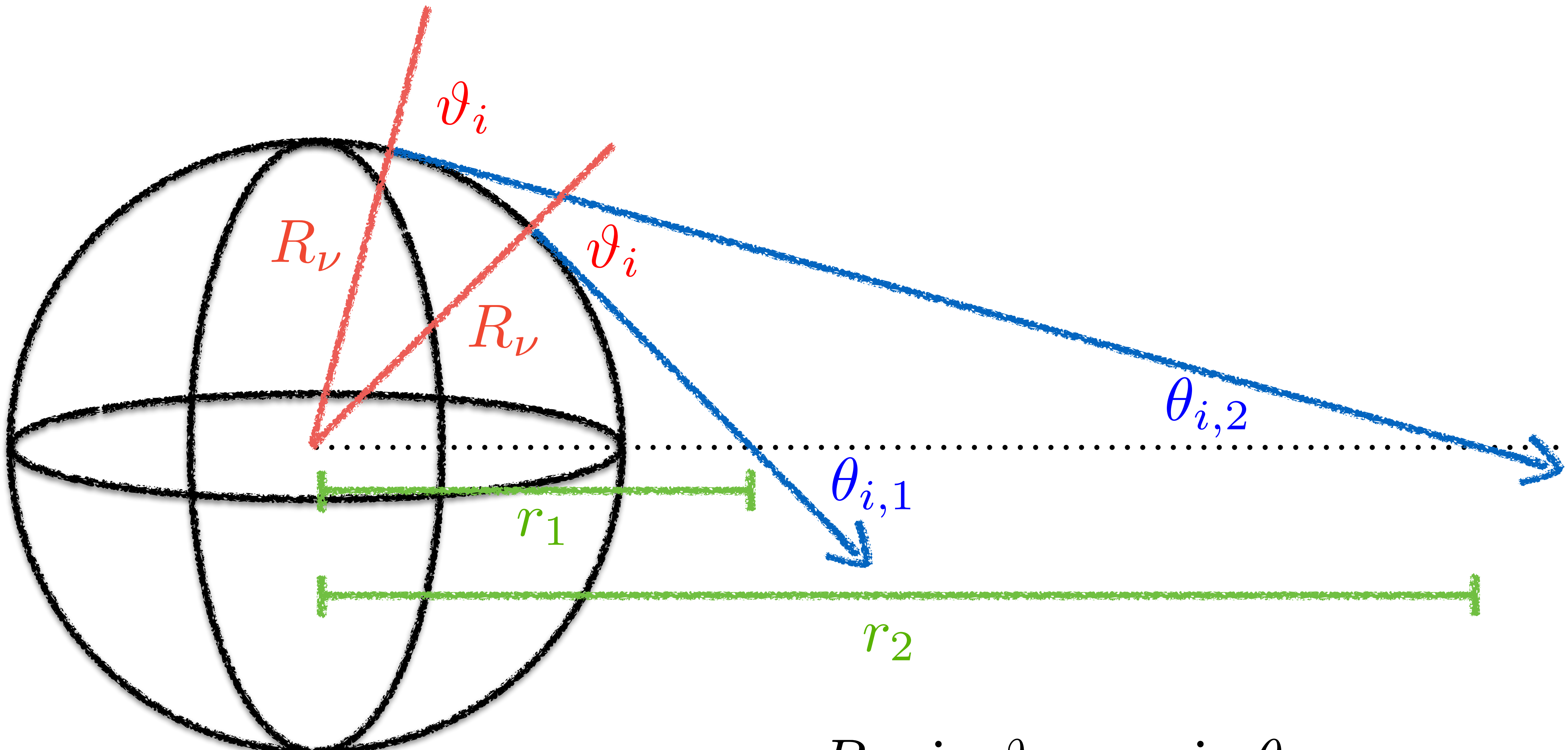
Basic Trigonometry is our Friend, as well



$$R_\nu \sin\vartheta_i = r \sin\theta_i$$

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2}G_\mathrm{F} \textstyle\sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right) n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^\dagger_{\nu,\mathrm{j}} \\ &-\sqrt{2}G_\mathrm{F} \textstyle\sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right) n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^\dagger_{\bar{\nu},\mathrm{j}} \end{aligned}$$

Basic Trigonometry is our Friend, as well

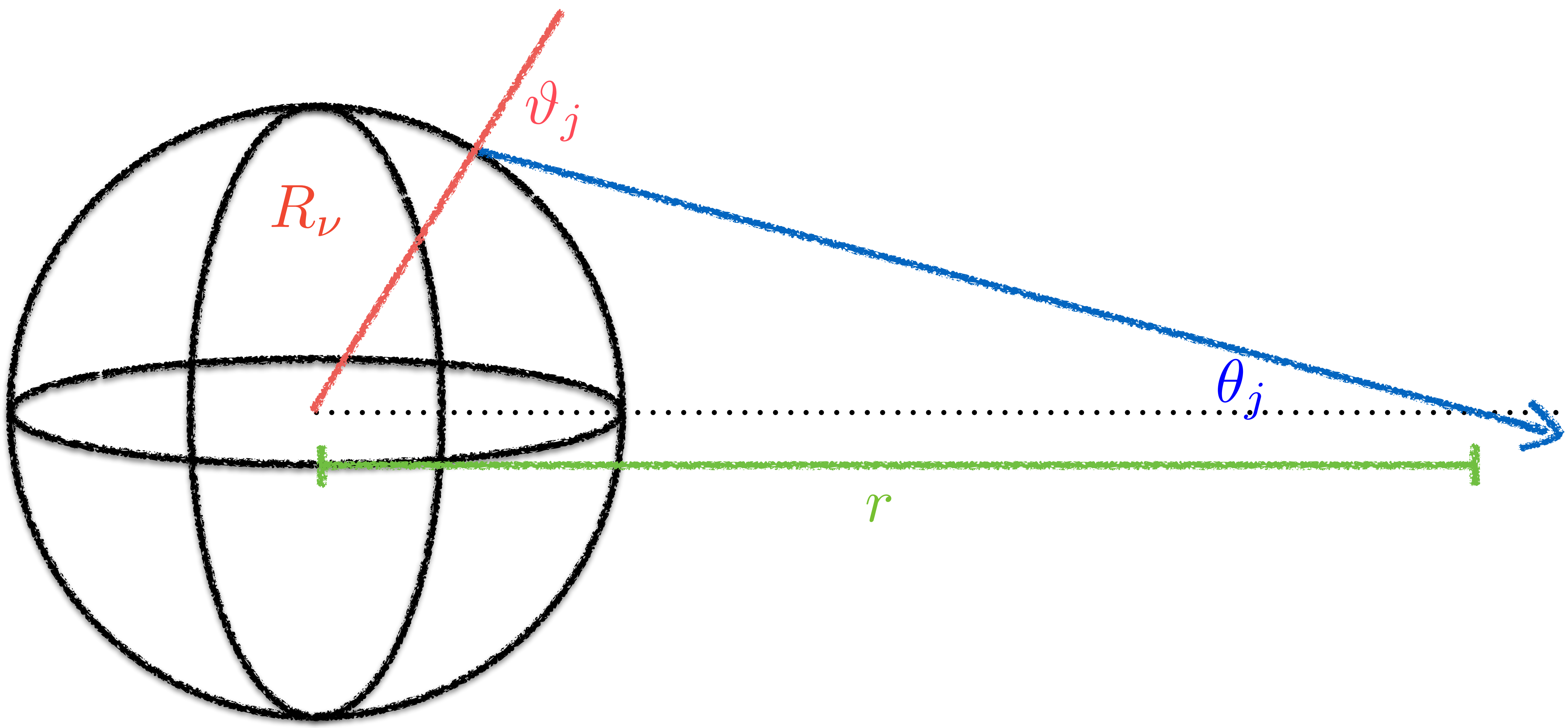


$$R_\nu \sin\vartheta_i = r \sin\theta_i$$

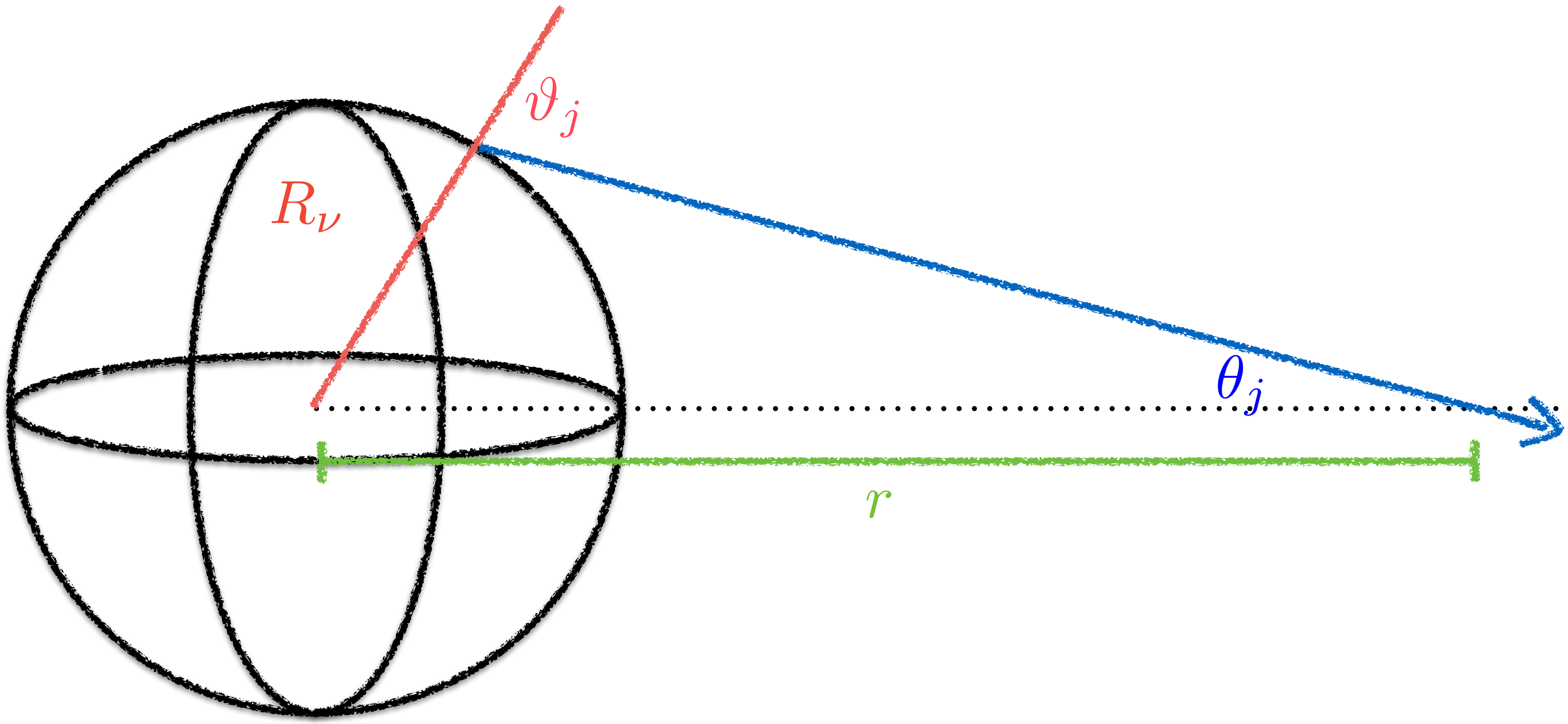
$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_\mathrm{F} \sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^\dagger_{\nu,\mathrm{j}} \\ &\quad - \sqrt{2} G_\mathrm{F} \sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^\dagger_{\bar{\nu},\mathrm{j}} \end{aligned}$$

explicit function of $r,\ \vartheta_i,\ \vartheta_j$

Basic Trigonometry is our Friend, Part 2

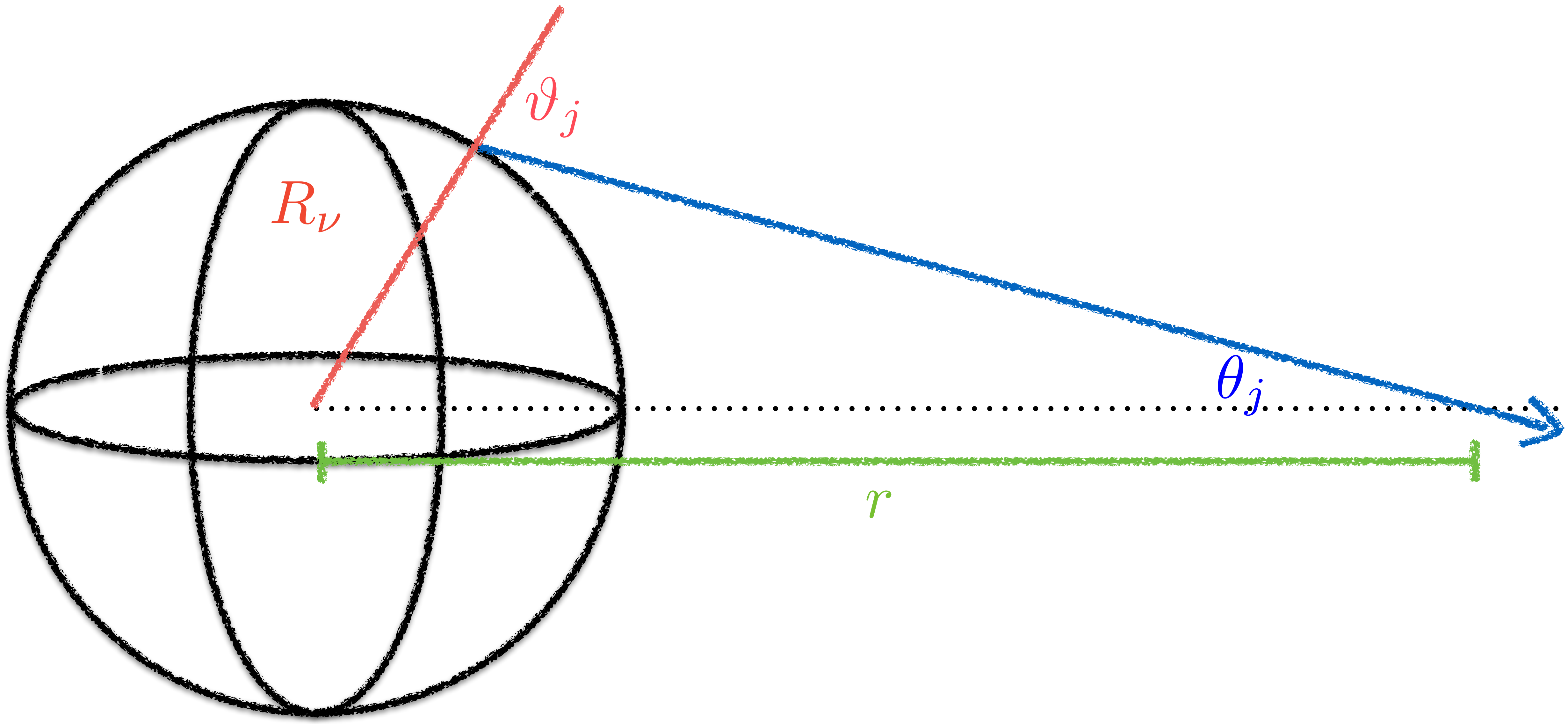


Basic Trigonometry is our Friend, Part 2



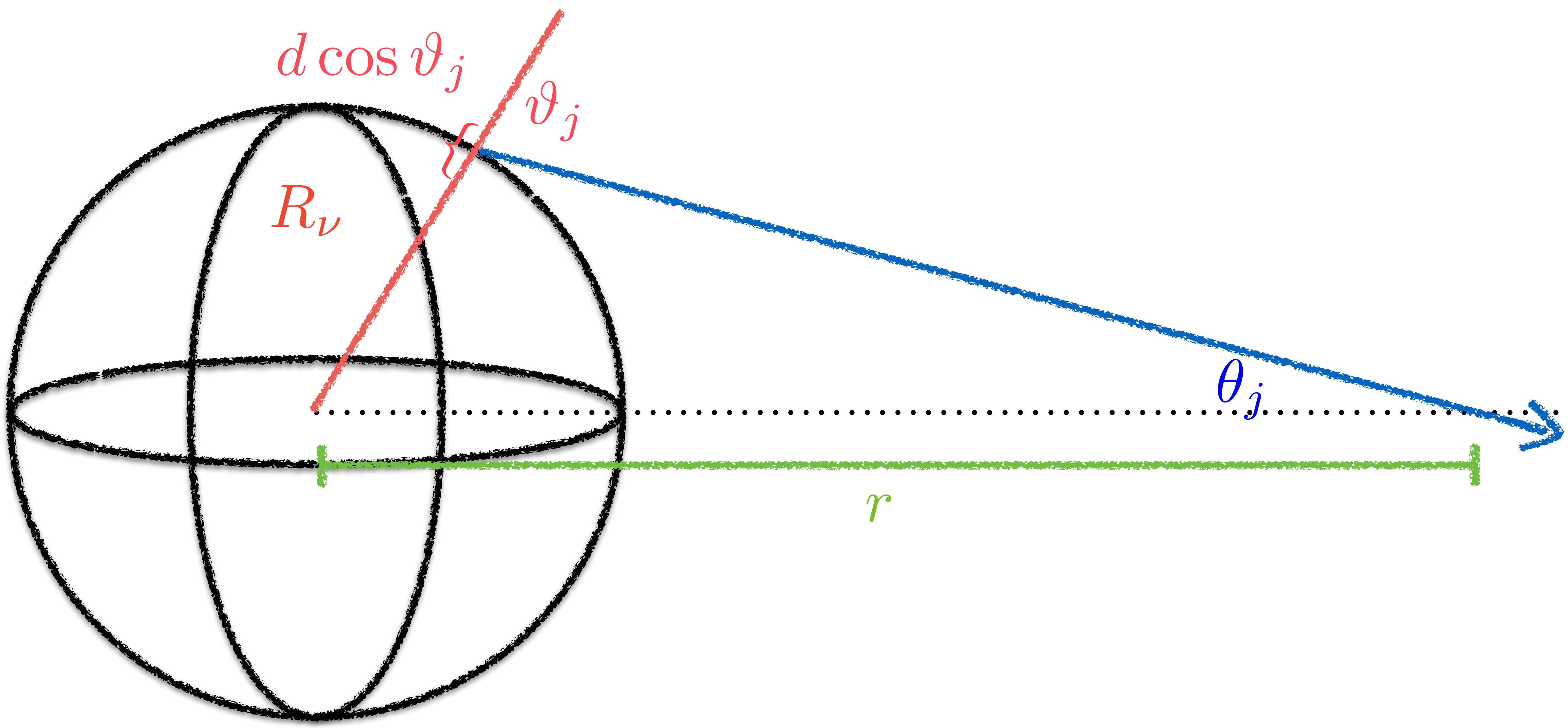
$$
\begin{aligned}
H_{\nu\nu,\mathrm{i}} &= \sqrt{2}G_{\mathrm{F}} \textstyle\sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^{\dagger}_{\nu,\mathrm{j}} \\
&- \sqrt{2}G_{\mathrm{F}} \textstyle\sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^{\dagger}_{\bar{\nu},\mathrm{j}}
\end{aligned}
$$

Basic Trigonometry is our Friend, Part 2



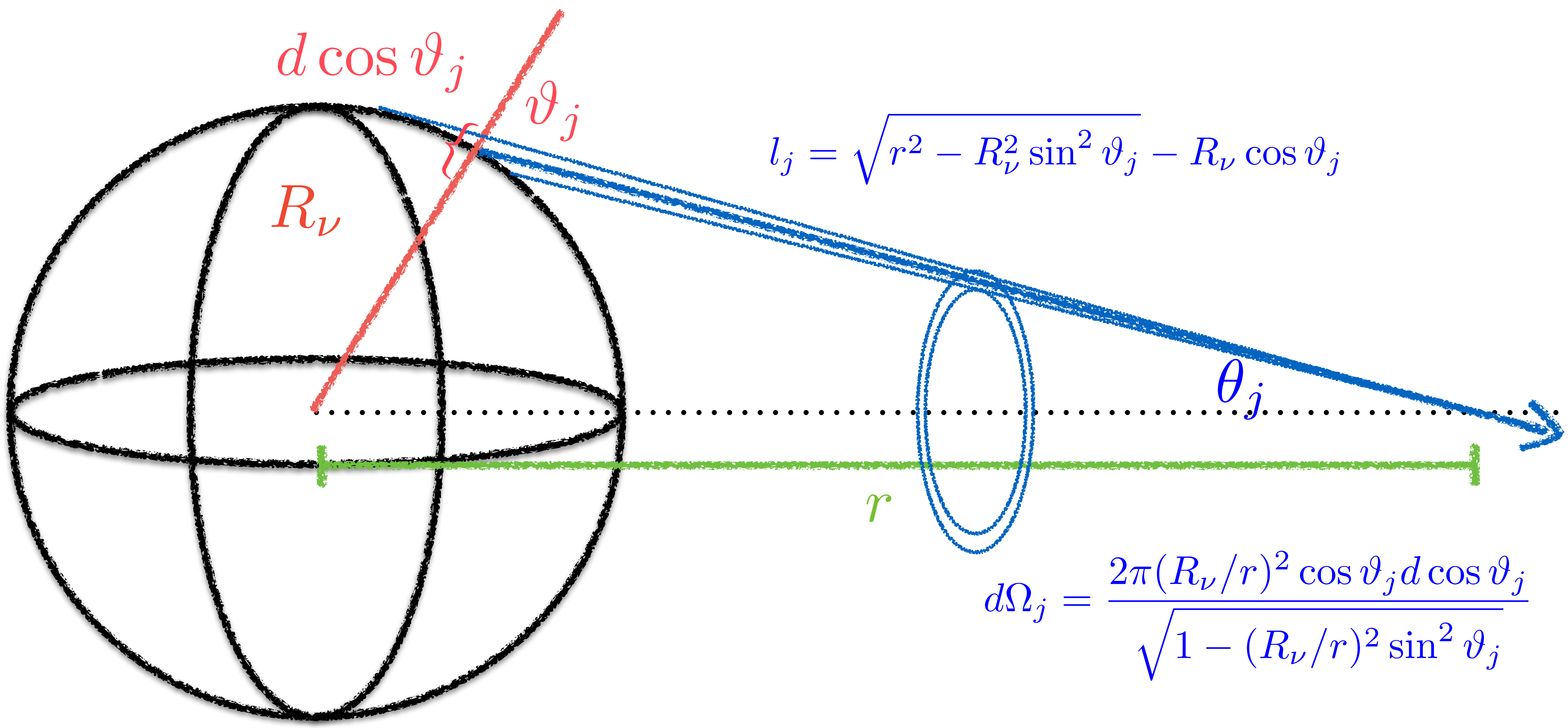
$$
\begin{aligned}
H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_\mathrm{F} \sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^\dagger_{\nu,\mathrm{j}} \\
&- \sqrt{2} G_\mathrm{F} \sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^\dagger_{\bar{\nu},\mathrm{j}}
\end{aligned}
$$

Basic Trigonometry is our Friend, Part 2



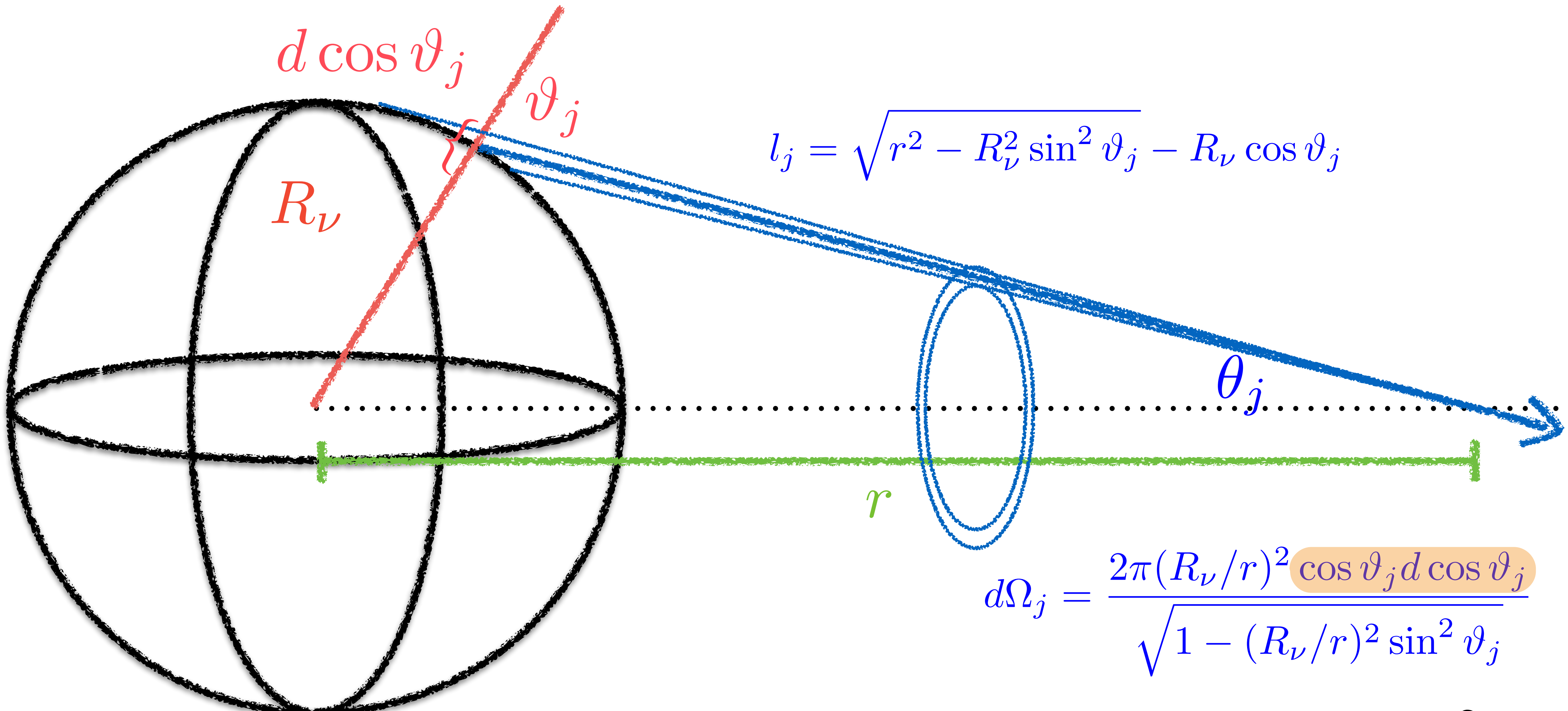
$$H_{\nu\nu,\mathrm{i}} = \sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^\dagger_{\nu,\mathrm{j}}$$
$$-\sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^\dagger_{\bar{\nu},\mathrm{j}}$$

Basic Trigonometry is our Friend, Part 2



$$
\begin{aligned}
H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^{\dagger}_{\nu,\mathrm{j}} \\
&\quad -\sqrt{2} G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^{\dagger}_{\bar{\nu},\mathrm{j}}
\end{aligned}
$$

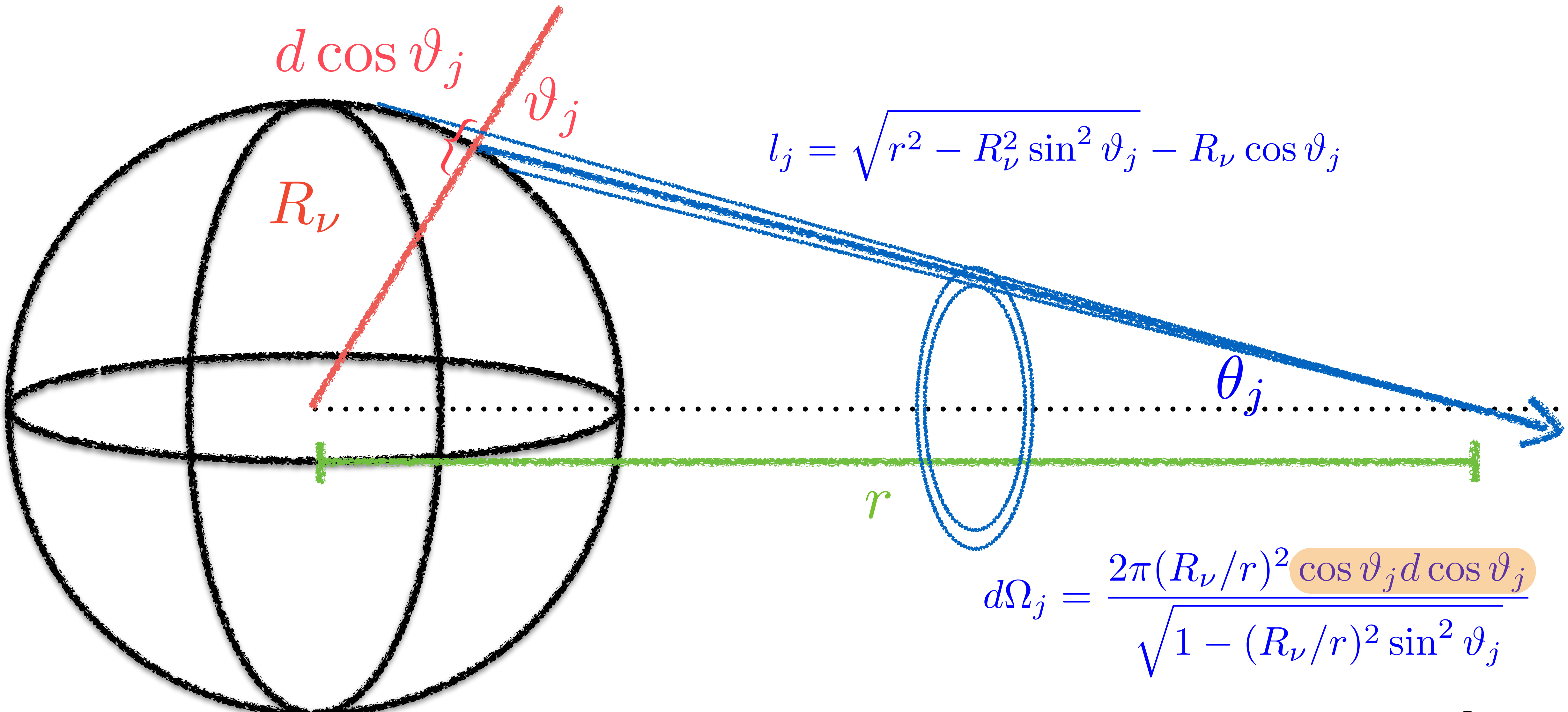
Basic Trigonometry is our Friend, Part 2



Big Hint:bin evenly in $\cos^2\vartheta$

$$
\begin{aligned}
H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_{\mathrm{F}} \textstyle\sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^{\dagger}_{\nu,\mathrm{j}} \\
&\quad - \sqrt{2} G_{\mathrm{F}} \textstyle\sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^{\dagger}_{\bar{\nu},\mathrm{j}}
\end{aligned}
$$

Basic Trigonometry is our Friend, Part 2



$$l_j = \sqrt{r^2 - R_\nu^2 \sin^2\vartheta_j} - R_\nu \cos\vartheta_j$$

$$d\Omega_j = \frac{2\pi (R_\nu/r)^2 \cos\vartheta_j d\cos\vartheta_j}{\sqrt{1-(R_\nu/r)^2\sin^2\vartheta_j}}$$

Big Hint:bin evenly in $\cos^2\vartheta$

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2} G_\mathrm{F} \textstyle\sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^\dagger_{\nu,\mathrm{j}} \\ &\quad - \sqrt{2} G_\mathrm{F} \textstyle\sum_\mathrm{j} \left(1 - \hat{k}_\mathrm{i} \cdot \hat{k}_\mathrm{j}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^\dagger_{\bar{\nu},\mathrm{j}} \end{aligned}$$

explicit functions of $r,\ \vartheta_j,\ E_j$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \theta_i,\ \phi_i\right])$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\,[r,\ \cancel{\theta_i},\ \cancel{\phi_i}])$$

$$H_{\nu\nu,i}(r,\ \theta_i,\ \phi_i,\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\,[r,\ E_j,\ \theta_j,\ \phi_j])$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \cancel{\theta_i},\ \cancel{\phi_i}\right])$$

$$H_{\nu\nu,i}(r,\ \theta_i,\ \cancel{\phi_i},\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\left[r,\ E_j,\ \theta_j,\ \cancel{\phi_j}\right])$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\,[r,\ \cancel{\theta_i},\ \cancel{\phi_i}])$$

$$H_{\nu\nu,i}(r,\ \cancel{\theta_i}\to\vartheta_i,\ \cancel{\phi_i},\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^\dagger_{\nu,j}\,[r,\ E_j,\ \cancel{\theta_j}\to\vartheta_j,\ \cancel{\phi_j}])$$

Re-examine our Variables

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Affine Parameter, r

$$H_{vac,i}\left(E_i,\ \delta m^2,\ \theta_V,\ \delta\right)$$

$$H_{e,i}(n_e\left[r,\ \cancel{\theta_i},\ \cancel{\phi_i}\right])$$

$$H_{\nu\nu,i}(r,\ \cancel{\theta_i}\to\vartheta_i,\ \cancel{\phi_i},\ \sum_j n_{\nu,j}\psi_{\nu,j}\psi^{\dagger}_{\nu,j}\left[r,\ E_j,\ \cancel{\theta_j}\to\vartheta_j,\ \cancel{\phi_j}\right])$$

Now this is becoming manageable.

Really, We're Down to 3 Dimensions

- The only dimensions left which might need fine resolution are r, E, and ϑ.

- The size of a single $\psi_{\nu,j}$ is set by the SU(3) symmetry of neutrino flavors: 288 bytes.

- The size of the system of coupled states we are solving is now [ncosth,negy,3,3] x 2.

- ~100 kB per process, but ncosth^2 messages need to be passed ~100 GB message traffic per time step!

Really, We're Down to 3 Dimensions

- The only dimensions left which might need fine resolution are r, E, and ϑ.
- The size of a single $\psi_{\nu,j}$ is set by the SU(3) symmetry of neutrino flavors: 288 bytes.
- The size of the system of coupled states we are solving is now [ncosth,negy,3,3] x 2.
- $\sim$100 kB per process, but ncosth^2 messages need to be passed $\sim$100 GB message traffic per time step!

“Exploit Data Locality” - Bronson Messer

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^{\dagger}_{\nu,\mathrm{j}} \\ &-\sqrt{2}G_{\mathrm{F}}\sum_{\mathrm{j}}\left(1-\hat{k}_{\mathrm{i}}\cdot\hat{k}_{\mathrm{j}}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^{\dagger}_{\bar{\nu},\mathrm{j}} \end{aligned}$$

↑

$$(1-\cos\theta_{\mathrm{ij}})$$

“Exploit Data Locality” - Bronson Messer

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2}G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\nu,\mathrm{j}} \psi_{\nu,\mathrm{j}} \psi^{\dagger}_{\nu,\mathrm{j}} \\ &\quad - \sqrt{2}G_{\mathrm{F}} \sum_{\mathrm{j}} \left(1 - \hat{k}_{\mathrm{i}} \cdot \hat{k}_{\mathrm{j}}\right) n_{\bar{\nu},\mathrm{j}} \psi_{\bar{\nu},\mathrm{j}} \psi^{\dagger}_{\bar{\nu},\mathrm{j}} \end{aligned}$$

↑

$$(1 - \cos\theta_{\mathrm{ij}})$$

↑

$$(1 - \cos\theta_i \cos\theta_j)$$

“Exploit Data Locality” - Bronson Messer

$$\begin{aligned} H_{\nu\nu,\mathrm{i}} &= \sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\nu,\mathrm{j}}\psi_{\nu,\mathrm{j}}\psi^\dagger_{\nu,\mathrm{j}} \\ &-\sqrt{2}G_\mathrm{F}\sum_\mathrm{j}\left(1-\hat{k}_\mathrm{i}\cdot\hat{k}_\mathrm{j}\right)n_{\bar{\nu},\mathrm{j}}\psi_{\bar{\nu},\mathrm{j}}\psi^\dagger_{\bar{\nu},\mathrm{j}} \end{aligned}$$

↑

$$(1-\cos\theta_\mathrm{ij})$$

↑

$$(1-\cos\theta_i\cos\theta_j)$$

Perform a partial sum locally

$$H_{\nu\nu,1} = \sqrt{2}G_F\sum_j\left(n_{\nu,j}\psi_{\nu,j}\psi^\dagger_{\nu,j} - n_{\bar{\nu},j}\psi_{\bar{\nu},j}\psi^\dagger_{\bar{\nu},j}\right)$$

$$H_{\nu\nu,2} = \sqrt{2}G_F\sum_j\cos\theta_j\left(n_{\nu,j}\psi_{\nu,j}\psi^\dagger_{\nu,j} - n_{\bar{\nu},j}\psi_{\bar{\nu},j}\psi^\dagger_{\bar{\nu},j}\right)$$

} 288 Bytes

How I learned to stop worrying and love Allreduce()

$$ncores \left\{ \begin{array}{l} H_{\nu\nu,1} \quad H_{\nu\nu,2} \\ H_{\nu\nu,1} \quad H_{\nu\nu,2} \\ H_{\nu\nu,1} \quad H_{\nu\nu,2} \end{array} \right. \rightarrow H^{tot}_{\nu\nu,1} \quad H^{tot}_{\nu\nu,2}$$

$$ncores \times \ 288 \text{ bytes} \sim O(100\,kB)$$

$$\rightarrow H_{\nu\nu,i} = H_{\nu\nu,1} - \cos\theta_i \times H_{\nu\nu,2}$$

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

The form of the above Hamiltonian equation screams out for a first order implicit solution method.

$$\psi_{n+1} = \left[I + \frac{1}{i}\Delta r H_{tot}\right]^{-1}\psi_n$$

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

~~The form of the above Hamiltonian equation screams out for a first order implicit solution method.~~

$$\psi_{n+1} = \left[I + \frac{1}{i}\Delta r H_{tot}\right]^{-1}\psi_n$$

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

~~The form of the above Hamiltonian equation screams out for a first order implicit solution method.~~

$$\psi_{n+1} = \left[I + \frac{1}{i}\Delta r H_{tot}\right]^{-1}\psi_n$$

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

~~The form of the abov~~

~~n equation screams out for a first order i n method.~~

$$\psi_{n+1} = \left[\;\right]^{-1} \psi_n$$

Now we have this down to single process sized problem

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

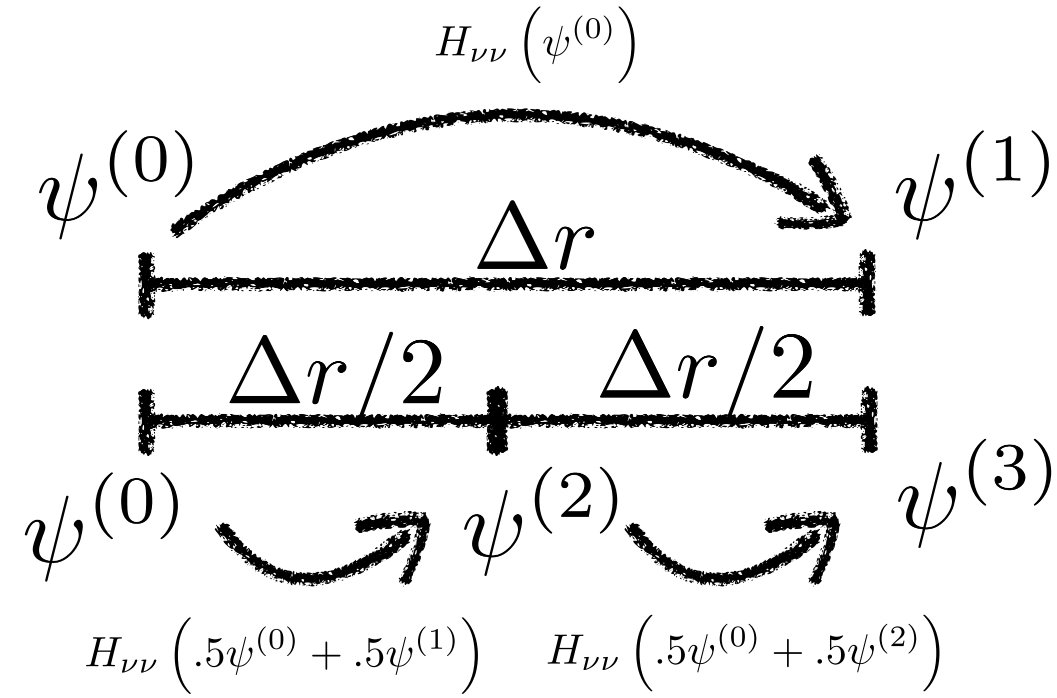
Each set of equations is now down to 3X3 (X2) with negy different wave functions stored locally ~(a few) thousand per core.

The form of the abov … n equation screams out fo a first o der i … n method

REJECTED

$$\psi_{n+1} = \left[\quad \right] \psi_n$$

Why does the obvious thing fail?



- Basic Leapfrog algorithm:
- High frequency oscillations.

$$i\frac{d}{dt}\psi_{\nu,i} = H_{tot}\psi_{\nu,i} \implies \text{local solutions where } \omega_{osc} \propto diag\left(H_{tot}\right)$$

$$l_{osc} = \frac{2\pi}{\omega_{osc}} \sim 10\,\text{cm} \qquad R_{\text{Flavor Transformation}} \sim 10^3\,\text{km}$$

- This is bad news for tracking complex phases in wave functions

$$Err = Re(\psi^{(1)} - \psi^{(3)})^2 + Im(\psi^{(1)} - \psi^{(3)})^2 \sim \frac{\Delta r}{l_{osc}} \sim 10^{-6}$$

Find the Local Eigen Basis

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

- Employ the Magnus method to work explicitly in the eigen basis of the local Hamiltonian.

$$\psi_{\nu,\mathrm{i}}\left(r+\Delta r\right) \simeq \exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right)\psi_{\nu,\mathrm{i}}\left(r\right)$$

$$\sum_b H_{ab}V_{bc} = \zeta_c V_{ac}, \quad a,b,c = 1,2,3$$

$$\exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right) = V\begin{pmatrix} \mathrm{e}^{-i\zeta_1\Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2\Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3\Delta r} \end{pmatrix} V^\dagger$$

} Computationally expensive, but potentially much longer step size

Find the Local Eigen Basis

$$i\frac{\partial}{\partial t}\psi_{\nu,\mathrm{i}} = \left(H_{\mathrm{vac,i}} + H_{\mathrm{e,i}} + H_{\nu\nu,\mathrm{i}}\right)\psi_{\nu,\mathrm{i}}$$

- Employ the Magnus method to work explicitly in the eigen basis of the local Hamiltonian.

$$\psi_{\nu,\mathrm{i}}\left(r+\Delta r\right) \simeq \exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right)\psi_{\nu,\mathrm{i}}\left(r\right)$$

$$\sum_b H_{ab}V_{bc} = \zeta_c V_{ac}, \quad a,b,c = 1,2,3$$

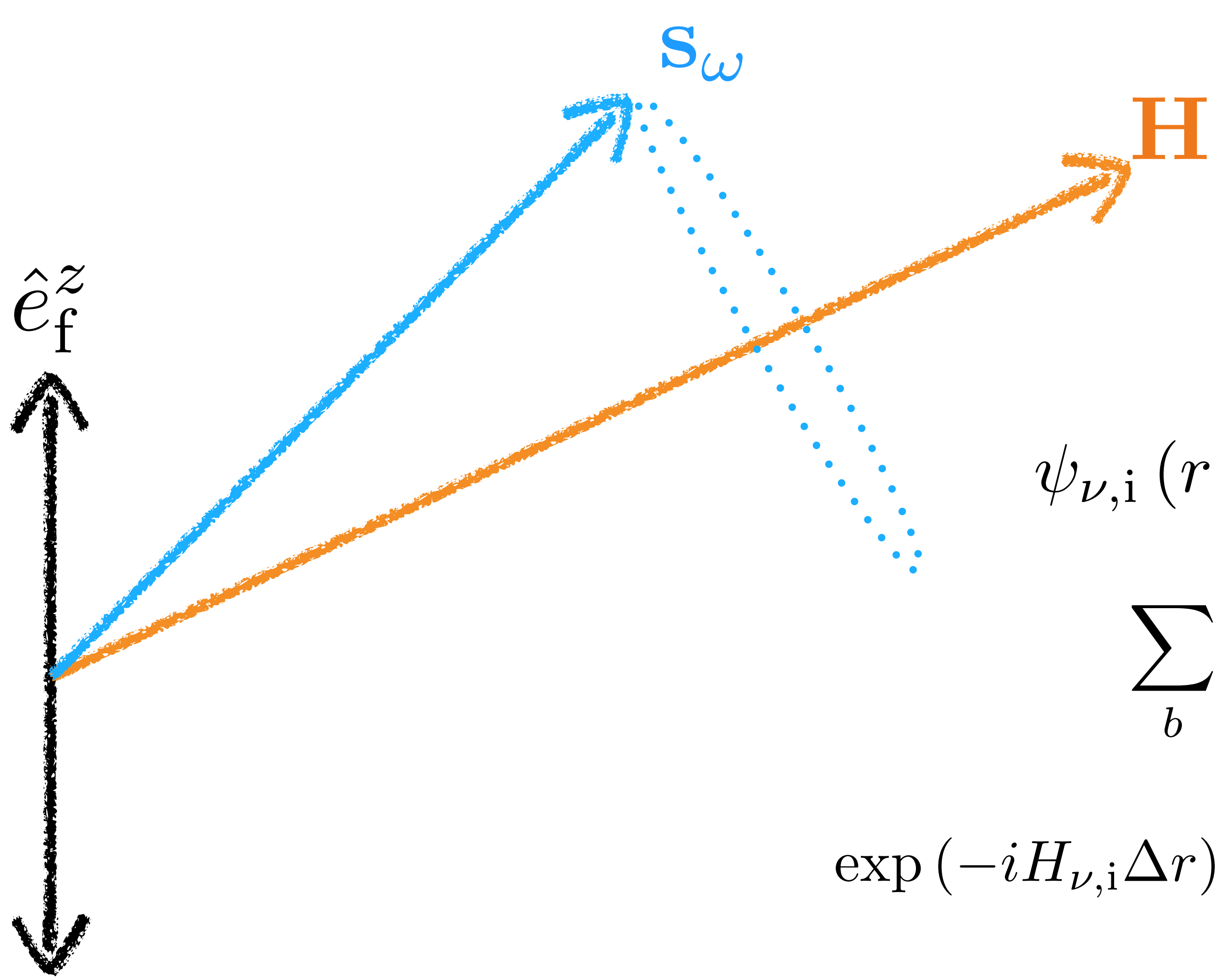
$$\exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right) = V\begin{pmatrix} \mathrm{e}^{-i\zeta_1\Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2\Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3\Delta r}\end{pmatrix}V^\dagger$$

Computationally expensive, but potentially much longer step size

Poster Child for GPU implementable calculation (MAGMA)

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



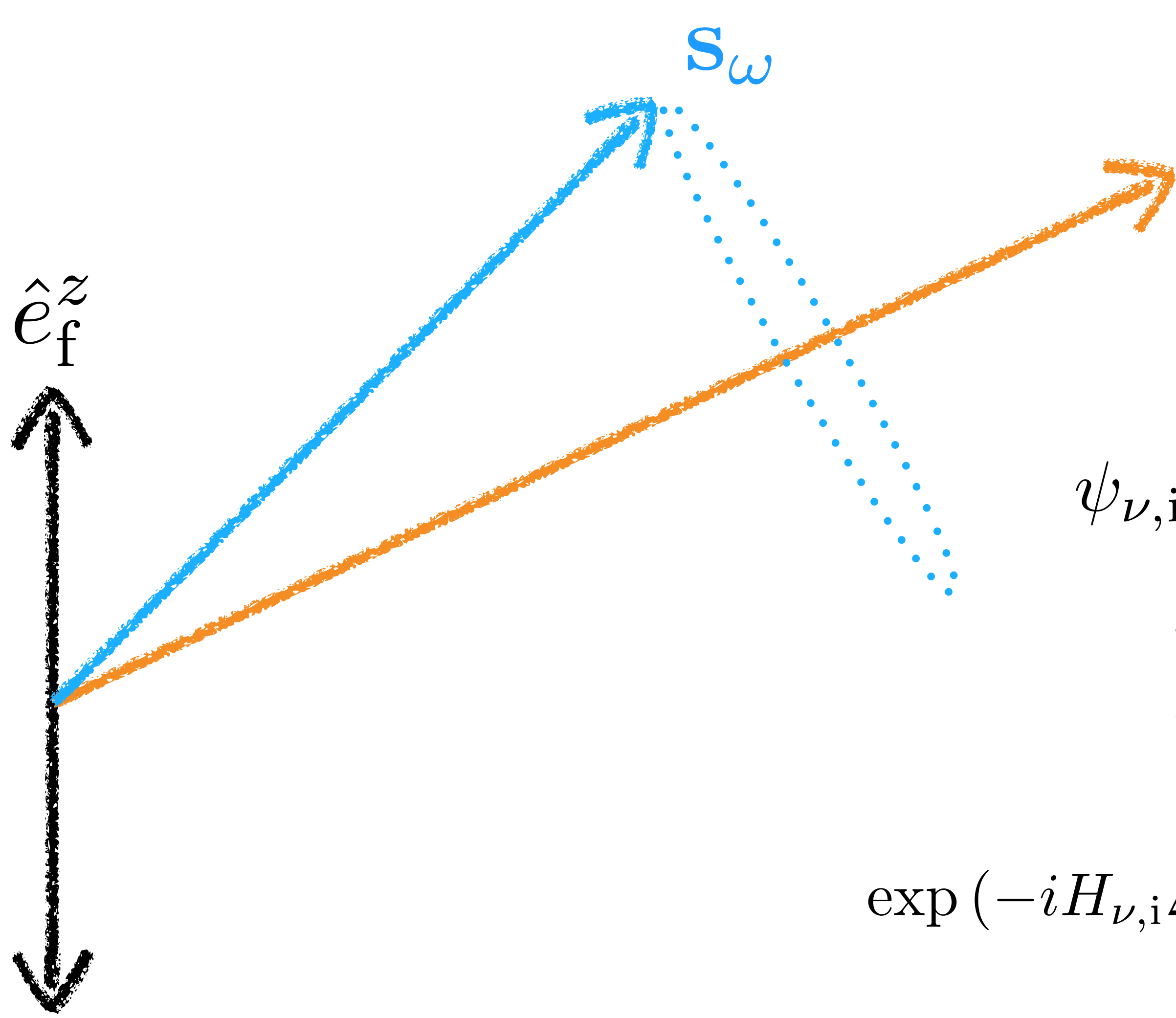
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab}V_{bc} = \zeta_c V_{ac}, \quad a,b,c = 1,2,3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1\Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2\Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3\Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



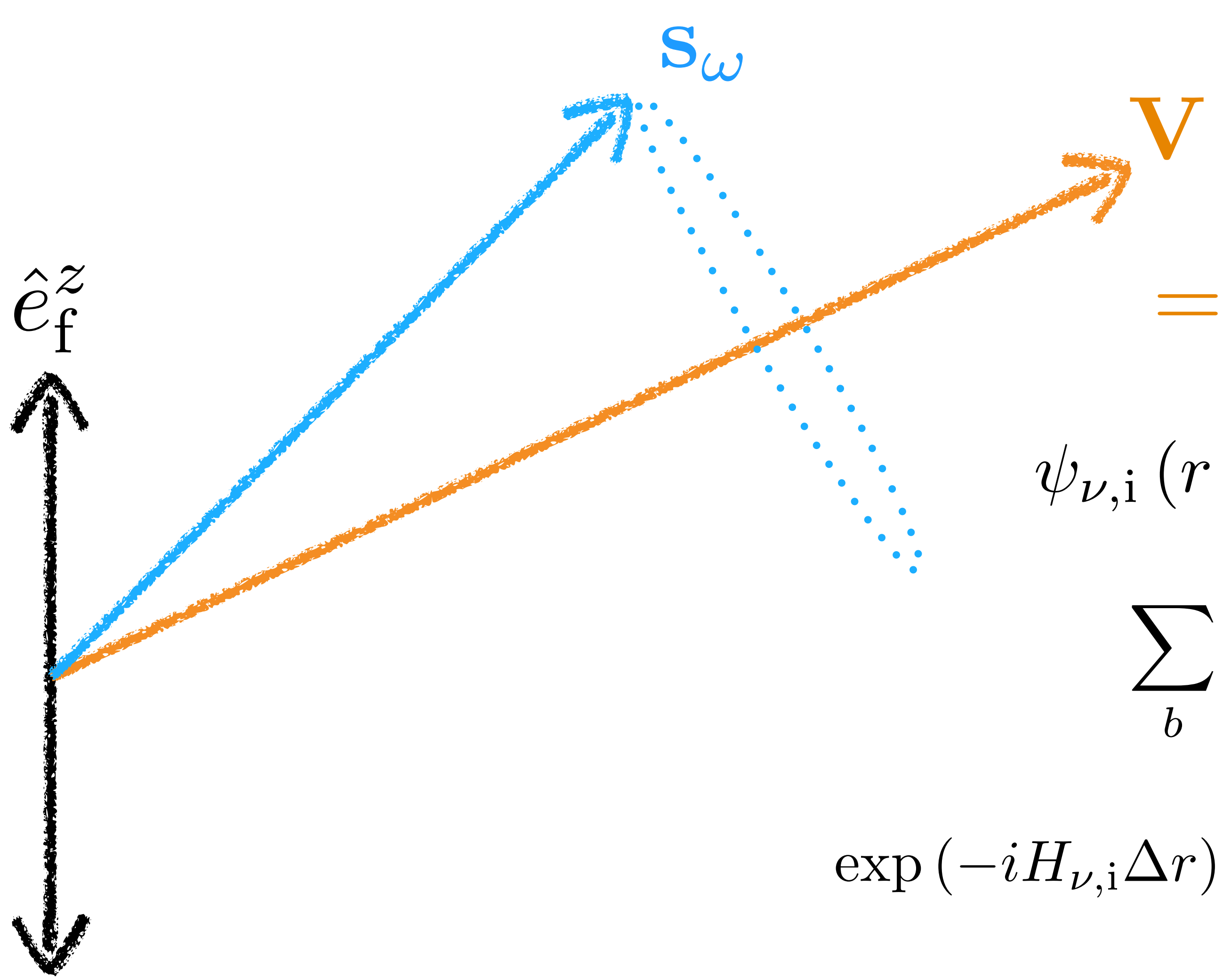
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \rightarrow SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

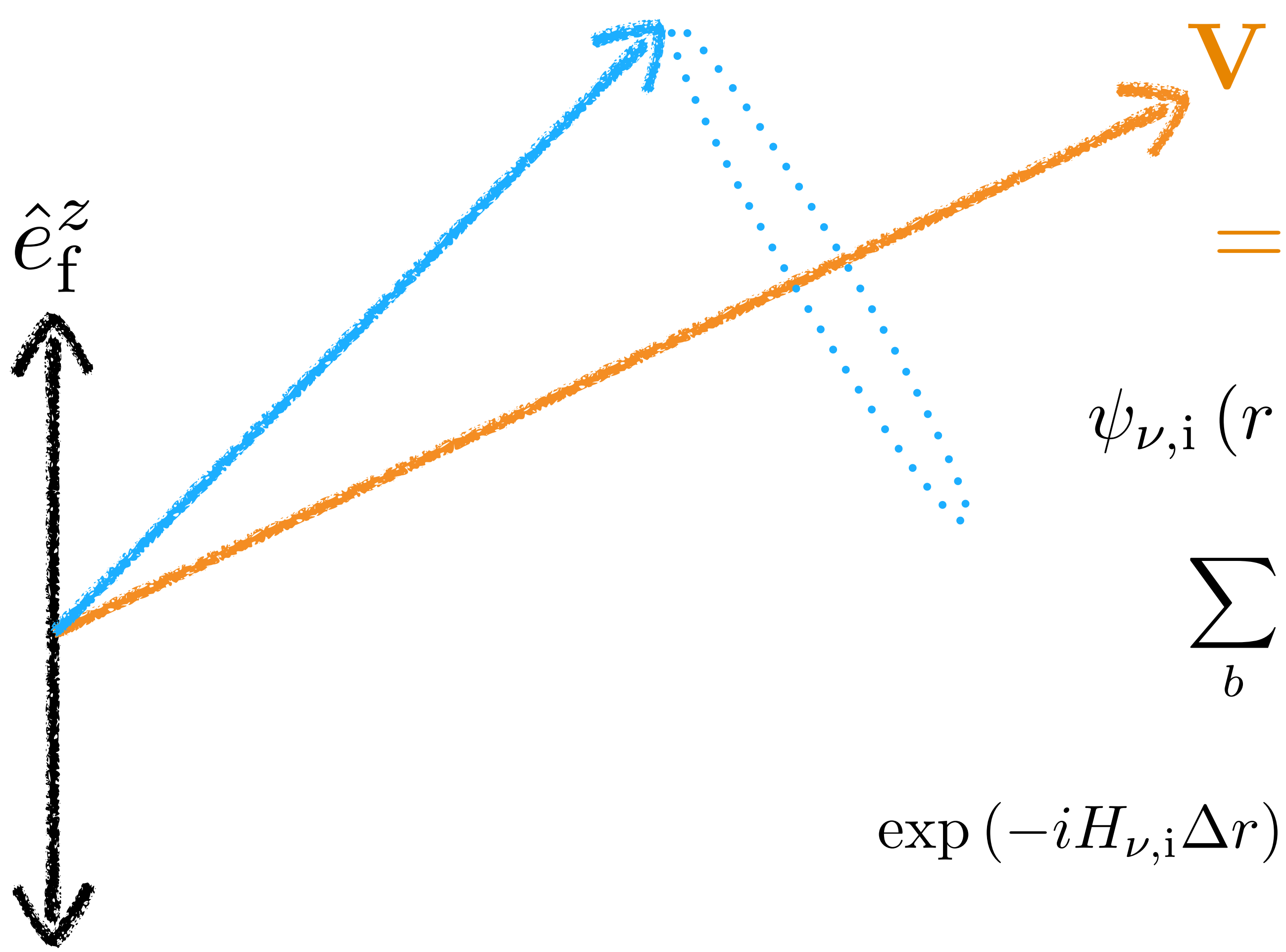
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

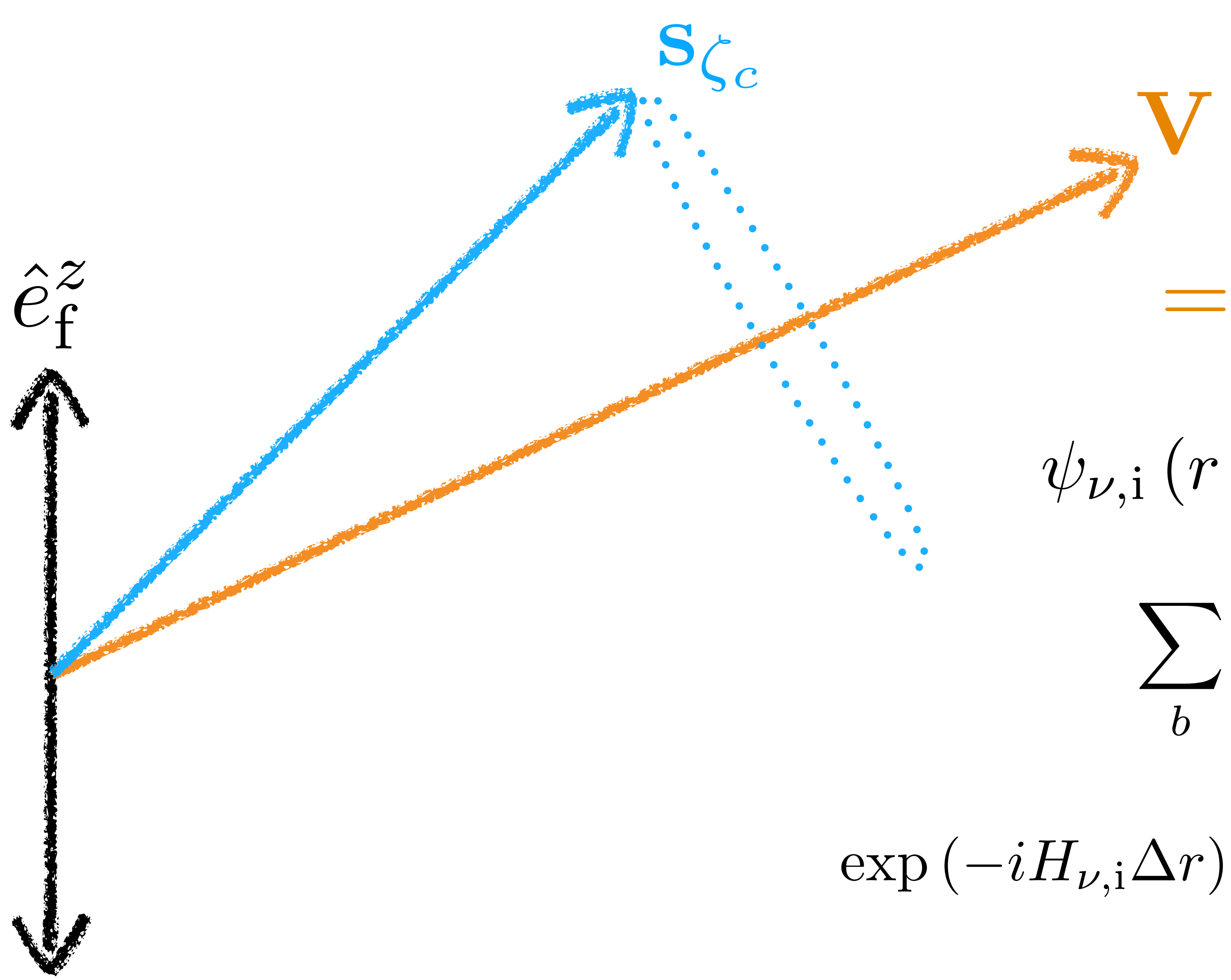
$$\psi_{\nu,\mathrm{i}}\left(r + \Delta r\right) \simeq \exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right)\psi_{\nu,\mathrm{i}}\left(r\right)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp\left(-iH_{\nu,\mathrm{i}}\Delta r\right) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

$$\psi_{\nu,\rm i}\,(r + \Delta r) \simeq \exp\left(-iH_{\nu,\rm i}\Delta r\right)\psi_{\nu,\rm i}\,(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

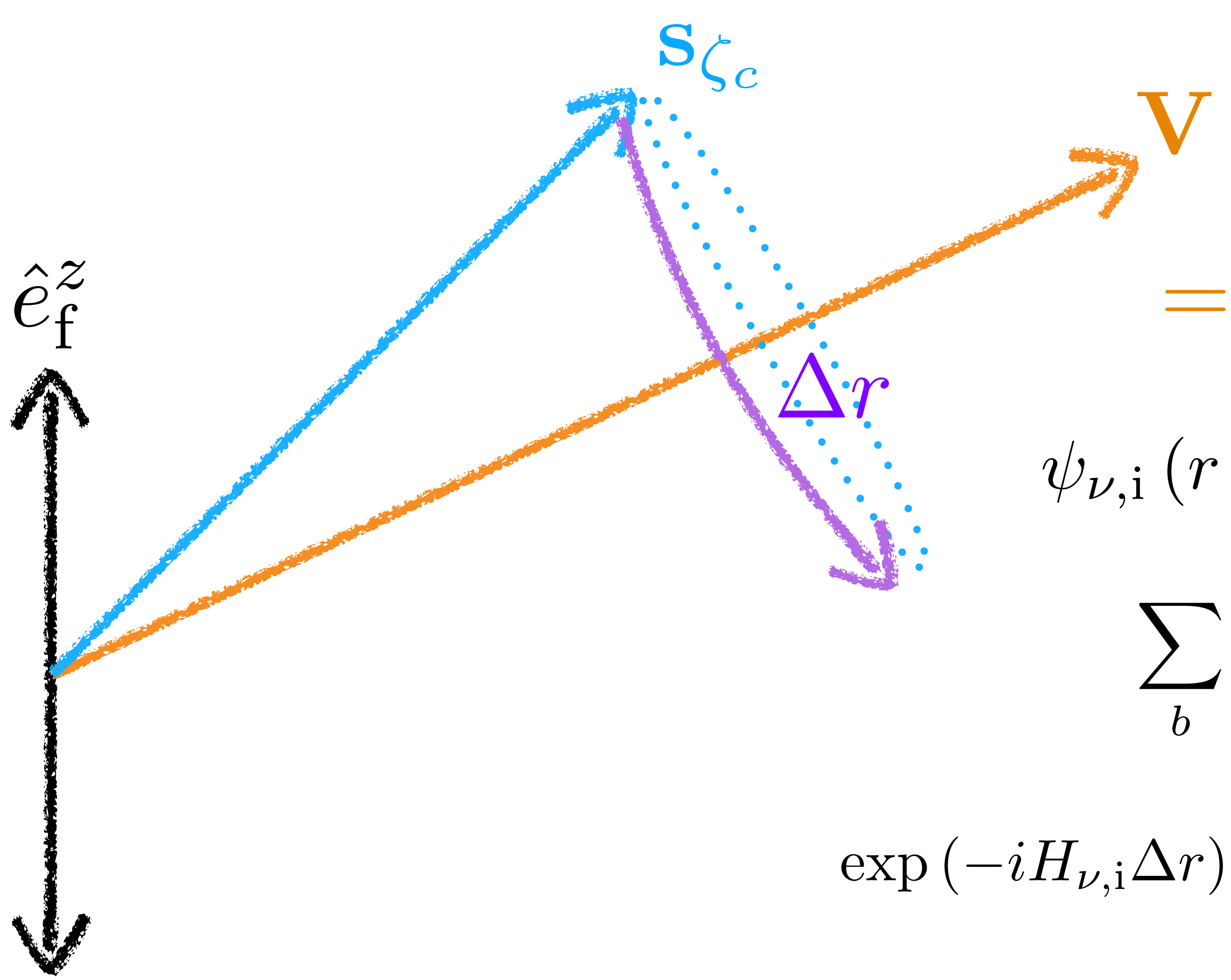
$$\exp\left(-iH_{\nu,\rm i}\Delta r\right) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu$$

$$SU(2) \to SO(3)$$

$$\frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

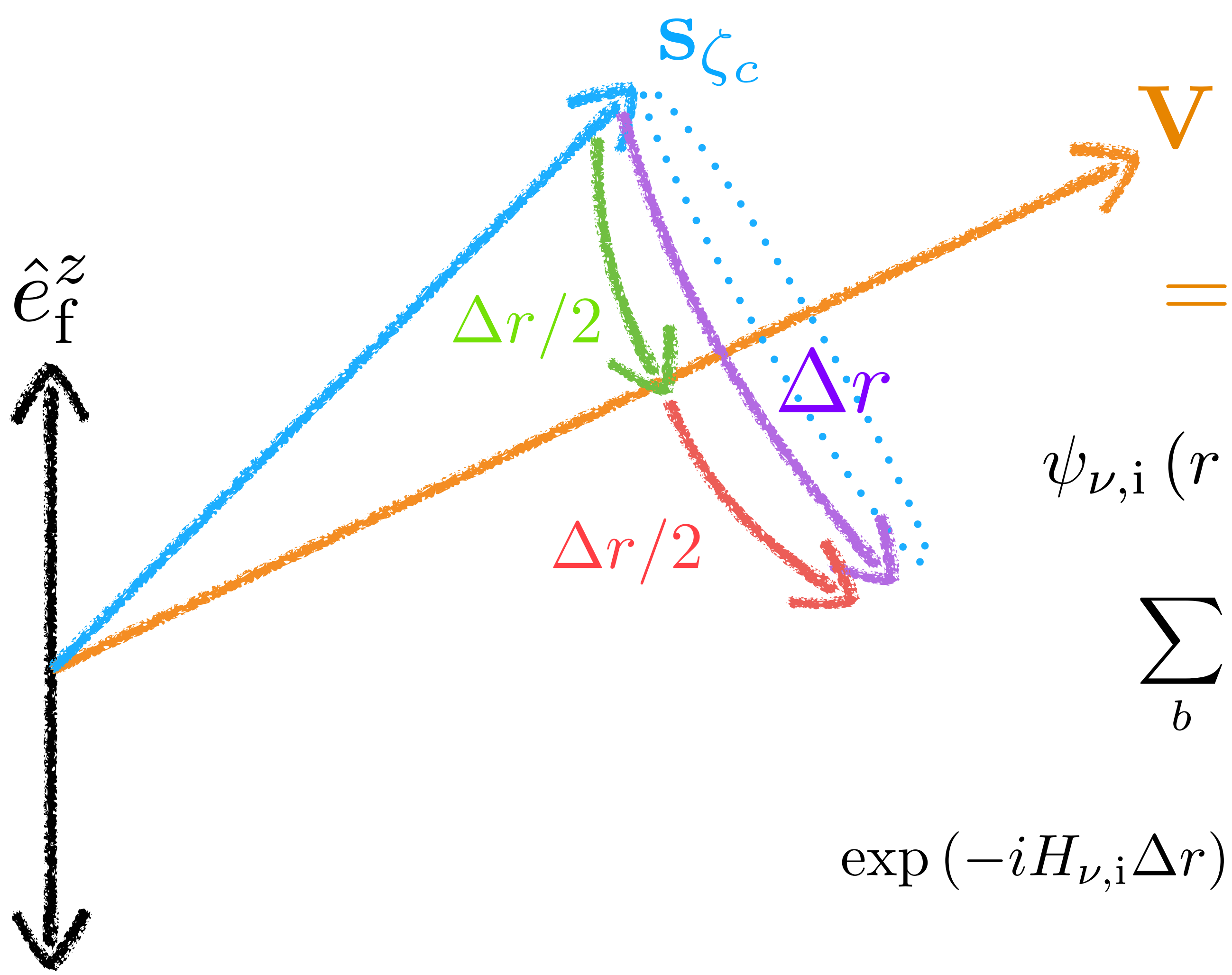
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

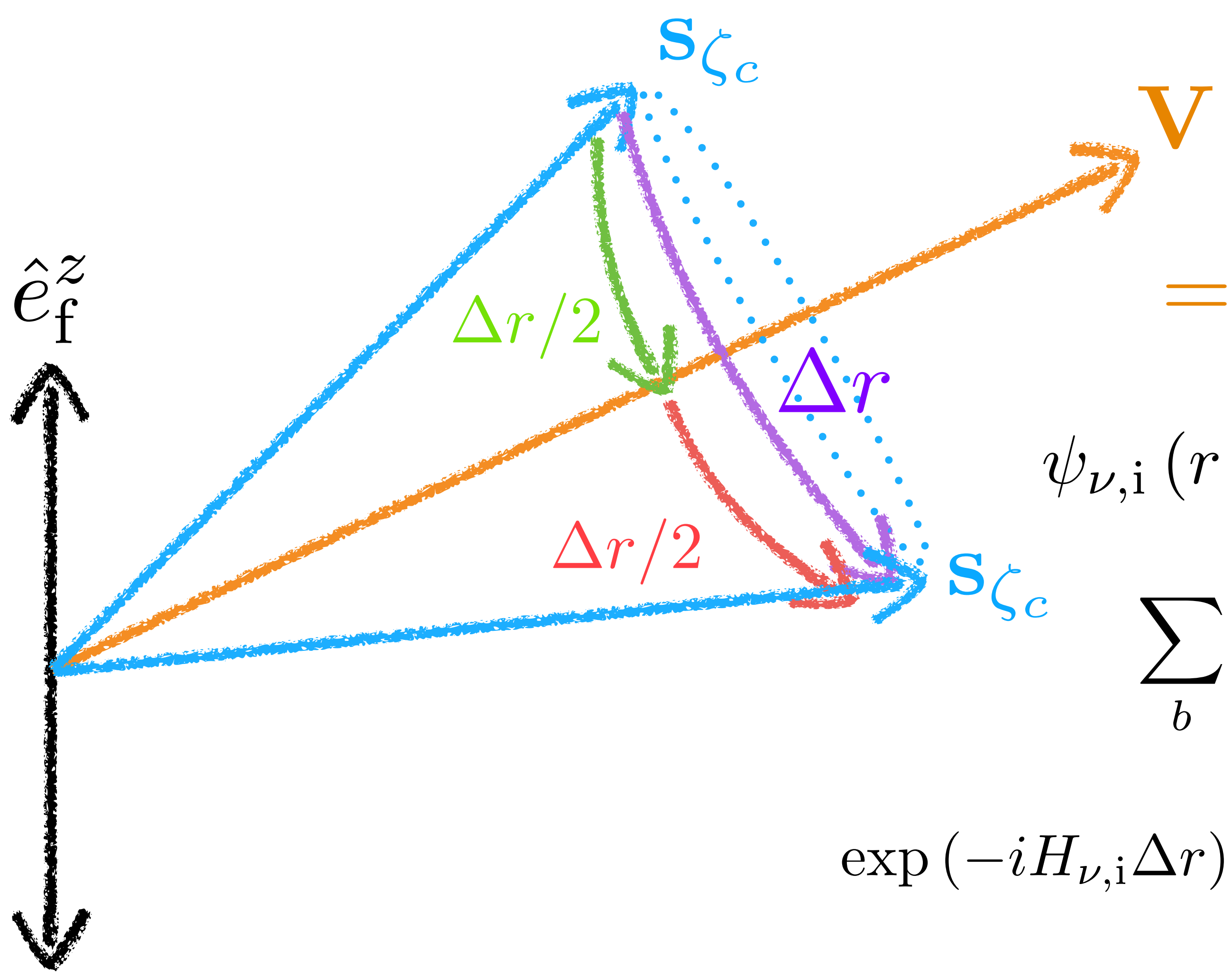
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}} \Delta r) \psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}} \Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

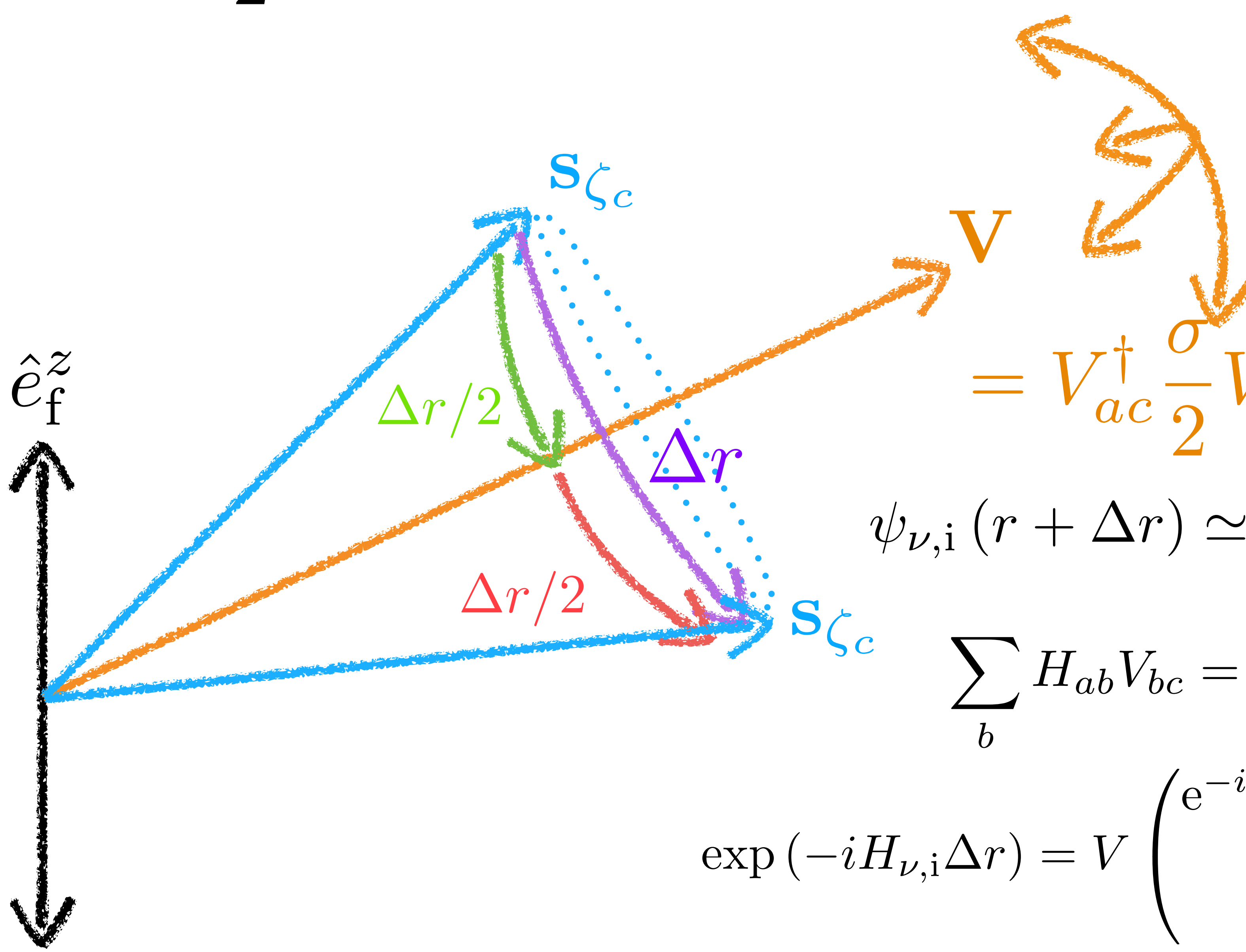
$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab}V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1\Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2\Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3\Delta r} \end{pmatrix} V^\dagger$$

Visualizing the Magnus Method

$$\mathbf{s}_\nu \equiv \psi_\nu^\dagger \frac{\sigma}{2} \psi_\nu \qquad SU(2) \to SO(3) \qquad \frac{d}{dt}\mathbf{s} = \mathbf{s} \times \mathbf{H}$$



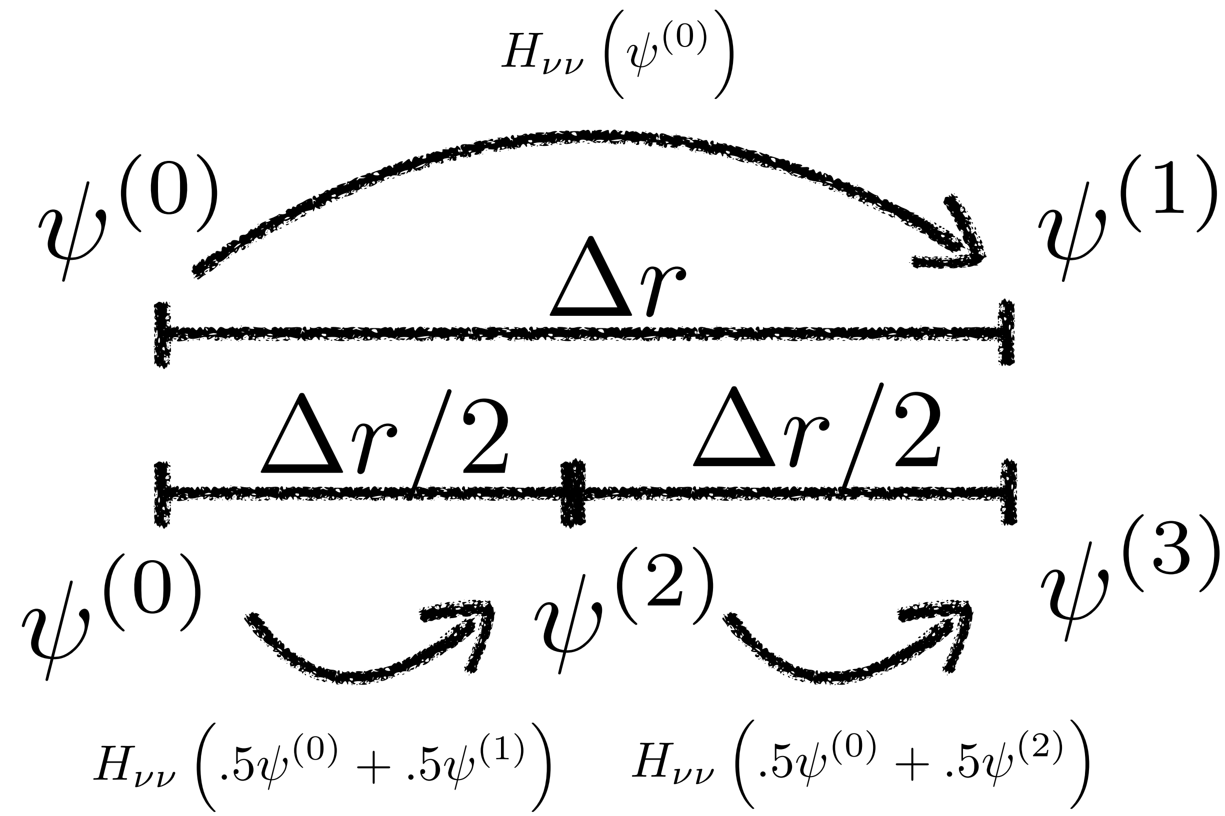
$$= V_{ac}^\dagger \frac{\sigma}{2} V_{ac}$$

$$\psi_{\nu,\mathrm{i}}(r + \Delta r) \simeq \exp(-iH_{\nu,\mathrm{i}}\Delta r)\psi_{\nu,\mathrm{i}}(r)$$

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

$$\exp(-iH_{\nu,\mathrm{i}}\Delta r) = V \begin{pmatrix} \mathrm{e}^{-i\zeta_1 \Delta r} & 0 & 0 \\ 0 & \mathrm{e}^{-i\zeta_2 \Delta r} & 0 \\ 0 & 0 & \mathrm{e}^{-i\zeta_3 \Delta r} \end{pmatrix} V^\dagger$$

Back to our Original Idea



- Basic Leapfrog algorithm:
- Rotating about local basis.

$$\sum_b H_{ab} V_{bc} = \zeta_c V_{ac}, \quad a, b, c = 1, 2, 3$$

- An improvement for tracking complex phases

$$Err = Re\left(\psi^{(1)} - \psi^{(3)}\right)^2 + Im\left(\psi^{(1)} - \psi^{(3)}\right)^2 \sim \frac{\Delta r}{2\pi/\zeta_c} \text{ or } \frac{\Delta r}{\Delta V_{ac}} \sim 10^{-6}$$

$$\text{typically } \Delta r \geq l_{osc} \implies \sim 10^6 \text{ integration steps}$$

Now there is a plan!

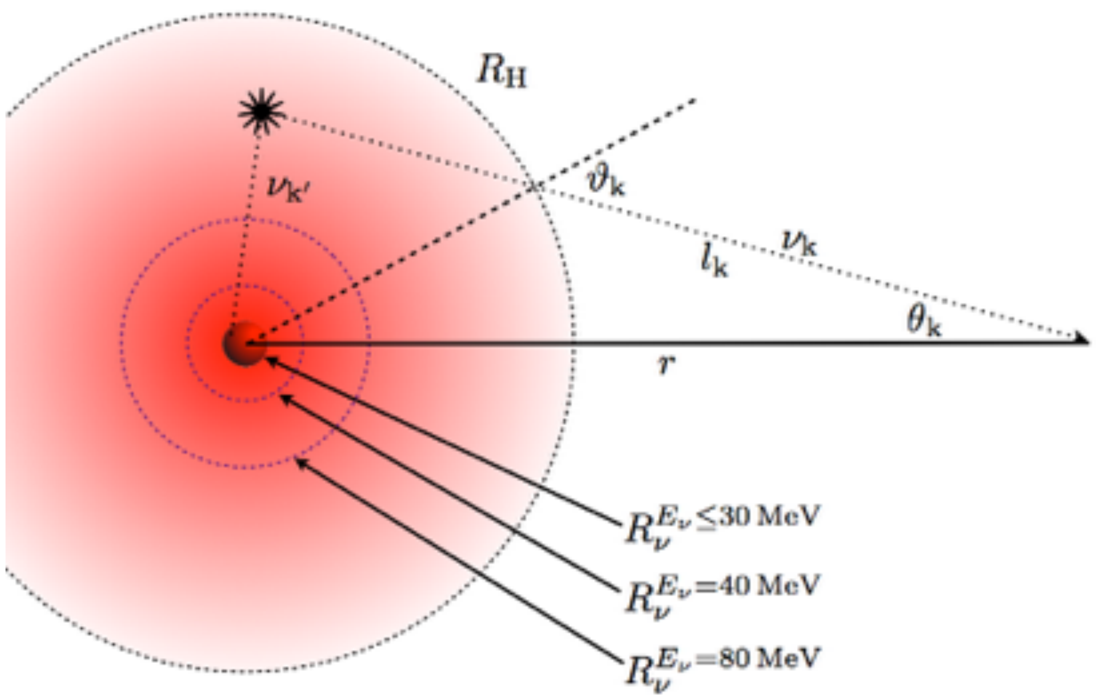
- Step 1: Exploit the symmetry of the problem. 6 Dimensions are reduced to 3.
- Step 2: Be efficient with your message passing and perform as much computation on local distributed processes (like a GPU) as you can get away with.
- Step 3: Think physically. If it looks like a duck, and quacks like a duck, it's probably a duck (to a reasonable approximation).

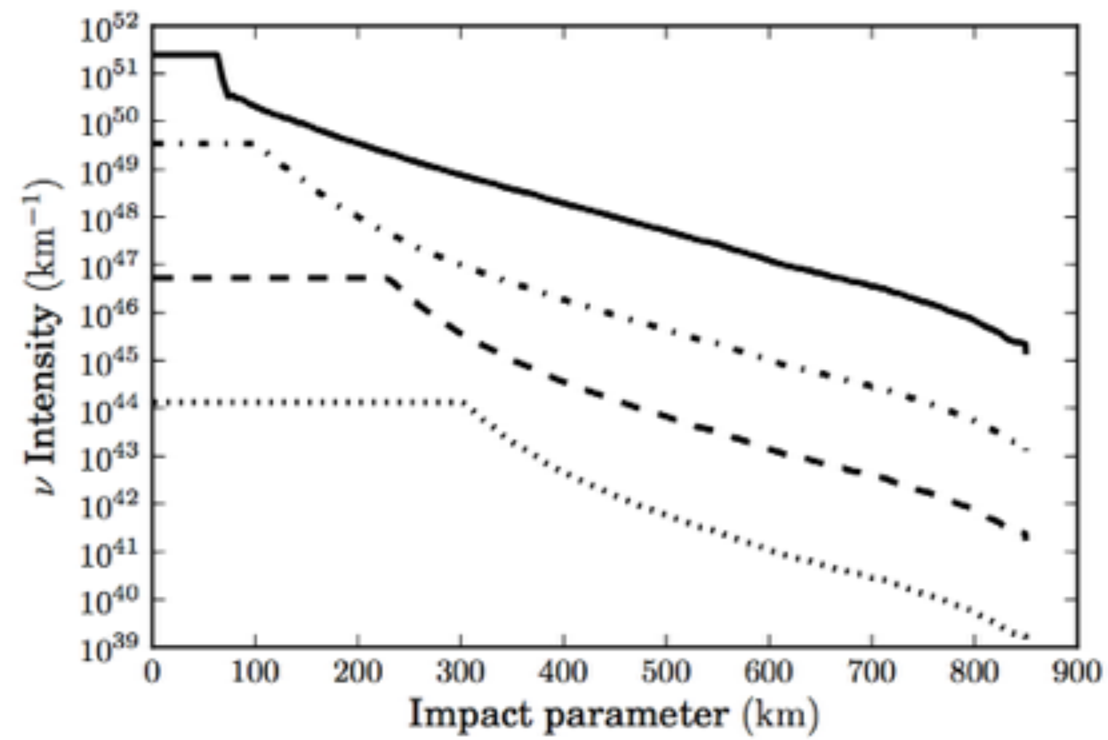
Not all simplicity is necessary

$$f_\nu(E_\nu,\vartheta_k) \equiv \frac{1}{F_2(\eta_\nu(\vartheta_k))\,T_\nu^3(\vartheta_k)} \frac{E_\nu^2}{\exp(E_\nu/T_\nu(\vartheta_k) - \eta_\nu(\vartheta_k)) + 1}$$

$$\mathrm{d}n_\nu(E_\nu,\vartheta_k) = \frac{2\pi j_\nu(E_\nu,\vartheta_k)\cos\vartheta_k \mathrm{d}(\cos\vartheta_k)\,R_H^2}{r^2\left(\sqrt{1-(\sin\vartheta_k R_H/r)^2} - \cos\vartheta_K R_H/r\right)}$$

$$j_\nu(E_\nu,\vartheta_k) = \frac{L_\nu(\vartheta_k)}{4\pi^2 R_H^2 \langle E_\nu(\vartheta_k)\rangle} f_\nu(E_\nu,\vartheta_k)$$





Local memory usage is increased by 20 MB, or ~5%