Here is the derivation of partial volume of a sphere that lies outside of the simulation cube when the sphere lands near an edge of the cube. The corner case is not accounted for since the cube is periodic in one axis and the spherical cap lying outside when the sphere is near the face is a simple, known integral.

The problem is decomposed into the computation of the volume of two spherical caps at right angles that have a region of overlap. The caps are distance a and b away from the centre of the sphere, where $a^2 + b^2 < R^2$ for R the radius of the sphere, so that the corner lies within the sphere. The volume of each of the caps $V1$ is given simply by the standard formula for a spherical cap:

$$V_1 = \frac{\pi h^2}{3}(3R - h)$$

where $h = R - a$

After calculating the volume of the two caps, we must subtract the volume of the pickle-shaped intersection of the two caps since we have counted it twice. To do this, I formulate the problem as an integral under a curve by first projecting the sphere and intersecting planes of the cube faces onto the x-y plane. This is done taking the z-axis to run parallel to the edge of the cube. The centre of the circle of the sphere projection is located a distance a left of the y-axis and a distance b below the x-axis. Now we just need to integrate the area under the curve from $x = 0$ to where the curve intersects the x axis.

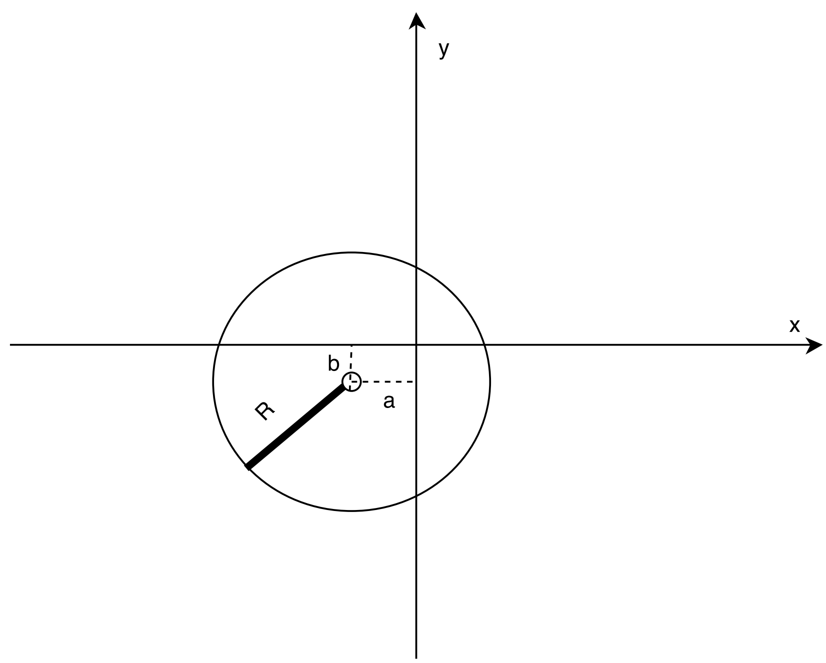

Figure 1: Circular section of sphere at cube edge

To find the equation of this curve, we simply solve the equation of the circle for y:

$$(x + a)^2 + (y + b)^2 = R^2$$

since the circle is located at $(-a, -b)$, so the solution above the x-axis is

$$y = \sqrt{R^2 - (x + a)^2} - b$$

and it intersects the x-axis when $y = 0$ so at

$$x = \sqrt{R^2 - b^2} - a$$

So now the integral to solve for the area at one intersection of our pickle is

$$\int_0^{\sqrt{R^2-b^2}-a} \left[\sqrt{R^2 - (x+a)^2} - b\right] dx$$

The second term is trivial and for the first term we make the substitution

$$\begin{aligned} (x + a) &= R \sin\theta \\ \Rightarrow dx &= R \cos\theta d\theta \end{aligned}$$

and the limits change to

$$\left[0, \sqrt{R^2 - b^2} - a\right] \rightarrow \left[\sin^{-1}\left(\frac{q}{R}\right), \sin^{-1}\left(\frac{\sqrt{R^2 - b^2}}{R}\right)\right]$$

So the integral of the first term goes as

$$\begin{aligned} &R^2 \int_{\sin^{-1}\left(\frac{q}{R}\right)}^{\sin^{-1}\left(\frac{\sqrt{R^2-b^2}}{R}\right)} \sqrt{1 - \sin^2\theta} \cos\theta d\theta \\ =&R^2 \int_{\sin^{-1}\left(\frac{q}{R}\right)}^{\sin^{-1}\left(\frac{\sqrt{R^2-b^2}}{R}\right)} \cos^2\theta d\theta \\ =&\frac{R^2}{2} \int_{\sin^{-1}\left(\frac{q}{R}\right)}^{\sin^{-1}\left(\frac{\sqrt{R^2-b^2}}{R}\right)} (1 + \cos 2\theta)\, d\theta \\ =&\frac{R^2}{2} (\theta + \sin\theta\cos\theta)\Big|_{\sin^{-1}\left(\frac{q}{R}\right)}^{\sin^{-1}\left(\frac{\sqrt{R^2-b^2}}{R}\right)} \end{aligned}$$

Now $\cos\sin^{-1}(x) = \sqrt{1 - x^2}$ so after evaluating the integral at the limits and also including the integral of the second term b above, we have for the area

$$\frac{1}{2}\left[R^2 \sin^{-1}\frac{\sqrt{R^2 - b^2}}{R} - R^2 \sin^{-1}\frac{a}{R} + R\sqrt{R^2 - b^2}\sqrt{1 - \frac{R^2 - b^2}{R^2}} - aR\sqrt{1 - \frac{a^2}{R^2}}\right] - b\sqrt{R^2 - b^2} - ab$$

and after some simplifying

$$\frac{1}{2}\left[R^2 \sin^{-1}\frac{\sqrt{R^2 - b^2}}{R} - R^2 \sin^{-1}\frac{a}{R} - b\sqrt{R^2 - b^2} - a\sqrt{R^2 - a^2} - 2ab\right]$$

Finally, we have to integrate along the length of the pickle. To do this, we integrate along the z-axis, summing the contributions of each intersection of the pickle. This looks like shrinking the radius of the circle in the figure above. The radius ρ of the circle goes as $\sqrt{R^2 - z^2}$ as shown in figure 2. So we replace all instances of R in the last expression with $\rho(z)$ and integrate with respect to z from $z = 0$ up until where ρ reaches the origin (and multiplying by two), which is when $\rho = \sqrt{a^2 + b^2}$. To make the integral a little easier, R is also factored out and all lengths are given in terms of R.

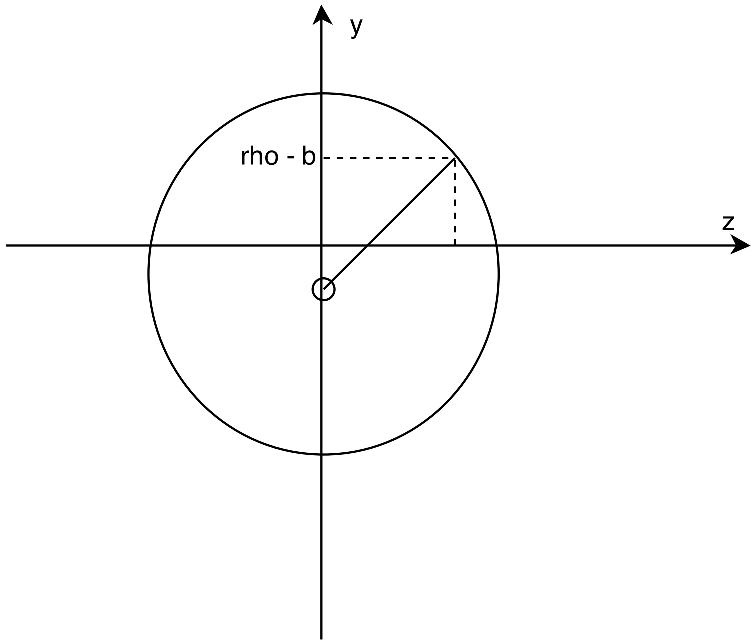

Figure 2: Finding the dependence of ρ on z

$$\int_0^{\sqrt{R^2-a^2-b^2}} \left[\rho^2(z)\sin^{-1}\frac{\sqrt{\rho^2(z)-b^2}}{\rho(z)} - \rho^2(z)\sin^{-1}\frac{a}{\rho(z)} - b\sqrt{\rho^2(z)-b^2} - a\sqrt{\rho^2(z)-a^2} - 2ab\right] dz$$

$$\int_0^{\sqrt{R^2-a^2-b^2}} \left[\left(R^2-z^2\right)\sin^{-1}\frac{\sqrt{R^2-z^2-b^2}}{\sqrt{R^2-z^2}} - \left(R^2-z^2\right)\sin^{-1}\frac{a}{\sqrt{R^2-z^2}} - b\sqrt{R^2-z^2-b^2} - a\sqrt{R^2-z^2-a^2} - 2ab\right] dz$$

To simplify the integral, a, b, and z are replaced with $\alpha = \frac{a}{R}$, $\beta = \frac{b}{R}$, and $\zeta = \frac{z}{R}$ respectively.

$$R^3\int_0^{\sqrt{1-\alpha^2-\beta^2}} \left[\left(1-\zeta^2\right)\sin^{-1}\frac{\sqrt{1-\zeta^2-\beta^2}}{\sqrt{1-\zeta^2}} - \left(1-\zeta^2\right)\sin^{-1}\frac{\alpha}{\sqrt{1-\zeta^2}} - \beta\sqrt{1-\zeta^2-\beta^2} - \alpha\sqrt{1-\zeta^2-\alpha^2} - 2\alpha\beta\right] d\zeta$$

Now integrate this term by term. The square root terms are done the same way as the square root term above and the inverse sine terms will be integrated by parts.