Numerical solution of the temperature derivative of radial distribution function at constant volume and pressure derivative of the diffusion coefficient related to the Grüneisen parameter, γ_G.

Shreya Singh, Rahul Kumar, Raj Kumar Mishra* and R. Lalneihpuii*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi- 221005, India

*Corresponding authors Email: maneihi.chem@bhu.ac.in, rkmishra.chem@bhu.ac.in

Part 1: Numerical solution of the temperature derivative of radial distribution function at constant volume.

$$g(r) = 1 + \frac{1}{2\pi^2\rho}\int_0^\infty k^2[S(k)-1]\,\frac{\sin(kr)}{kr}\,dk \tag{1}$$

$$\left[\frac{\partial g(r)}{\partial T}\right]_V = \frac{1}{2\pi^2\rho}\int_0^\infty k^2\,\frac{\sin(kr)}{kr}\frac{\partial}{\partial T}[S(k)-1]\,dk \tag{2}$$

$$\left[\frac{\partial g(r)}{\partial T}\right]_V = \frac{1}{2\pi^2\rho}\int_0^\infty k^2\,\frac{\sin(kr)}{kr}\frac{\partial}{\partial T}[S(k)]dk \tag{3}$$

$$\frac{\partial}{\partial T}[S(k)] = \frac{\partial}{\partial T}\left[\frac{1}{1-\rho C(k)}\right] \tag{4}$$

$$\frac{\partial}{\partial T}[S(k)] = -[1-\rho C(k)]^{-2}\frac{\partial}{\partial T}[1-\rho C(k)] \tag{5}$$

$$\frac{\partial}{\partial T}[S(k)] = -[1-\rho C(k)]^{-2}\left[-\rho\frac{\partial}{\partial T}C(k)\right] \tag{6}$$

$$\frac{\partial}{\partial T}[S(k)] = -[1-\rho C(k)]^{-2}\left[-\rho\frac{\partial}{\partial T}\left[\frac{24\eta\epsilon}{k_BT}\right](x^{-3})[\sin\lambda x-\lambda x\cos\lambda x+x\cos x-\sin x]\right] \tag{7}$$

Here $x = k\sigma$

$$\frac{\partial}{\partial T}[S(k)] = -[1-\rho C(k)]^{-2}(-\rho)\left[\left(-\frac{24\eta\epsilon}{k_BT^2}\right)(x^{-3})[\sin\lambda x-\lambda x\cos\lambda x+x\cos x-\sin x]\right] \tag{8}$$

$$\frac{\partial}{\partial T}[S(k)] = -[1-\rho C(k)]^{-2}\rho\left[\frac{24\eta\epsilon}{k_BT^2}(x^{-3})[\sin\lambda x-\lambda x\cos\lambda x+x\cos x-\sin x]\right] \tag{9}$$

$$\left[\frac{\partial g(r)}{\partial T}\right]_V = \frac{1}{2\pi^2\rho}\int_\sigma^{\lambda\sigma} k^2\,\frac{\sin(kr)}{kr}\left[-\frac{24\eta\epsilon}{k_BT^2}\rho[1-\rho C(k)]^{-2}(x^{-3})[\sin\lambda x-\lambda x\cos\lambda x+ x\cos x-\sin x]\right] \tag{10}$$

$$\left[\frac{\partial g(r)}{\partial T}\right]_V = -\frac{1}{2\pi^2 r}\frac{24\eta\epsilon}{k_BT^2}\int_\sigma^{\lambda\sigma}[1-\rho C(k)]^{-2}(x^{-3})\,[\sin\lambda x-\lambda x\cos\lambda x+x\cos x- \sin x]\,k\sin kr\;dk \tag{11}$$

$$\left[\frac{\partial g(r)}{\partial T}\right]_V = -\frac{1}{2\pi^2 r}\frac{24\eta\epsilon}{k_BT^2}\int_\sigma^{\lambda\sigma} S(k)^2\;U(k)\;\;k\sin kr\;\;dk \tag{12}$$

Where $U(k) = (k\sigma)^{-3}[sin(k\sigma\lambda) - k\sigma\lambda cos(k\sigma\lambda) + k\sigma\, cos(k\sigma) - sin(k\sigma)]$

Part 2: Numerical solution of the pressure derivative of the diffusion coefficient related to the Grüneisen parameter, γ_G.

$$D = \frac{k_B T}{\xi} \quad (1)$$

$$\left[\frac{\partial lnD}{\partial P}\right]_T = -\frac{1}{\xi}\left[\frac{\partial \xi^H}{\partial P} + \frac{\partial \xi^S}{\partial P} + \frac{\partial \xi^{SH}}{\partial P}\right]_T \quad (2)$$

$$\xi^H = \frac{8}{3}\rho g(\sigma)\sigma^2(\pi m k_B T)^{\frac{1}{2}} \quad (3)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \frac{8}{3}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\frac{\partial \rho}{\partial P}\ g(r) + \left(\frac{\partial g(r)}{\partial P}\right)_{r=\sigma}\rho\right]_T \quad (4)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \frac{8}{3}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\rho\beta_T g(r) + \left(\frac{\partial g(r)}{\partial P}\right)_T\rho\right]_{r=\sigma} \quad (5)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \xi^H\beta_T + \frac{8}{3}\rho\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\frac{\partial g(r)}{\partial P}\right]_T \quad (6)$$

$$g(r) = 1 + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\ \sin kr\ \ dk \quad (7)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = \frac{\partial}{\partial P}\left[\frac{1}{2\pi^2\rho}\int_0^\infty \frac{k\{S(k)-1\}\sin kr}{r}dk\right] \quad (8)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = \frac{1}{2\pi^2\rho}\frac{\partial}{\partial P}\left(\frac{1}{r}\right)\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2 r}\frac{\partial}{\partial P}\left(\frac{1}{\rho}\right)\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k\frac{\partial S(k)}{\partial P}\sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\frac{\partial \sin kr}{\partial P}dk \quad (9)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = \frac{1}{2\pi^2\rho}\left[-\frac{1}{r^2}\frac{\partial r}{\partial P}\right]\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2 r}\left[-\frac{1}{\rho^2}\frac{\partial \rho}{\partial P}\right]\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k\frac{\partial S(k)}{\partial P}\sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\cos kr\ k\frac{\partial r}{\partial P}dk \quad (10)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = -\frac{1}{2\pi^2\rho r^2}\frac{\partial r}{\partial P}\int_0^\infty k[S(k)-1]\ \sin kr\ dk - \frac{1}{2\pi^2 r\rho^2}\frac{\partial \rho}{\partial P}\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k\frac{\partial S(k)}{\partial P}\sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\cos kr\ k\frac{\partial r}{\partial P}dk \quad (11)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = -\frac{1}{2\pi^2\rho r^2}\left(-\frac{r}{3}\beta_T\right)\int_0^\infty k[S(k)-1]\ \sin kr\ dk - \frac{1}{2\pi^2 r\rho^2}(\rho\beta_T)\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k\frac{\partial S(k)}{\partial P}\sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\cos kr\ k\left(-\frac{r}{3}\beta_T\right)\ dk \quad (12)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = \frac{1}{2\pi^2\rho r}\frac{\beta_T}{3}\int_0^\infty k[S(k)-1]\ \sin kr\ dk - \frac{1}{2\pi^2\rho r}\beta_T\int_0^\infty k[S(k)-1]\ \sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k\frac{\partial S(k)}{\partial P}\sin kr\ dk + \frac{1}{2\pi^2\rho r}\int_0^\infty k[S(k)-1]\cos kr\ k\left(-\frac{r}{3}\beta_T\right)\ dk \quad (13)$$

$$\left[\frac{\partial g(r)}{\partial P}\right]_T = \frac{\beta_T}{3}[g(r)-1] - \beta_T[g(r)-1] + \frac{1}{2\pi^2\rho r}\int_0^\infty kZ'(k)\sin kr\ dk - \frac{\beta_T}{6\pi^2\rho}\int_0^\infty k^2[S(k)-1]\cos kr\ \ dk \quad (14)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \frac{8}{3}\sigma^2\rho\beta_T(\pi m k_B T)^{\frac{1}{2}}\, g(r) + \frac{8}{3}\rho\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\frac{\beta_T}{3}[g(r)-1] - \beta_T[g(r)-1] + \frac{1}{2\pi^2\rho r}\int_0^\infty kZ'(k)\sin kr\, dk - \frac{\beta_T}{6\pi^2\rho}\int_0^\infty k^2[S(k)-1]\cos k\sigma\ dk\right] \quad (15)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \frac{8}{3}\sigma^2\rho\beta_T(\pi m k_B T)^{\frac{1}{2}}\, g(r) - \frac{2}{3}\beta_T[g(r)-1] \times \frac{8}{3}\sigma^2\rho(\pi m k_B T)^{\frac{1}{2}} + \frac{8}{3}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\frac{1}{2\pi^2 r}\int_0^\infty kZ'(k) sinkr\, dk - \frac{\beta_T}{6\pi^2}\int_0^\infty k^2[S(k)-1]\cos k\sigma\ dk\right] \quad (16)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \xi^H\beta_T - \frac{2}{3}\beta_T\left[\frac{8}{3}\sigma^2\rho(\pi m k_B T)^{\frac{1}{2}}\, g(r) - \frac{8}{3}\sigma^2\rho(\pi m k_B T)^{\frac{1}{2}}\right] + \frac{8}{3}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\left[\frac{1}{2\pi^2 r}\int_0^\infty kZ'(k) sinkr\, dk - \frac{\beta_T}{6\pi^2}\int_0^\infty k^2[S(k)-1]\cos k\sigma\ dk\right] \quad (17)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \xi^H\beta_T - \frac{2}{3}\beta_T\left[\xi^H - \frac{8}{3}\sigma^2\rho(\pi m k_B T)^{\frac{1}{2}}\right] + \frac{4}{3\pi^2}\sigma(\pi m k_B T)^{\frac{1}{2}}\int_0^\infty kZ'(k) sinkr\, dk - \frac{4\beta_T}{9\pi^2}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\int_0^\infty k^2[S(k)-1]\cos k\sigma\ dk \quad (18)$$

$$\left[\frac{\partial \xi^H}{\partial P}\right]_T = \xi^H\beta_T - \frac{2}{3}\beta_T\xi^H + \frac{16}{9}\beta_T\sigma^2\rho(\pi m k_B T)^{\frac{1}{2}} + \frac{4}{3\pi^2}\sigma(\pi m k_B T)^{\frac{1}{2}}\int_0^\infty kZ'(k) sinkr\, dk - \frac{4\beta_T}{9\pi^2}\sigma^2(\pi m k_B T)^{\frac{1}{2}}\int_0^\infty k^2[S(k)-1]\cos k\sigma\ dk \quad (19)$$

$$\xi^S = -\frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\tilde{G}(k)dk \quad (20)$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = -\frac{1}{12\pi^2}\frac{\partial\rho}{\partial P}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\tilde{G}(k)dk - \frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\frac{\partial\tilde{G}(k)}{\partial P}dk \quad (21)$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = -\frac{1}{12\pi^2}\rho\beta_T\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\tilde{G}(k)dk - \frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\frac{\partial\tilde{G}(k)}{\partial P}dk \quad (22)$$

$$\tilde{G}(k) = \frac{[S(k)-1]}{\rho} \quad (23)$$

$$\frac{\partial[\tilde{G}(k)]}{\partial P} = \frac{1}{\rho}\left[\frac{\partial}{\partial P}\tilde{S}(k)\right] + [S(k)-1]\frac{\partial}{\partial P}\left(\frac{1}{\rho}\right) \quad (24)$$

$$\frac{\partial[\tilde{G}(k)]}{\partial P} = \frac{1}{\rho}Z'(k) - [S(k)-1]\left(\frac{1}{\rho^2}\right)\frac{\partial\rho}{\partial P} \quad (25)$$

$$\frac{\partial[\tilde{G}(k)]}{\partial P} = \frac{1}{\rho}Z'(k) - \frac{[S(k)-1]\beta_T}{\rho} \quad (26)$$

$$\frac{\partial[\tilde{G}(k)]}{\partial P} = \frac{1}{\rho}Z'(k) - \tilde{G}(k)\beta_T \quad (27)$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = -\frac{1}{12\pi^2}\rho\beta_T\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\tilde{G}(k)dk - \frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}}\int_0^\infty k^3\,\phi^{SW}(k)\left[\frac{1}{\rho}Z'(k) - \frac{[S(k)-1]\beta_T}{\rho}\right]dk \quad (28)$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = \xi^s \beta_T - \frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}} \int_0^\infty k^3\, \phi^{SW}\,(k)\,\frac{Z'(k)}{\rho}\,dk - \left[-\frac{\rho}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}} \int_0^\infty k^3\, \phi^{SW}\,(k)\tilde{G}(k)\beta_T dk\right] \tag{29}$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = \xi^s \beta_T - \xi^s \beta_T - \frac{1}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}} \int_0^\infty k^3\, \phi^{SW}\,(k) Z'(k) dk \tag{30}$$

$$\left[\frac{\partial \xi^S}{\partial P}\right]_T = -\frac{1}{12\pi^2}\left(\frac{\pi m}{k_B T}\right)^{\frac{1}{2}} \int_0^\infty k^3\, \phi^{SW}\,(k) Z'(k) dk \tag{31}$$

$$\xi^{SH} = -\frac{1}{3}\rho g(\sigma)\left(\frac{m}{\pi k_B T}\right)^{\frac{1}{2}} \int_0^\infty [k\sigma \cos k\sigma - \sin k\sigma]\phi^{SW}\,(k)\,dk \tag{32}$$

$$\left[\frac{\partial \xi^{SH}}{\partial P}\right]_T = -\frac{1}{3}\rho g(\sigma)\left(\frac{m}{\pi k_B T}\right)^{\frac{1}{2}} \frac{\partial \rho}{\partial P}\int_0^\infty [k\sigma \cos k\sigma - \sin k\sigma]\,\phi^{SW}\,(k) dk + \left(-\frac{1}{3}\right)\rho\,\frac{\partial g(\sigma)}{\partial P}\left(\frac{m}{\pi k_B T}\right)^{\frac{1}{2}} \int_0^\infty [k\sigma \cos k\sigma - \sin k\sigma]\phi^{SW}\,(k)\,dk \tag{33}$$

$$\left[\frac{\partial \xi^{SH}}{\partial P}\right]_T = -\frac{1}{3} g(\sigma)\left(\frac{m}{\pi k_B T}\right)^{\frac{1}{2}} \rho\beta_T \int_0^\infty [k\sigma \cos k\sigma - \sin k\sigma]\,\phi^{SW}\,(k) dk - \left(-\frac{1}{3}\right)\rho\left(\frac{m}{\pi k_B T}\right)^{\frac{1}{2}} \int_0^\infty [k\sigma \cos k\sigma - \sin k\sigma]\phi^{SW}\;\,dk\left[-\frac{2}{3}\beta_T[g(\sigma)-1] + \frac{1}{2\pi^2\rho\sigma}\int_0^\infty k\,Z'(k)\sin kr\,dk - \frac{\beta_T}{6\pi^2\rho}\int_0^\infty k^2[S(k)-1]\cos k\sigma\;\,dk\right] \tag{34}$$

$$\left[\frac{\partial \xi^{SH}}{\partial P}\right]_T = \xi^{SH}\beta_T + \frac{\xi^{SH}}{g(\sigma)}\left[-\frac{2}{3}\beta_T[g(\sigma)-1] + \frac{1}{2\pi^2\rho\sigma}\int_0^\infty kZ'(k)\sin k\sigma\,dk - \frac{\beta_T}{6\pi^2\rho}\int_0^\infty k^2[S(k)-1]\cos k\sigma\;\,dk\right] \tag{35}$$

$$\frac{\partial S(k)}{\partial P} = -\frac{1}{[1-\rho\tilde{C}(k)]^2}(-1)\frac{\partial}{\partial P}\left[\rho\tilde{C}(k)\right]; \quad S(k) = \frac{1}{1-\rho\tilde{C}(k)} \tag{36}$$

$$\frac{\partial S(k)}{\partial P} = [S(k)]^2\frac{\partial}{\partial P}\left[\rho\tilde{C}(k)\right] \tag{37}$$

$$\rho\tilde{C}(k) = -\frac{24\eta}{(k\sigma)^6}\Big[\alpha(k\sigma)^3(\sin k\sigma - k\sigma\cos k\sigma) + \beta(k\sigma)^2\{2k\sigma\sin k\sigma - (k^2\sigma^2 - 2)\cos k\sigma - 2\} + \gamma\{(4k^3\sigma^3 - 24k\sigma)\sin k\sigma - (k^4\sigma^4 - 12k^2\sigma^2 + 24)\cos k\sigma + 24\} - \left(\frac{\varepsilon}{k_B T}\right)(k\sigma)^3(\sin\lambda k\sigma - \lambda k\sigma\cos\lambda k\sigma + k\sigma\cos k\sigma - \sin k\sigma)\Big] \tag{38}$$

$$\alpha = \frac{(1+2\eta)^2}{(1-\eta)^4} \tag{39}$$

$$\beta = -\frac{6\eta\left(1+\frac{\eta}{2}\right)^2}{(1-\eta)^4} \tag{40}$$

$$\gamma = \frac{\eta(1+2\eta)^2}{2(1-\eta)^4} \tag{41}$$

$$\rho\tilde{C}(k) = -\frac{24\eta}{(k\sigma)^6}\left[\alpha P' + \beta Q' + \gamma R' - \frac{\varepsilon S'}{k_B T}\right] \tag{42}$$

$$P' = (k\sigma)^3(\sin k\sigma - k\sigma\cos k\sigma) \tag{43}$$

$$Q' = (k\sigma)^2\{2k\sigma \sin k\sigma - (k^2\sigma^2 - 2)\cos k\sigma - 2\} \tag{44}$$

$$R' = \{(4k^3\sigma^3 - 24k\sigma)\sin k\sigma - (k^4\sigma^4 - 12k^2\sigma^2 + 24)\cos k\sigma + 24\} \tag{45}$$

$$S' = (k\sigma)^3(\sin \lambda k\sigma - \lambda k\sigma \cos \lambda k\sigma + k\sigma \cos k\sigma - \sin k\sigma) \tag{46}$$

$$\frac{\partial[\rho\tilde{C}(k)]}{\partial P} = -\frac{24}{(k\sigma)^6}\left[\alpha P' + \beta Q' + \gamma R' - \frac{\varepsilon S'}{k_B T}\right]\frac{\partial \eta}{\partial P} + \left(-\frac{24\eta}{(k\sigma)^6}\right)\left[P'\frac{\partial \alpha}{\partial P} + Q'\frac{\partial \beta}{\partial P} + R'\frac{\partial \gamma}{\partial P} - \frac{\partial}{\partial P}\left(\frac{\varepsilon S'}{k_B T}\right)\right] \tag{47}$$

$$\eta = \frac{\pi\rho\sigma^3}{6} \tag{48}$$

$$\frac{\partial \eta}{\partial P} = \frac{\pi\sigma^3}{6}\frac{\partial \rho}{\partial P} \tag{49}$$

$$\frac{\partial \eta}{\partial P} = \frac{\pi\rho\beta_T\sigma^3}{6} \tag{50}$$

$$\frac{\partial \eta}{\partial P} = \eta\beta_T \tag{51}$$

$$\frac{\partial \alpha}{\partial P} = \frac{\partial}{\partial P}\left[\frac{(1+2\eta)^2}{(1-\eta)^4}\right] \tag{52}$$

$$\frac{\partial \alpha}{\partial P} = 4\alpha\eta\beta_T\left[\frac{2+\eta}{(1+2\eta)(1-\eta)}\right] \tag{53}$$

$$\frac{\partial \beta}{\partial P} = -6\frac{\partial}{\partial P}\left[\frac{\eta\left(1+\frac{\eta}{2}\right)^2}{(1-\eta)^4}\right] \tag{54}$$

$$\frac{\partial \beta}{\partial P} = \beta\beta_T\left[\frac{\eta^2+9\eta+2}{(2+\eta)(1-\eta)}\right] \tag{55}$$

$$\frac{\partial \gamma}{\partial P} = \frac{\partial}{\partial P}\left[\frac{\eta(1+2\eta)^2}{2(1-\eta)^4}\right] \tag{56}$$

$$\frac{\partial \gamma}{\partial P} = \gamma\beta_T\left[\frac{2\eta^2+9\eta+1}{(1+2\eta)(1-\eta)}\right]$$

$$\frac{\partial[\rho\tilde{C}(k)]}{\partial P} = -\frac{24\eta\beta_T}{(k\sigma)^6}\left[\alpha P' + \beta Q' + \gamma R' - \frac{\varepsilon S'}{k_B T}\right] - \frac{24\eta\beta_T}{(k\sigma)^6}\left[P' 4\alpha\eta\left(\frac{2+\eta}{(1+2\eta)(1-\eta)}\right) + Q'\beta\left(\frac{\eta^2+9\eta+2}{(2+\eta)(1-\eta)}\right) + R'\gamma\left(\frac{2\eta^2+9\eta+1}{(1+2\eta)(1-\eta)}\right)\right] \tag{57}$$

$$\frac{\partial S(k)}{\partial P} = \frac{\beta_T[S(k)][S(k)-1]}{\alpha P' + \beta Q' + \gamma R' - \frac{\varepsilon S'}{k_B T}}\left[\alpha P' + \beta Q' + \gamma R' - \frac{\varepsilon S'}{k_B T} + P' 4\alpha\eta\left(\frac{2+\eta}{(1+2\eta)(1-\eta)}\right) + Q'\beta\left(\frac{\eta^2+9\eta+2}{(2+\eta)(1-\eta)}\right) + R'\gamma\left(\frac{2\eta^2+9\eta+1}{(1+2\eta)(1-\eta)}\right)\right] \tag{58}$$

$$\frac{\partial S(k)}{\partial P} = Z'(k) \tag{59}$$

$$\phi^{SW}(k) = \frac{4\pi\varepsilon}{k^3}[\lambda k\sigma \cos \lambda k\sigma - \sin \lambda k\sigma - k\sigma \cos k\sigma + \sin k\sigma] \tag{60}$$

Abbreviations of symbols used in the manuscript:

D: Diffusion Coefficient.

k_B: Boltzmann Constant.

T: Working Temperature.

P: Pressure.

ξ: Friction Coefficient.

ξ^H: Friction coefficient of the hard part of the potential function.

ξ^S: Friction coefficient of the soft part of the potential function.

ξ^{SH}: Friction coefficient of the soft-hard part of the potential function.

ρ: Number density.

$g(\sigma)$: Radial distribution function (at $r = \sigma$).

$g(r)$: Radial distribution function.

σ: Hard sphere diameter.

m: Atomic mass of liquid metals.

β_T: Isothermal compressibility factor.

r: Position of atoms with respect to reference atom.

$S(k)$: Structure factor.

k: Momentum vector.

ε: Depth of square well.

λ: Related to width of square well potential

η: Packing fraction.

$\tilde{C}(k)$: Total direct correlation function in momentum space.