Erratum: Velocity autocorrelation function for simple liquids and its application to liquid metals and alloys [Phys. Rev. E 70, 051201 (2004)]

Kirit N. Lad and Arun Pratap

(Received 18 April 2006; published 30 May 2006)

DOI: 10.1103/PhysRevE.73.059902 PACS number(s): 61.20.Lc, 66.10.−x, 66.30.Fq, 61.25.Mv, 99.10.Cd

Equations (17), (18), and (25) are incorrect. The correct equations are

$$c_1 = -\frac{Y_n[2(n+1)\gamma] - \gamma Y_{n+1}[2(n+1)\gamma]}{\gamma\{J_n[2(n+1)\gamma]Y_{n+1}[2(n+1)\gamma] - J_{n+1}[2(n+1)\gamma]Y_n[2(n+1)\gamma]\}}, \tag{17}$$

$$c_2 = \frac{J_n[2(n+1)\gamma] - \gamma J_{n+1}[2(n+1)\gamma]}{\gamma\{J_n[2(n+1)\gamma]Y_{n+1}[2(n+1)\gamma] - J_{n+1}[2(n+1)\gamma]Y_n[2(n+1)\gamma]\}}, \tag{18}$$

$$\frac{d^2\psi}{dt^2} + \beta_0\frac{d\psi}{dt} + \omega_0^2\psi = 0. \tag{25}$$

One of the two functions represented in Fig. 1 is found to be wrong. The mistake resulted due to an error in the compilation of the program. Subsequently, the values of γ, c_1, and c_2 also change as shown in Table I. Fortunately, these changes do not introduce any appreciable change in the results for the velocity autocorrelation function (VACF). The corrected Fig. 1 is as below.

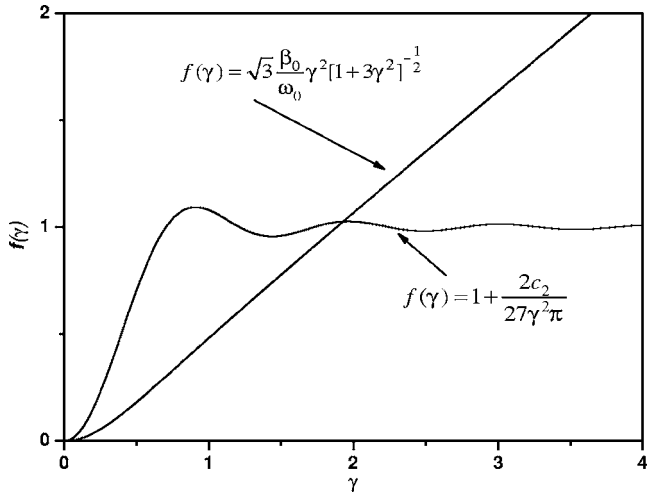

FIG. 1. Two sides of Eq. (32) plotted as a function of γ for the case of $\beta_0 \neq \omega_0$.

TABLE I. Parameters used to calculate velocity autocorrelation function. These are the corrected values of γ, c_1, and c_2.

			$Li_{0.61}Na_{0.39}$		$Li_{0.70}Mg_{0.30}$	
	Li	Na	Li-Li	Na-Na	Li-Li	Mg-Mg
γ	1.9262	1.9849	1.8523	1.508	1.8511	1.4252
c_1	1.5529	0.0123	3.1426	−3.2519	3.1636	−3.2175
c_2	4.1429	4.4817	3.01	−0.6612	2.9863	0.4792

