## 11.G.2. Diffusion Coefficient

Since $\hat{C}^-$ is a linear operator [see (11.106)], (11.194) implies $\Delta_x$ is linear in $p_x$. In order to have a finite contribution to the integral in (11.191), we must have

$$\Delta_x(\mathbf{p}) = p_x\, g(p^2)$$

where $g$ is some function to be determined.

Expanding $g$ in terms of the Sonine polynomials, we set

$$\Delta_x(\mathbf{p}) = p_x \sum_{l=0}^{\infty} d_l\, S_q^l\left(\beta \frac{p^2}{2m}\right) \tag{11.202}$$

where the argument of $S_q^l$ was chosen such that the orthogonality relations (11.201) takes the form

$$\langle S_q^l \mid S_q^{l'} \rangle_q = \frac{\beta}{m} \int_0^\infty d\,p\, p\, e^{-\beta p^2/2m} \left(\beta \frac{p^2}{2m}\right)^q S_q^l\left(\beta \frac{p^2}{2m}\right) S_q^{l'}\left(\beta \frac{p^2}{2m}\right) \tag{11.202a}$$
$$= \delta_{l\,l'} \frac{\Gamma(q+l+1)}{l!}$$

Using the following *Mathematica* code

$$\left(\int_0^\pi \mathtt{Sin}[\theta]^3\, d\theta\right) \int_0^{2\pi} \mathtt{Cos}[\phi]^2\, d\phi$$

$$\frac{4\pi}{3}$$

we get, for an arbitrary function $h(p)$,

$$\int d\,\mathbf{p}\; e^{-\beta p^2/2m}\, p_x^2\, h(p) = \int_0^\pi \sin\theta\, d\,\theta \int_0^{2\pi} d\,\phi\, (p \sin\theta \cos\phi)^2 \int_0^\infty d\,p\; p^2\, h(p)$$
$$= \frac{4\pi}{3} \int_0^\infty d\,p\; e^{-\beta p^2/2m}\, p^4\, h(p)$$

(11.202b)

Putting (11.202) into (11.191) gives

$$D = -\frac{1}{m^2}\left(\frac{\beta}{2\pi m}\right)^{3/2} \sum_{l=0}^{\infty} d_l \int d\,\mathbf{p}\; e^{-\beta p^2/2m}\, p_x^2\, S_q^l\left(\beta \frac{p^2}{2m}\right)$$
$$= -\frac{1}{m^2}\left(\frac{\beta}{2\pi m}\right)^{3/2} \frac{4\pi}{3} \sum_{l=0}^{\infty} d_l \int_0^\infty d\,p\; e^{-\beta p^2/2m}\, p^4\, S_q^l\left(\beta \frac{p^2}{2m}\right) \tag{11.202c}$$

Since

$$S_q^0\left(\beta \frac{p^2}{2m}\right) = 1 \qquad [\text{ see (11.199) }]$$

the $p$-integral in (11.202c) is proportional to (11.202a) for $l' = 0$ if we set

$$p^{1+2q} = p^4 \qquad \to \qquad q = \frac{3}{2}$$

In which case, (11.202a) simplifies to

$$\langle S_{3/2}^l \mid S_{3/2}^{l'} \rangle_{3/2} = \frac{\beta}{m}\left(\frac{\beta}{2m}\right)^{3/2} \int_0^\infty d\,p\; e^{-\beta p^2/2m}\, p^4\, S_{3/2}^l\left(\beta \frac{p^2}{2m}\right) S_{3/2}^{l'}\left(\beta \frac{p^2}{2m}\right)$$

$$= \frac{3\beta}{4\pi m}\left(\frac{\beta}{2m}\right)^{3/2} \int d\boldsymbol{p}\; e^{-\beta p^2/2m}\, p_x^2\, S_{3/2}^{l}\left(\beta \frac{p^2}{2m}\right) S_{3/2}^{l'}\left(\beta \frac{p^2}{2m}\right)$$
$$= \delta_{l\,l'} \frac{\Gamma\left(l+\frac{5}{2}\right)}{l!}$$

(11.202d)

Setting $l' = 0$ gives

$$\left\langle S_{3/2}^{l} \mid 1 \right\rangle_{3/2} = \frac{\beta}{m}\left(\frac{\beta}{2m}\right)^{3/2} \int_0^\infty d\,p\; e^{-\beta p^2/2m}\; p^4\, S_{3/2}^{l}\left(\beta \frac{p^2}{2m}\right)$$
$$= \delta_{l\,0}\, \Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}\; \delta_{l\,0} \qquad (11.202e)$$

where $\Gamma\left(\frac{5}{2}\right)$ was evaluated using either (11.198) or the following *Mathematica* code

```
Gamma[5/2]
```

$$\frac{3\sqrt{\pi}}{4}$$

Putting (11.202e) into (11.202c) gives

$$D = -\frac{1}{m^2}\left(\frac{\beta}{2\pi m}\right)^{3/2} \frac{4\pi}{3} \sum_{l=0}^{\infty} d_l\, \frac{3}{4}\sqrt{\pi}\; \delta_{l\,0}\, \frac{m}{\beta}\left(\frac{2m}{\beta}\right)^{3/2}$$
$$= -\frac{1}{m\beta}\, d_0$$

(11.203)

In order to calculate $d_0$, we put (11.202) into (11.194) and get

$$\hat{C}^-\, \Delta_x = \sum_{l=0}^{\infty} d_l\, \hat{C}^-\left[p_x\, S_{3/2}^{l}\left(\beta \frac{p^2}{2m}\right)\right] = p_x$$

(11.204a)

From (11.202d), we have

$$\frac{3\beta}{4\pi m}\left(\frac{\beta}{2m}\right)^{3/2} \int d\boldsymbol{p}\; e^{-\beta p^2/2m}\, p_x^2\, S_{3/2}^{l'}\left(\beta \frac{p^2}{2m}\right) = \frac{3}{4}\sqrt{\pi}\; \delta_{l'\,0} \qquad (11.204b)$$

Therefore, $\left(\frac{\beta}{2\pi m}\right)^{3/2} \int d\boldsymbol{p}\; e^{-\beta p^2/2m}\, p_x\, S_{3/2}^{l'}\left(\beta \frac{p^2}{2m}\right) \times (11.204\,a)$ gives

$$\sum_{l=0}^{\infty} D_{l'\,l}\, d_l = \frac{m}{\beta}\, \delta_{l'\,0}$$

(11.204)

where

$$D_{l'\,l} = \left(\frac{\beta}{2\pi m}\right)^{3/2} \int d\boldsymbol{p}\; e^{-\beta p^2/2m}\, p_x\, S_{3/2}^{l'}\left(\beta \frac{p^2}{2m}\right)\, \hat{C}^-\left[p_x\, S_{3/2}^{l}\left(\beta \frac{p^2}{2m}\right)\right] \qquad (11.205)$$

In matrix form, (11.204) becomes

$$\mathbb{D}\,\mathbb{d} = \begin{pmatrix} D_{00} & D_{01} & D_{02} & \cdots \\ D_{10} & D_{11} & D_{12} & \cdots \\ D_{20} & D_{21} & D_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} d_0 \\ d_1 \\ d_2 \\ \vdots \end{pmatrix} = \frac{m}{\beta} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

(11.205a)

(11.204) can be solved by truncating the sum at $l = \nu$ to give

$$\sum_{l=0}^{\nu} D_{l' l}^{(\nu)} d_l^{(\nu)} = \frac{m}{\beta} \delta_{l' 0} \qquad l' = 0, 1, \ldots, \nu$$

(11.206)

The corresponding matrix form is the $(\nu + 1)$-dimensional version of (11.205a)

$$\mathbb{D}^{(\nu)} \mathbb{d}^{(\nu)} = \frac{m}{\beta} \mathbb{i}^{(\nu)}$$

(11.206a)

$$\rightarrow \qquad \mathbb{d}^{(\nu)} = \frac{m}{\beta} \left[ \mathbb{D}^{(\nu)} \right]^{-1} \mathbb{i}^{(\nu)}$$

$$\therefore \qquad d_0^{(\nu)} = \frac{m}{\beta} \left[ \mathbb{D}^{(\nu)} \right]_{00}^{-1}$$

(11.207)

(11.203) thus becomes

$$D = -\frac{1}{\beta^2} \lim_{\nu \to \infty} \left[ \mathbb{D}^{(\nu)} \right]_{00}^{-1} \qquad (11.208)$$

For the lowest order approximation, $\nu = 0$, we have

$$\mathbb{D}^{(0)} = D_{00}$$

where, from (11.205),

$$D_{00} = \left( \frac{\beta}{2\pi m} \right)^{3/2} \int d\boldsymbol{p}\, e^{-\beta p^2/2m} p_x S_{3/2}^0 \left( \beta \frac{p^2}{2m} \right) \hat{C}^- \left[ p_x S_{3/2}^0 \left( \beta \frac{p^2}{2m} \right) \right]$$

$$= \left( \frac{\beta}{2\pi m} \right)^{3/2} \int d\boldsymbol{p}\, e^{-\beta p^2/2m} p_x \hat{C}^- p_x \qquad \text{[ (11.199) used. ]}$$

$$= \left\langle p_x, \hat{C}^- p_x \right\rangle \qquad \text{[ (11.98) used. ]}$$

$$= \left\langle p_x \hat{C}^- p_x \right\rangle_\beta \qquad \text{[ thermal average ]}$$

(11.209a)

Hence,

$$D = -\frac{1}{\beta^2 D_{00}}$$

(11.209)

For $\nu = 1$, we have

$$\mathbb{D}^{(1)} = \begin{pmatrix} D_{00} & D_{01} \\ D_{10} & D_{11} \end{pmatrix}$$

$$\rightarrow \qquad \left[ \mathbb{D}^{(1)} \right]^{-1} = \frac{1}{D_{00} D_{11} - D_{01} D_{10}} \begin{pmatrix} D_{11} & -D_{01} \\ -D_{10} & D_{00} \end{pmatrix}$$

$$\therefore \qquad D = -\frac{1}{\beta^2}\frac{D_{11}}{D_{00}D_{11}-D_{01}D_{10}}$$
$$= -\frac{1}{\beta^2}\frac{1}{D_{00}}\frac{D_{00}D_{11}}{D_{00}D_{11}-D_{01}D_{10}}$$
$$= -\frac{1}{\beta^2}\frac{1}{D_{00}}\left(1-\frac{D_{01}D_{10}}{D_{00}D_{11}}\right)^{-1} \tag{11.210}$$

Putting (11.106) into (11.209a) gives

$$D_{00} = 2\left(\frac{\beta}{2\pi m}\right)^{3/2}\int d\boldsymbol{p}\; e^{-\beta p^2/2m}\int d\boldsymbol{p}'\, p_x\int d\Omega\; v\,\sigma(\Theta,v)\; f^{0}{}'\left(p_{fx}-p_x\right)$$
$$= n_0\left(\frac{\beta}{2\pi m}\right)^{3}\int d\boldsymbol{p}\int d\boldsymbol{p}'\; e^{-\beta\left(p^2+p'^2\right)/2m}\,p_x\int d\Omega\; v\,\sigma(\Theta,v)\left(p_{fx}-p_x\right) \tag{11.210a}$$

where (11.87) was used and we have replaced the impact parameter $b$ with the scattering angle $\Theta$ in the CM frame.

Converting to the CM coordinates, we have [see §11.C.1.1]

$$d\boldsymbol{p}\,d\boldsymbol{p}' = (M\mu)^3\, d\boldsymbol{V}_{\rm CM}\; d\boldsymbol{v} = m^6\, d\boldsymbol{V}_{\rm CM}\; d\boldsymbol{v}$$
$$\frac{1}{2m}\left(p^2+p'^2\right) = \frac{1}{2}M V_{\rm CM}^2+\frac{1}{2}\mu v^2 = m V_{\rm CM}^2+\frac{1}{4}m v^2$$
$$\boldsymbol{p} = m\boldsymbol{V}_{\rm CM}-\mu\boldsymbol{v} = m\boldsymbol{V}_{\rm CM}-\frac{1}{2}m\boldsymbol{v} \qquad \boldsymbol{p}_f = m\boldsymbol{V}_{\rm CM}-\frac{1}{2}m\boldsymbol{v}_f$$
$$\boldsymbol{p}' = m\boldsymbol{V}_{\rm CM}+\mu\boldsymbol{v} = m\boldsymbol{V}_{\rm CM}+\frac{1}{2}m\boldsymbol{v} \qquad \boldsymbol{p}_f' = m\boldsymbol{V}_{\rm CM}+\frac{1}{2}m\boldsymbol{v}_f$$
$$\boldsymbol{v}_f\cdot\boldsymbol{v} = v^2\cos\Theta$$

Note: velocities are used partly to conform with Reichl's narrative in Ex.11.4, and partly because there is no good symbol for the relative momentum $\mu\boldsymbol{v}$.

(11.210a) becomes

$$D_{00} = n_0\left(\frac{\beta}{2\pi m}\right)^{3} m^8\int d\boldsymbol{V}_{\rm CM}\int d\boldsymbol{v}\; e^{-\beta m\left(V_{\rm CM}^2+\frac{1}{4}v^2\right)}\left(V_{{\rm CM}\,x}-\frac{1}{2}v_x\right)\int d\Omega\; v\,\sigma(\Theta,v)\,\frac{1}{2}\left(-v_{fx}+v_x\right)$$
$$= \frac{n_0}{32}\left(\frac{\beta}{\pi m}\right)^{3/2} m^5\int d\boldsymbol{v}\; e^{-\beta m v^2/4}\; v_x\,v\int d\Omega\;\sigma(\Theta,v)\left(v_{fx}-v_x\right) \tag{11.210b}$$

where

$$\int d\boldsymbol{V}_{\rm CM}\, e^{-\beta m V_{\rm CM}^2}\left(V_{{\rm CM}\,x}-\frac{1}{2}v_x\right) = \int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta\, d\theta\int_0^{\infty}dV\, e^{-\beta m V^2}\; V^2\left(V\cos\phi\sin\theta-\frac{1}{2}v_x\right)$$
$$= -\frac{1}{2}\left(\frac{\pi}{m\beta}\right)^{3/2} v_x$$

was evaluated using the following code.

```
Assuming[β > 0 && m > 0, ∫_0^{2π} ∫_0^π ∫_0^∞ Sin[θ] (V Cos[ϕ] Sin[θ] - 1/2 vx) V^2 e^{-β m V^2} dV dθ dϕ]
```

$$-\frac{\pi^{3/2}\,v_x}{2\,(m\,\beta)^{3/2}}$$

Consider now the more general form of the scattering integral

$$\mathcal{I} = \int d\Omega\ \sigma(\Theta, v) \left( \mathbf{v}_f - \mathbf{v} \right)$$
$$= \int_0^{2\pi} d\alpha \int_{-1}^{1} d\cos\Theta\ \sigma(\Theta, v) \left( \mathbf{v}_f - \mathbf{v} \right)$$

For a given $\mathbf{p} = \mu\,\mathbf{v}$, $\mathbf{p}_f = \mu\,\mathbf{v}_f$ lies on the scattering cone shown in Fig.a. Since $\sigma(\Theta, v)$ is independent of the azimuth angle $\alpha$, the component of $(\mathbf{v}_f - \mathbf{v})$ perpendicular to $\mathbf{v}$ cancels out in the $\alpha$ integral so that

$$\mathcal{I} = -2\pi \int_{-1}^{1} d\cos\Theta\ \sigma(\Theta, v)\, w_{//}\, \hat{\mathbf{v}}$$

(11.210c)

where $w_{//}$ is the magnitude of the component of $\mathbf{w} = \mathbf{v}_f - \mathbf{v}$ (anti-) parallel to $\mathbf{v}$. Using the cross-sectional view of the cone shown in Fig.b., we have, since $v = v_f$ for elastic scattering,

$$w = |\ \mathbf{v}_f - \mathbf{v}\ | = 2\,v \sin\frac{\Theta}{2}$$
$$w_{//} = \sqrt{\left(2\,v \sin\frac{\Theta}{2}\right)^2 - (v \sin\Theta)^2} = v\sqrt{4\sin^2\frac{\Theta}{2} - 4\sin^2\frac{\Theta}{2}\cos^2\frac{\Theta}{2}}$$
$$= 2\,v \sin^2\frac{\Theta}{2}$$

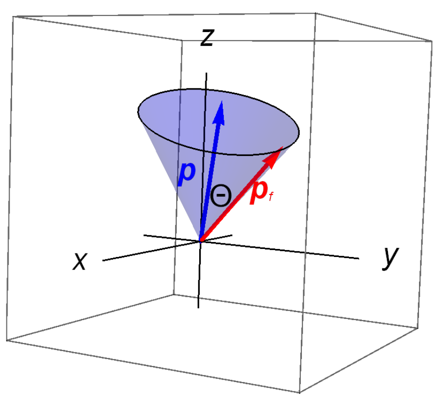


Fig.a

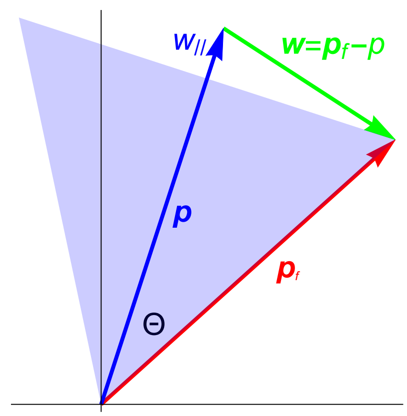


Fig.b

Hence, (11.210c) becomes

$$\mathcal{I} = -4\pi \int_{-1}^{1} d\cos\Theta\ \sigma(\Theta, v) \sin^2\frac{\Theta}{2}\, \mathbf{v}$$

and (11.210b) becomes

$$D_{00} = -\frac{n_0}{8}\pi \left(\frac{\beta}{\pi m}\right)^{3/2} m^5 \int d\mathbf{v}\ e^{-\beta m v^2/4}\, v_x^2\, v \int_{-1}^{1} d\cos\Theta\ \sigma(\Theta, v) \sin^2\frac{\Theta}{2} \qquad (11.210d)$$

Ex.11.1 of §11.1.2 studied the case of a point particle of mass $m$ scattering off an immobile sphere of radius $R$. The results there are readily converted to the present case of scattering between two hard spheres of mass $m$ and radius $R$ with the following substitutions

$$m \to \mu = \frac{m}{2} \qquad R \to 2R \qquad \sigma(b, v) \to \sigma_{CM}(\Theta, v)$$

Hence, for (1) in Ex.11.1,

$$\sigma(b, v) = \frac{R^2}{4} \qquad \rightarrow \qquad \sigma_{CM}(\Theta, v) = \frac{(2R)^2}{4} = R^2$$

(11.210d) thus becomes

$$D_{00} = -\frac{n_0}{8}\pi\left(\frac{\beta}{\pi m}\right)^{3/2} m^5 R^2 \int d\mathbf{v}\, e^{-\beta m v^2/4}\, v_x^2\, v \int_{-1}^{1} d\cos\Theta\, \sin^2\frac{\Theta}{2}$$
$$= -\frac{n_0}{8}\pi\left(\frac{\beta}{\pi m}\right)^{3/2} m^5 R^2 \int d\mathbf{v}\, e^{-\beta m v^2/4}\, v_x^2\, v$$

where

```
∫_0^π Sin[Θ] Sin[Θ/2]^2 dΘ
```

1

In spherical coordinates,

$$D_{00} = -\frac{n_0}{8}\pi\left(\frac{\beta}{\pi m}\right)^{3/2} m^5 R^2 \int_0^{2\pi} d\phi \int_{-1}^{1} d\cos\theta \int_0^{\infty} d v\, e^{-\beta m v^2/4}\, v^5 \sin^2\theta \cos^2\phi$$
$$= -\frac{n_0}{8}\pi\left(\frac{\beta}{\pi m}\right)^{3/2} m^5 R^2 \frac{256\pi}{3 m^3 \beta^3}$$

where

```
Assuming[β > 0 && m > 0, (∫_0^{2π} Cos[ϕ]^2 dϕ) (∫_0^π Sin[θ]^3 dθ) ∫_0^∞ v^5 e^{-β m v^2/4} dv]
```

$$\frac{256\pi}{3\, m^3 \beta^3}$$

Hence,

$$D_{00} = -\frac{32}{3} n_0 R^2 \sqrt{\frac{\pi m}{\beta^3}}$$

(11.210e)

(11.209) then gives

$$D = \frac{3}{32 n_0 R^2}\sqrt{\frac{k_B T}{m\pi}} \qquad (11.211)$$