Erratum: Analytic understanding and control of dynamical friction [Phys. Rev. B 97, 104104 (2018)]

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We have identified an inaccuracy in the main result of the original paper, namely Eq. (1).

The error arises when incorporating viscous dissipation in the substrate through the exponential term $e^{-\gamma|t|/2}$ directly into the structure factor $S_{nn}(x, x'; t)$, as given by Eq. (10). Specifically, in the original paper, in deriving Eq. (1) from Eq. (6) we accounted for dissipation by broadening the Dirac $\delta(Qv_{\rm SL} - \omega(Q))$ of Eq. (5) into a Lorentzian, as described by Eq. (11). However, the successive calculation leading to Eq. (1) still relies on the relation $Qv_{\rm SL} = \omega(Q)$ which in reality is just approximate, after the broadening of the Dirac delta.

To rectify this issue, we return to Eq. (4) of the original paper, expressed in terms of the imaginary part of the density-density susceptibility. For clarity, we report this initial expression here:

$$F(v_{\rm SL}) = -2\int_0^\infty \frac{dQ}{2\pi} Q\,{\rm Im}\,\chi^R_{nn}(Q, Q; Qv_{\rm SL})|V_{\rm ext}(Q)|^2. \tag{1}$$

The correction involves the calculation of the friction force F directly from χ_{nn}, without involving the structure factor through the fluctuation-dissipation theorem.

We follow calculations analogous to those in Appendix B of the original paper, but applied here to the density-density susceptibility

$${\rm Im}\,\chi^R_{nn}(Q, Q; \omega > 0) = -\frac{i}{\hbar}\lim_{N\to\infty}\frac{1}{Na}{\rm Im}\int_0^\infty dt\, e^{i\omega t}\,\langle[\hat{n}_Q(t), \hat{n}_{-Q}(0)]\rangle. \tag{2}$$

By using Eqs. (B1), (B3), and the one-phonon approximation Eq. (B7) of the original paper, we obtain (in the thermodynamic limit)

$$\lim_{N\to\infty}\frac{1}{N}\langle[\hat{n}_Q(t), \hat{n}_{-Q}(0)]\rangle \sum_{j=-\infty}^{\infty} e^{-iQaj}\left(e^{-Q^2\Phi_j(t,\beta)} - e^{-Q^2\Phi_j^*(t,\beta)}\right) \simeq -2i\sum_{j=-\infty}^{\infty} e^{-iQaj}Q^2{\rm Im}\Phi_j(t, \beta). \tag{3}$$

From the definition of $\Phi_j(t, \beta)$ in Eq. (B6), and Eq. (B9) of the original paper, we arrive at

$${\rm Im}\,\chi^R_{nn}(Q, Q; \omega > 0) = -\frac{\pi Q^2}{2ma\omega(Q)}\,\delta(\omega - \omega(Q)). \tag{4}$$

Substitution of this damping-free expression into Eq. (1) leads to

$$F(v_{\rm SL}) = \frac{\pi}{ma}\int_0^\infty \frac{dQ}{2\pi}\frac{Q^3}{\omega(Q)}|V_{\rm ext}(Q)|^2\,\delta(Qv_{\rm SL} - \omega(Q)), \tag{5}$$

which is entirely equivalent to Eq. (6) of the original paper, where the fraction $(1 - e^{-\beta\hbar v_{\rm SL}Q})/(1 - e^{-\beta\hbar\omega(Q)}) \equiv 1$ due to the delta condition, leading to $v_{\rm SL}Q \equiv \omega(Q)$.

We now proceed to introduce damping into the susceptibility

$${\rm Im}\,\chi^{\rm R\,diss}_{nn}(Q, Q; t) = {\rm Im}\,\chi^R_{nn}(Q, Q; t)\,e^{-\gamma|t|/2} \tag{6}$$

rather than into the structure factor. Using this modified susceptibility in Eq. (1), the phonon decay induces the same kind of Lorentzian broadening of the Dirac delta in Eq. (5)

$$\delta(Qv_{\rm SL} - \omega(Q)) \to \frac{1}{\pi}\frac{\gamma/2}{(Qv_{\rm SL} - \omega(Q))^2 + (\gamma/2)^2}, \tag{7}$$

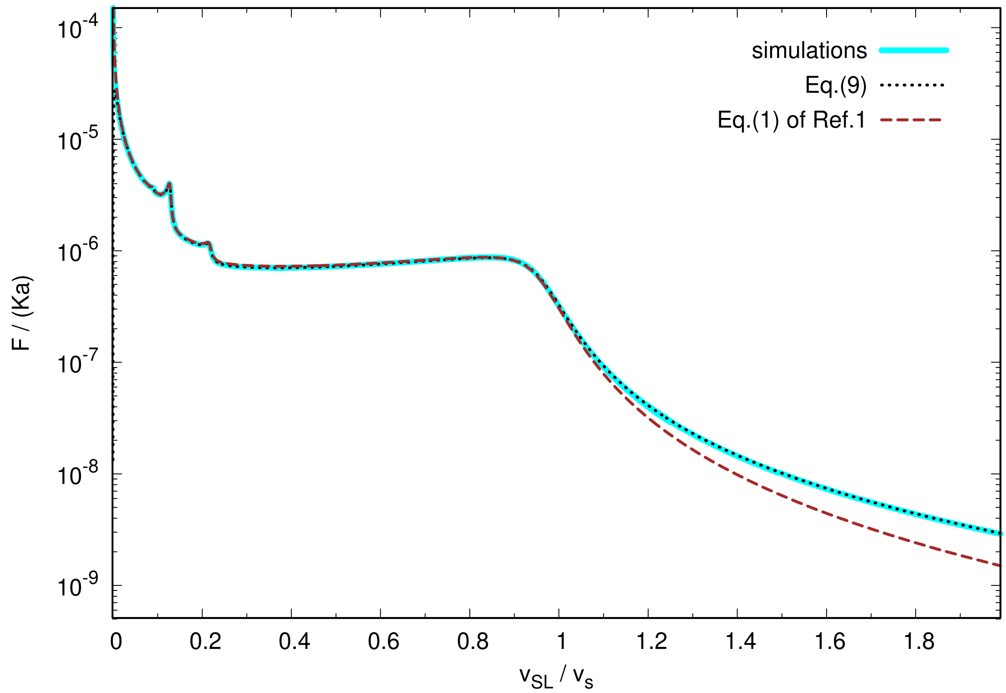

FIG. 1. Comparison of the slider-speed dependence of the friction force $F(v_{\rm SL})$ obtained from the two analytical expressions, the correct Eq. (9) and the incorrect Eq. (1) of the original paper, with that obtained through numerical simulations in the same conditions [$\epsilon = 5 \times 10^{-4}\, Ka^2$, $d = 0.475\, a$, $\sigma = 0.5\, a$, $\gamma = 0.1\, (mK)^{1/2}$]. Deviations of the incorrect Eq. (1) of the original paper dominate at supersonic speeds, where the exact Eq. (9) maintains an excellent agreement.

analogous to Eq. (11) of the original paper. The resulting correct expression of friction for a dissipative harmonic chain is therefore

$$F(v_{\rm SL}) = \frac{1}{2mav_{\rm SL}} \int_{-\infty}^{+\infty} dQ\, \frac{Qv_{\rm SL}}{\omega(Q)}\, Q^2 |V_{\rm ext}(Q)|^2\, \frac{1}{\pi}\, \frac{\gamma/2}{(Qv_{\rm SL} - \omega(Q))^2 + (\gamma/2)^2} \tag{8}$$

$$= \frac{1}{2ma} \int_{-\infty}^{+\infty} dQ\, \frac{Q^3}{\omega(Q)}\, |V_{\rm ext}(Q)|^2\, \frac{\frac{\gamma}{2\pi}}{(Qv_{\rm SL} - \omega(Q))^2 + \left(\frac{\gamma}{2}\right)^2}. \tag{9}$$

Compared to the incorrect Eq. (1) of the original paper, the first formulation (8) clarifies that an extra a factor $Qv_{\rm SL}/\omega(Q)$ must be included, and the integration must extend over the entire Q axis, because the Lorentzian contributes for $Q < 0$, too. This extension is not required for Eq. (5), which would acquire vanishing contributions if the Q integration was extended to negative values.

Equation (9) is the correct friction expression, that should be used in place of Eq. (1) of the original paper. Figure 1 compares the incorrect formula with the corrected expression (9), and with numerical simulations. The deviation between the two expressions is often small because the ratio $Qv_{\rm SL}/\omega(Q)$ in (8) systematically approaches unity for all Q points with maximum Lorentzian weight, thus explaining the fair agreement of the incorrect formula of the original paper with the numerical simulations. However, this maximum-weight resonance condition is hardly met for supersonic velocities: indeed, in that region of $v_{\rm SL} > v_{\rm s}$ the new correct expression (9) approaches the numerically simulated friction far better.

While Eq. (9) may suggest a risk of diverging integrand at all Q points where the phonon frequency $\omega(Q)$ vanishes, in practice the integrand is a perfectly regular function of Q. To clarify this point, we reformulate Eq. (9) as

$$F(v_{\rm SL}) = \frac{2v_{\rm SL}}{ma} \int_0^{+\infty} dQ\, Q^4\, |V_{\rm ext}(Q)|^2 \frac{\frac{\gamma}{2\pi}}{\left[(Qv_{\rm SL} - \omega(Q))^2 + \left(\frac{\gamma}{2}\right)^2\right]\left[(Qv_{\rm SL} + \omega(Q))^2 + \left(\frac{\gamma}{2}\right)^2\right]}, \tag{10}$$

demonstrating the absence of any singular point in the integration.

As a final side observation, Eq. (B1) in the original paper should be corrected to

$$\hat{n}_Q(t) = \sum_{j=1}^{N} e^{-iQaj}\, e^{-iQ\hat{u}_j(t)}. \tag{11}$$