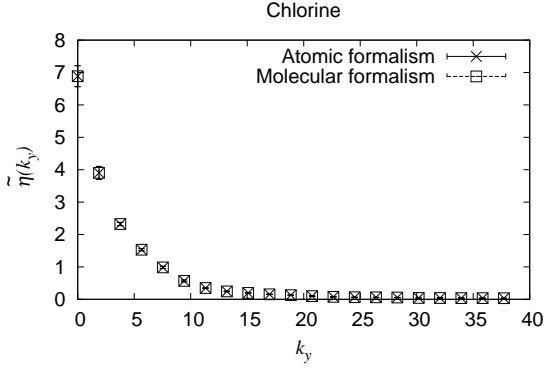


TABLE II: Zero frequency, zero wave-vector shear viscosity and fitted parameter values for monatomic and diatomic systems

		WCA	WCA	WCA	LJ	LJ	Chlorine
State Point	$\rho_a$	0.375	0.480	0.840	0.840	0.840	1.088
	$T$	0.765	0.765	1.000	0.765	1.0	0.97
System size	$N_a$	2048					1728
	$\eta_0$	0.265(0.273[20])	0.392	2.290	2.810	2.650	6.889
2-term Gaussian, $A_2 = 1 - A_1$ Eq. (27)	$A$	0.189(0.440[20])	0.309	0.155	0.093	0.107	0.407
	$\sigma_1$	12.48(4.750[20])	6.916	8.122	10.04	9.088	5.377
	$\sigma_2$	2.116(1.376[20])	1.835	2.592	2.778	2.759	1.236
	$s_r$	0.007(0.005[20])	0.013	0.044	0.021	0.027	0.082
2-term Gaussian Eq. (27)	$A_1$	0.792	0.687	0.874	0.907	0.892	0.592
	$A_2$	0.174	0.254	0.155	0.094	0.106	0.407
	$\sigma_1$	2.245	2.113	2.592	2.776	2.765	1.237
	$\sigma_2$	13.36	7.745	8.124	10.02	9.127	5.377
	$s_r$	0.007	0.011	0.035	0.022	0.031	0.081
4-term Gaussian Eq. (27)	$A_1$	0.432	0.566	0.778	0.689	0.868	0.398
	$A_2$	0.394	0.248	0.118	0.190	0.047	0.538
	$A_3$	0.120	0.138	0.088	0.114	0.089	0.055
	$A_4$	0.056	0.047	0.017	0.017	0.020	0.008
	$\sigma_1$	3.228	2.826	2.950	2.709	2.814	4.355
	$\sigma_2$	1.261	0.821	0.651	2.709	0.145	1.155
	$\sigma_3$	8.165	6.973	8.496	7.037	7.628	10.46
	$\sigma_4$	15.19	14.74	23.66	24.94	19.99	37.56
	$s_r$	0.008	0.002	0.012	0.014	0.024	0.018
	Lorentzian-type Eq. (28)	$\alpha$	0.198(0.180[20])	0.170	0.062	0.041	0.043
$\beta$		1.562(1.662[20])	1.715	2.326	2.602	2.572	1.667
$s_r$		0.002(0.005[20])	0.005	0.042	0.018	0.042	0.016

FIG. 1:  $\tilde{\eta}(k_y)$  versus  $k_y$  for chlorine calculated using atomic and molecular formalisms ( $\rho_a = 1.088$ ,  $T = 0.97$ ,  $N_a = 1728$ ).

statistical uncertainty in both atomic and molecular formalisms.

It has been shown previously that numerous one parameter functions failed to capture the behaviour of the reciprocal space kernel data [20]. We therefore present the best fits with two or more fitting parameters. We have identified two functional forms that fit the data well:

an  $N_G$  term Gaussian function

$$\tilde{\eta}_G(k_y) = \eta_0 \sum_j^{N_G} A_j \exp(-k_y^2/2\sigma_j^2) \quad A_j, \sigma_j \in \mathbb{R}_+ \quad (27)$$

and a Lorentzian type function

$$\tilde{\eta}_L(k_y) = \frac{\eta_0}{1 + \alpha |k_y|^\beta} \quad \alpha, \beta \in \mathbb{R}_+, \quad (28)$$

We present the best fits of the data to (i) a two-term Gaussian function with freely estimated amplitudes (i.e. unconstrained fitting) termed as  $\tilde{\eta}_{G_2}$ , (ii) to a two-term Gaussian function with interdependent amplitudes (i.e. constrained fitting  $\sum_j^{N_G} A_j = 1$ ) given by Hansen *et al.* [20] and termed as  $\tilde{\eta}_{G_{2H}}$ , (iii) to a four-term Gaussian function with freely estimated amplitudes, termed as  $\tilde{\eta}_{G_4}$  and (iv) to the Lorentzian type function, Eq. (28). In order to measure the magnitude of the residuals we use the residual standard deviation defined as  $s_r = \sqrt{\sum_{n=1}^{n_s} r^2 / (n_s - n_p)}$  where  $n_s$  is the number of data points,  $n_p$  is the number of fitting parameters, and  $r$  is the residual [48]. After an iterative curve fitting procedure the accurate estimation of  $\eta_0$  was kept fixed allowing all other parameters in Eqs. (27) and (28) to be used as fitting parameters. In Table II we have listed the fitting parameters for monatomic and diatomic molecular fluids and compared to the previous results where possible.