Theory of noncontact friction for atom-surface interactions

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The noncontact (van der Waals) friction is an interesting physical effect which has been the subject of controversial scientific discussion. The “direct” friction term due to the thermal fluctuations of the electromagnetic field leads to a friction force proportional to \( 1/Z^5 \) (where \( Z \) is the atom-wall distance). The “backaction” friction term takes into account the feedback of thermal fluctuations of the atomic dipole moment onto the motion of the atom and scales as \( 1/Z^8 \). We investigate noncontact friction effects for the interactions of hydrogen, ground-state helium and metastable helium atoms with \( \alpha \)-quartz (SiO\(_2\)), gold (Au) and calcium difluorite (CaF\(_2\)). We find that the backaction term dominates over the direct term induced by the thermal electromagnetic fluctuations inside the material, over wide distance ranges. The friction coefficients obtained for gold are smaller than those for SiO\(_2\) and CaF\(_2\) by several orders of magnitude.

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I. INTRODUCTION

Noncontact friction arises in atom-surface interactions; the theoretical treatment has given rise to some discussion [1–11]. In a simplified understanding, for an ion flying by a dielectric surface (“wall”), the quantum friction effect can be understood in terms of Ohmic heating of the material by the motion of the image charge inside the medium. Alternatively, one can understand it in terms of the thermal fluctuations of the electric fields in the vicinity of the dielectric, and the backreaction onto the motion of the ion or atom in the vicinity of the “wall”.

It has recently been argued that one cannot separate the van-der-Waals force, at finite temperature, from the friction effect [9]. The backaction effect is due to the fluctuations of the atomic dipole moment [9], which are mirrored by the wall and react back onto the atom; this leads to an additional contribution to the friction force. In contrast to the “direct” term created by the electromagnetic field fluctuations inside the medium [5] (proportional to \( 1/Z^5 \) where \( Z \) is the atom-wall distance), the backaction term leads to a \( 1/Z^8 \) effect. A comparison of the magnitude of these two effects, for realistic dielectric response functions of materials, and using a detailed model of the atomic polarizability, is the subject of the current paper. While the \( 1/Z^8 \) effect is parametrically suppressed for large atom-wall separations, the numerical coefficients may still change the hierarchy of the effects.

We should also note that the direct term [5, 9] can be formulated as an integral over the imaginary part of the polarizability, and of the dielectric response function of the material. Recently, we found a conceptually interesting “one-loop” dominance for the imaginary part of the polarizability [12, 13]. The imaginary part of the polarizability describes a process where the atom emits radiation at the same frequency as the incident laser radiation, but in a different direction. Note that, by contrast, Rabi flopping involves continuous absorption and emission into the laser mode; the laser-dressed states [14, 15] are superpositions of states \(|g, n_L + 1\rangle\) and \(|e, n_L\rangle\), where \( n_L \) is the number of laser photons while \(|g\rangle\) and \(|e\rangle\) denote the atomic ground and excited states. \( A \text{ priori} \), this Rabi flopping may proceed off resonance.

FIG. 1. Feynman diagrams contributing to the imaginary part of the polarizability. A photon is absorbed from a bath (denoted by the external crosses), while a second photon of equal frequency (nonresonant with respect to an atomic transition) is emitted (Cutkosky rules).

By contrast, when the ac Stark shift of an atomic level is formulated perturbatively and the second-order shift of the atomic level in the external laser field is evaluated using a second-quantized formalism (see Sec. III of Ref. [16]), a resonance condition has to be fulfilled in order for an imaginary part of the energy shift to be generated. Namely, the final state of atom+field in the decay process has to have exactly the same energy as the reference state of atom+field. This is possible only at exact resonance, when the emitted photon has just the right frequency to compensate the “quantum jump” of the bound electron from an excited state to an energetically lower state [16–18]. The ac Stark shift is propor-
tional to the atomic polarizability. Its tree-level imaginary part [12, 13] corresponds to spontaneous emission of the atom at an exact resonance frequency, still, not necessarily along the same direction as the incident laser photon. When quantum electrodynamics is involved, it is seen that due to quantum fluctuations of the electromagnetic field, spontaneous emission is possible off resonance. In Refs. [12, 13], the imaginary part of the polarizability was found to be dominated by a self-energy correction to the ac Stark shift. Physically, the imaginary part of the polarizability corresponds to a “decay rate” of the reference state |φ, nL⟩ used in the calculation of the ac Stark shift, to a state |φ, nL − 1, 1⟩L, where |φ⟩ is the atomic reference state, the occupation number of the laser mode is nL, and there is either zero or one photon in the mode L. While the laser frequency is equal to the frequency of the emitted radiation (ωL = ωZ), the emission proceeds into a different direction as compared to the laser wave vector (k ≠ kL). Off resonance, the quantum electrodynamical one-loop effect calculated in Refs. [12, 13] thus dominates the imaginary part of the polarizability, not the tree-level term. This is quite surprising; the relevant Feynman diagrams are shown in Fig. 1. The peculiar behavior of the imaginary part of the polarizability suggests a detailed numerical study of the noncontact friction integral [5, 9], and comparison, of the direct and backaction terms.

This paper is organized as follows. In Sec. II, we attempt to shed some light on the derivation of the effect. Full SI mksÅ units are kept throughout the derivation. The numerical calculations of noncontact friction for the hydrogen and helium interactions with α-quartz, gold, and CaF2 are described in Sec. III, where we shall use atomic units for for frequency data and friction coefficients in Tables I—V. We employ a convenient fit to the vibrational and interband excitations of the α-quartz and CaF2 lattices. Finally, conclusions are drawn in Sec. IV.

II. DERIVATION

Our derivation is in part inspired by Ref. [9]; we supplement the discussion with some explanatory remarks and simplified formulas where appropriate. The electric field at the position of the atomic dipole (i.e., at the position of the atom) is written as

$$\vec{E}(t) = \vec{E}_0 e^{-i\omega t} + \vec{E}_1 e^{-i(\omega + \omega_0) t},$$  (1)

where ω is the angular frequency component of the (thermal) fluctuation, and ω0 describes a small displacement of the atom’s position itself. The contribution proportional to E1 is included as a result of a backaction term, which takes the variation of the spontaneous and induced fields over the spatial amplitude of the oscillatory motion of the atom into account [see Eq. (9)]. Hence, the angular frequency of the motion (ω0) is added to the thermal frequency, and the term is proportional to exp[−i(ω + ω0) t]. The displacement of the atom is of angular frequency ω0,

$$\vec{u}(t) = \vec{u}_0 e^{-i\omega_0 t}, \quad \vec{r}(t) = \vec{r}_0 + \vec{u}(t).$$  (2)

The dipole density of the isolated atom is supposed to perform oscillations of the form

$$\vec{d}(\vec{r}, t) = \vec{d}_0 \delta(3)(\vec{r} - \vec{r}_0) e^{-i\omega t} + \vec{p}_1(\vec{r}, \omega) e^{-i(\omega + \omega_0) t},$$

$$\vec{p}_1(\vec{r}, \omega) = \vec{d}_1 \delta(3)(\vec{r} - \vec{r}_0) - \vec{d}_0 e^{i\omega t} \nabla \delta(3)(\vec{r} - \vec{r}_0).$$  (3)

Here, the second term is generated by the displacement of the atom, i.e., by the expansion of the Dirac δ function δ(3)(r - r0 - ω(t)) to first order in u(t). While the atomic dipole moment is a sum of a fluctuating term d0 and an induced term (by the corresponding frequency component of the electric field at the position of the atom),

$$d_{0i} = d_{1i}^{f} + \alpha(\omega) E_{0i},$$  (4)

the frequency component for ω + ω0 only contains an induced term, d1 = α(ω + ω0) E0.

Let Gij(\vec{r}, \vec{r}', ω) denote the frequency component of the Green tensor which determines the electric field generated at position \vec{r}' by a point dipole at \vec{r}. In the non-retardation approximation [Eq. (1) of Ref. [5]], it reads

$$g(\vec{r}, \vec{r}', \omega) = \frac{1}{4\pi\epsilon_0} \left( \frac{1}{|\vec{r}' - \vec{r}|} \right) \left( \begin{array}{c} e(\omega) - 1 \\ e(\omega) + 1 \end{array} \right),$$

$$G_{ij}(\vec{r}, \vec{r}', \omega) = - \nabla_i \nabla_j g(\vec{r}, \vec{r}', \omega).$$  (5)

Here, \hat{n} = \hat{e}_z is the surface normal (the surface of the dielectric is the xy plane). The result

$$G_{zz}(\vec{0}, \vec{r}_z, \omega) = \frac{2}{\epsilon^2 - 1} \frac{e(\omega) - 1}{e(\omega) + 1} \frac{2}{\epsilon}, \quad \vec{r}_z = \hat{e}_z Z,$$  (6)

reflects the fact that a dipole oriented in parallel to the z axis generates a mirror dipole which also is oriented in parallel to the z axis (not antiparallel, see the dipoles in Fig. 2). Because of this, the second term on the right-hand side of Eq. (6) has the same sign as the first term.

FIG. 2. (Color online.) Mirroring a dipole in the xy plane. A dipole aligned along the x axis gives rise to an antiparallel mirror dipole, whereas a dipole aligned along the z axis gives rise to a parallel mirror dipole. Recall that mirror charges have the opposite sign as compared to the original ones.
Self-consistency dictates that the field \( \vec{E}_0 = \vec{E}_0(\vec{r}_0) \) at the position of the atom is equal to the sum of the field generated by the dipole moment \( d_0 \), and the fluctuating component \( E_i^s(\vec{r}_0, \omega) \) of the electric field,

\[
E_{0i} = G_{ii}(\vec{r}_0, \vec{r}_0, \omega) d_{0i} + E_i^s(\vec{r}_0, \omega) \nonumber
\]

\[
= G_{ii}(\vec{r}_0, \vec{r}_0, \omega) \alpha(\omega) E_{0i} + G_{ii}(\vec{r}_0, \vec{r}_0, \omega) d_{0i}^f + E_i^s(\vec{r}_0, \omega),
\]

where no summation over \( i \) is carried out (one has \( G_{ii} = G_{ii} \delta_{ij} \) at equal spatial coordinates). So,

\[
E_{0i} = \frac{G_{ii}(\vec{r}_0, \vec{r}_0, \omega) d_{0i}^f + E_i^s(\vec{r}_0, \omega)}{1 - G_{ii}(\vec{r}_0, \vec{r}_0, \omega) \alpha(\omega)},
\]

\[
d_{0i} = \frac{d_{0i}^f + \alpha(\omega) E_i^s(\vec{r}_0, \omega)}{1 - \alpha(\omega) G_{ii}(\vec{r}_0, \vec{r}_0, \omega)},
\]

where in Eq. (8b) we have taken into account Eq. (4). The electric field \( \vec{E}_0 \) and the dipole moment \( d_0 \) are given in terms of fluctuating terms; the denominators in Eq. (8) take the backaction into account. For \( \vec{E}_1 \), one observes that the gradient term in the expression of \( \vec{p}_1(\vec{r}, \omega) \) [Eq. (3)], in the non-fluctuating contribution \( \int d^3 \vec{r} G_{ij}(\vec{r}, \vec{r}, \omega + \omega_0) p_{ij}(\vec{r}, \omega) \), needs to be treated by partial integration. Adding the term due to the fluctuations of the atom’s position, and due to the spontaneous fluctuations of the electromagnetic field, one obtains

\[
E_{1i} = G_{ii}(\vec{r}_0, \vec{r}_0, \omega + \omega_0) \alpha(\omega + \omega_0) E_{1i},
\]

\[
+ \vec{u}_0 \cdot \vec{\nabla}_r (E_i^s(\vec{r}, \omega) + G_{ij}(\vec{r}_0, \vec{r}, \omega + \omega_0) d_{0j} + G_{ij}(\vec{r}, \vec{r}_0, \omega) d_{0j}|_{\vec{r}=\vec{r}_0}.
\]

This equation can be trivially solved for \( \vec{E}_1 \). The thermal fluctuations are described by the following equations [5],

\[
\langle d_i^f d_j^f \rangle = \frac{2 \Theta(\omega, T)}{\omega} \delta_{ij} \Im \frac{\alpha(\omega)}{1 - \alpha(\omega) G_{ii}(\vec{r}_0, \vec{r}_0, \omega)},
\]

\[
\langle E_i(\vec{r}) E_j(\vec{r}') \rangle = \frac{2 \Theta(\omega, T)}{\omega} \Im \{ G_{ij}(\vec{r}, \vec{r}', \omega) \}.
\]

where \( \Theta(\omega, T) = \frac{\hbar \omega}{\omega + n(\omega)} = \frac{\hbar \omega}{[\exp(\beta \hbar \omega) - 1]^{-1}}, \) and \( \beta = 1/(k_B T) \) is the Boltzmann constant. With the help of \( \rho = -\vec{\nabla} \cdot \vec{p} \) and \( \vec{j} = \partial_t \vec{p} \), one formulates a time-dependent force,

\[
\vec{F}(t) = \int d^3 r \left( \rho(\vec{r}, t) \vec{E}^s(\vec{r}, t) + \vec{j}(\vec{r}, t) \times \vec{B}^s(\vec{r}, t) \right)
\]

\[
= \vec{F}_s(t) + \vec{u}_0 \cdot \frac{\partial}{\partial \vec{r}} \vec{F}_s(t) + \vec{F}_f(\omega, \omega_0) e^{-i\omega_0 t}.
\]

Here, \( F_s(t) \) is the static van-der-Waals force, \( \vec{u}_0 \cdot \frac{\partial}{\partial \vec{r}} \vec{F}_s(t) \) describes the variation of the van-der-Waals force with the oscillating position of the atom, and \( \vec{F}_f(\omega, \omega_0) \) is a Fourier component of the friction force. An integration over the thermal fluctuations of all Fourier components of the friction force gives the total friction force,

\[
\vec{F}_f = \frac{1}{2} \int_0^\infty \frac{d\omega}{2\pi} \omega_0 \frac{\partial}{\partial \omega_0} \langle \vec{F}(\omega, \omega_0) \rangle |_{\omega_0 = 0}
\]

\[
= i \omega_0 [\eta_x (u_0 x \hat{e}_x + u_0 y \hat{e}_y) + \eta_z u_0 \hat{e}_z] - \eta_x (v_x \hat{e}_x + v_y \hat{e}_y) - \eta_z v_z \hat{e}_z.
\]

Here, \( \eta_x \) and \( \eta_z \) are the friction coefficient for motion along the \( x \) and \( z \) directions, respectively. The additional assumption of a small mechanical motion with velocity \( \vec{v} = \partial_t \vec{u}_0 e^{-i\omega_0 t} \) \( |_{t=0} = -i\omega_0 \vec{u}_0 \) is made.

The result for \( \eta_x \) is obtained as,

\[
\eta_x = \frac{\beta \hbar^2}{2\pi} \int_0^\infty \frac{d\omega}{\sinh^2(\frac{1}{2} \beta \hbar \omega)} \left[ \sum_{\ell=x,y,z} \frac{\partial^2}{\partial x \partial x} \text{Im} G_{\ell\ell}(\vec{r}, \vec{r}, \omega) \Im \left( \frac{\alpha(\omega)}{1 - \alpha(\omega) G_{\ell\ell}(\vec{r}, \vec{r}, \omega)} \right) \right]
\]

\[
- 2|\alpha(\omega)|^2 \text{Re} \left( \frac{1}{(1 - \alpha^*(\omega) D_{zz}(\vec{r}, \vec{r}, \omega))(1 - \alpha(\omega) G_{zz}(\vec{r}, \vec{r}, \omega)))} \left( \frac{\partial}{\partial x} G_{zz}(\vec{r}, \vec{r}, \omega) \right)^2 \right) \bigg|_{\vec{r}, \vec{r} = \vec{r}_0}
\]

\[
\approx \frac{\beta \hbar^2}{2\pi} \int_0^\infty \frac{d\omega}{\sinh^2(\frac{1}{2} \beta \hbar \omega)} \left[ \sum_{\ell=x,y,z} \frac{\partial^2}{\partial x \partial x} \text{Im} G_{\ell\ell}(\vec{r}, \vec{r}, \omega) \text{Im}[\alpha(\omega)] + \alpha(\omega)^2 \right]
\]

\[
\times \left\{ \sum_{\ell=x,y,z} \left( \frac{\partial^2}{\partial x \partial x} \text{Im} G_{\ell\ell}(\vec{r}, \vec{r}, \omega) \right) \text{Im}[G_{\ell\ell}(\vec{r}, \vec{r}, \omega)] - 2 \frac{\partial}{\partial x} \text{Im} \left[ G_{zz}(\vec{r}, \vec{r}, \omega) \right] \right\} \bigg|_{\vec{r}, \vec{r} = \vec{r}_0}.
\]

This result can be written as \( \eta_x = \eta_x^{(1)} + \eta_x^{(2)} \), where \( \eta_x^{(2)} \) is generated by the term in curly brackets in the integrand. With the help of \( \sum_{\ell} \frac{\partial^2}{\partial x \partial x} \text{Im} G_{\ell\ell}(\vec{r}, \vec{r}) = \text{Im} \left( \frac{\epsilon(\omega)-1}{\epsilon(\omega)+1} \right) \frac{3}{16\pi c_0} \), one verifies that the leading-order, linear term in the
polarizability (see Ref. [5]), from Eq. (13), is given as

$$\eta_z^{(1)} = \frac{\beta \hbar^2}{2\pi} \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \sum_{\ell=x,y,z} \partial^2 \partial_{\ell} \partial_{\ell'} \operatorname{Im} G_{\ell\ell}(r, r') \operatorname{Im} (\alpha(\omega)) = \frac{3\beta \hbar^2}{32\pi^2 \epsilon_0 Z^5} \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \operatorname{Im} \left(\frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}\right),$$

(14)

In Eq. (13), the term of second order in the polarization is given as follows,

$$\eta_z^{(2)} = \frac{\beta \hbar^2}{8\pi} \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \left[ \left\{ \frac{\partial^2}{\partial r^2} \operatorname{Im} G_{zz}(r, r, \omega) \right\} \operatorname{Im} G_{zz}(r, r, \omega) - 2 \left( \frac{\partial}{\partial z} \operatorname{Im} G_{zz}(r, r, \omega) \right)^2 \right]_{r=r'=r_z}$$

$$= \frac{9\beta \hbar^2}{4096 \pi^3 \epsilon_0^2 Z^8} \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \left[ \operatorname{Im} \left(\frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}\right) \right]^2.$$

(15)

For friction in the $z$ direction, one derives $\eta_z = \eta_z^{(1)} + \eta_z^{(2)}$, with $\eta_z^{(1)} = 2\eta_z^{(2)}$ and $\eta_z^{(2)} = 7\eta_x^{(2)}$, confirming Ref. [9]. The term $\eta_z^{(2)}$ is generated by the “backaction denominators” from Eqs. (8a) and (8b). For the numerical evaluation of the term $\eta_z^{(1)}$, the following result

$$\operatorname{Im}[\alpha(\omega)] = \operatorname{Im}[\alpha_R(\omega)] + \frac{\omega^3}{6\pi \epsilon_0 c^3} [\alpha(\omega)]^2,$$

(16a)

$$\operatorname{Im} [\alpha_R(\omega)] = \operatorname{Im} [\alpha_r(\omega)] - \operatorname{Im} [\alpha_r(-\omega)],$$

(16b)

$$\operatorname{Im} [\alpha_r(\omega)] = \frac{\pi}{2} \sum_m \frac{f_{m0}}{E_m - E} \delta(E_m - E + \hbar \omega),$$

(16c)

has recently been derived in Ref. [12]. Here, $f_{m0}$ are the oscillator strengths [19, 20] for the dipole transitions from the ground state of the atom with energy $E$ to the excited states $|m\rangle$ with energy $E_m$. The “one-loop” term in the result for $\operatorname{Im}[\alpha(\omega)]$, proportional to $\alpha(\omega)^2$, implies that the numerical evaluation of both $\eta_z^{(1)}$ and $\eta_z^{(2)}$ is related; because typical thermal wave vectors (inversely related to the thermal wavelengths) are much smaller than typical atomic transition frequencies, $\eta_z^{(2)}$ is the dominant term. The resonant, tree-level contribution to the atomic polarizability is denoted as $\operatorname{Im} [\alpha_r(\omega)]$.

The expression for $\operatorname{Im} [\alpha_r(\omega)]$ takes into account only resonant processes, with Dirac-$\delta$ peaks near the resonant transitions. However, this concept ignores the possibility of off-resonant driving of an atomic transition, where the atom would absorb an off-resonant photon and emit a photon of the same frequency as the absorbed, off-resonant one, but in a different spatial direction. Indeed, it has been argued in Ref. [21] that the off-resonant driving of an atomic transition mediates the dominant mechanism in the determination of the quantum friction force. The same argument applies to the atom-surface quantized radiation field (e.g., a laser field or a bath of thermal photons), the vertical internal lines denote the “cutting” of the diagram at the point where the photon is emitted, and the photon loop denotes the self-interaction of the atomic electron (the imaginary of the corresponding energy shift is directly proportional to the imaginary part of the polarizability [22]). The overall result is obtained by adding the (in this case dominant) one-loop “correction” to the resonant imaginary part of the polarizability.

### III. NUMERICAL EVALUATION

The structure of Eqs. (14) and (15), which we recall for convenience,

$$\eta_x^{(1)} = \frac{3\beta \hbar^2}{32\pi^2 \epsilon_0 Z^5} \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \operatorname{Im} \left(\frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}\right),$$

(17a)

$$\eta_x^{(2)} = \frac{9\beta \hbar^2}{4096 \pi^3 \epsilon_0^2 Z^8} \times \int_0^\infty \frac{d\omega}{\sin^2\left(\frac{\delta}{2} \beta \hbar \omega\right)} \left[ \operatorname{Im} \left(\frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1}\right) \right]^2,$$

(17b)

implies that, for the evaluation of the quantum friction coefficient in the vicinity of a dielectric, we need to have reliable data for both the imaginary part of the polarizability of the atom, $\operatorname{Im}[\alpha(\omega)]$, as well as the imaginary part of the dielectric response function, which is given as $\operatorname{Im}[\epsilon(\omega)] - \epsilon(\omega) + 1$. A related problem, namely, the calculation of black-body friction for an atom immersed in a thermal bath of photons, has recently been considered in Ref. [21]. It has been argued that the inclusion of the width $\Gamma_n$ of the virtual states in the expression for the polarizability is crucial for obtaining reliable predictions. The imaginary part of the polarizability is given in
TABLE I. Coefficients for the first few resonances for α-quartz according to the fitting formula (21) (ordinary and extraordinary optical axes). The \( \omega_k \) and \( \gamma_k \) are measured in atomic units, i.e., in units of the \( \hbar \), where \( \hbar \) is the Hartree energy. The fitting parameters have been obtained from data tabulated in Ref. [23] (see also Ref. [24]).

| Vibrational Excitations (Ordinary Axis) | \( k \) | \( \alpha_k \) | \( \omega_k \) | \( \gamma_k \) |
|----------------------------------------|------|-------------|-------------|-------------|
|                                        | 1    | 1.04 \times 10^{-2} | 1.83 \times 10^{-3} | 1.29 \times 10^{-5} |
|                                        | 2    | 8.53 \times 10^{-2} | 2.22 \times 10^{-3} | 1.83 \times 10^{-5} |
|                                        | 3    | 0.16 \times 10^{-2} | 3.18 \times 10^{-3} | 3.16 \times 10^{-5} |
|                                        | 4    | 1.06 \times 10^{-2} | 3.67 \times 10^{-3} | 3.20 \times 10^{-5} |
|                                        | 5    | 5.52 \times 10^{-2} | 5.23 \times 10^{-3} | 3.61 \times 10^{-5} |
|                                        | 6    | 4.55 \times 10^{-2} | 5.34 \times 10^{-3} | 3.89 \times 10^{-5} |

| Interband Excitations (Ordinary Axis) | \( k \) | \( \alpha_k \) | \( \omega_k \) | \( \gamma_k \) |
|---------------------------------------|------|-------------|-------------|-------------|
|                                       | 7    | 1.05 \times 10^{-2} | 3.89 \times 10^{-1} | 1.12 \times 10^{-2} |
|                                       | 8    | 4.71 \times 10^{-2} | 4.45 \times 10^{-1} | 5.28 \times 10^{-2} |
|                                       | 9    | 4.98 \times 10^{-2} | 5.37 \times 10^{-1} | 7.32 \times 10^{-2} |
|                                       | 10   | 1.06 \times 10^{-1} | 6.58 \times 10^{-1} | 1.30 \times 10^{-1} |
|                                       | 11   | 1.12 \times 10^{-1} | 8.26 \times 10^{-1} | 2.40 \times 10^{-1} |

| Vibrational Excitations (Extraordinary Axis) | \( k \) | \( \alpha_k \) | \( \omega_k \) | \( \gamma_k \) |
|-----------------------------------------------|------|-------------|-------------|-------------|
|                                               | 1    | 3.63 \times 10^{-2} | 1.74 \times 10^{-3} | 2.32 \times 10^{-5} |
|                                               | 2    | 8.45 \times 10^{-4} | 2.31 \times 10^{-3} | 1.52 \times 10^{-5} |
|                                               | 3    | 7.54 \times 10^{-2} | 2.42 \times 10^{-3} | 3.00 \times 10^{-5} |
|                                               | 4    | 1.08 \times 10^{-2} | 3.58 \times 10^{-3} | 3.49 \times 10^{-5} |
|                                               | 5    | 1.03 \times 10^{-1} | 5.31 \times 10^{-3} | 4.46 \times 10^{-5} |

| Interband Excitations (Extraordinary Axis) | \( k \) | \( \alpha_k \) | \( \omega_k \) | \( \gamma_k \) |
|---------------------------------------------|------|-------------|-------------|-------------|
|                                             | 6    | 1.05 \times 10^{-2} | 3.89 \times 10^{-1} | 1.12 \times 10^{-2} |
|                                             | 7    | 4.71 \times 10^{-2} | 4.45 \times 10^{-1} | 5.28 \times 10^{-2} |
|                                             | 8    | 4.98 \times 10^{-2} | 5.37 \times 10^{-1} | 7.32 \times 10^{-2} |
|                                             | 9    | 1.06 \times 10^{-1} | 6.58 \times 10^{-1} | 1.30 \times 10^{-1} |
|                                             | 10   | 1.12 \times 10^{-1} | 8.26 \times 10^{-1} | 2.40 \times 10^{-1} |

The relation (16c) into atomic units, we recall that the atomic units for charge \( e \), length (Bohr radius \( a_0 \)), and energy (Hartree \( E_h \)) are as follows,

\[
|e| = 1.60218 \times 10^{-19} \text{ C},
\]

\[
a_0 = \frac{\hbar}{\alpha \, m_e \, c} = 5.29177 \times 10^{-11} \text{ m},
\]

\[
E_h = m_e (\alpha \, c)^2 = 4.35974 \times 10^{-18} \text{ J} \approx 27.2 \text{ eV}.
\]

Here, \( |e| \) is the modulus of the elementary charge (we reserve the symbol \( e \) for the electron charge, see Ref. [31]), \( \alpha \) is Sommerfeld’s fine-structure constant, while \( m_e \) is the electron mass and \( c \) denotes the speed of light. The fundamental atomic unit of energy is obtained by multiplying the fundamental atomic mass unit by the fundamental atomic unit of velocity, which is \( \alpha \, c \). In atomic units, then, the reduced quantities fulfill the relations \( c = 1/\alpha \) and \( e = \hbar = m_e = 1 \), while \( \epsilon_0 = 1/(4\pi) \).

For completeness, we also indicate the explicit overall conversion from natural (n.u.) and atomic (a.u.) units to SI mksA for the polarizability, which reads as

\[
\alpha(\omega)|_{\text{SI}} = \frac{\epsilon_0 \, \hbar^3}{m^3 \, c^3} \alpha(\omega)|_{\text{n.u.}}.
\]

Judicious unit conversion helps to eliminate conceivable sources of numerical error in the final results for the friction coefficients. The hydrogen and helium polarizabilities, in the natural and atomic unit systems, are well known [32–38]. From now on, for the remainder of the current section, we switch to atomic units.

In our numerical calculations, we concentrate on the evaluation of dielectric response function of α-quartz (SiO₂), gold (Au), and calcium difluoride (CaF₂). Indeed, a collection of references on optical properties of solids has been given in Refs. [23, 25–29]. Following Ref. [24], we employ the following functional form for SiO₂ and CaF₂, which leads to a satisfactory fit of the available
Formula (21) leads to a satisfactory representation of the data (see Tables I and II),

\[ \rho(\omega) = \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 2} = \frac{[n(\omega) + i k(\omega)]^2 - 1}{[n(\omega) + i k(\omega)]^2 + 2} \approx \sum_{k=1}^{n} \alpha_k \frac{\omega_k^2}{\omega^2 - i \gamma_k \omega - \omega^2}. \]  

We have applied a model of this functional form to \(\alpha\)-quartz (ordinary and extraordinary axis), Au and CaF\(_2\). The form of \(\rho\) is inspired by the Clausius–Mossotti equation, which suggests that the expression \([\epsilon(\omega) - 1]/[\epsilon(\omega) + 2]\) should be identified as a kind of polarizability function of the underlying medium. This function, in turn, exactly has the functional form indicated on the right-hand side of Eq. (21). The dimensionless permittivity \(\epsilon(\omega)\) is obtained as \(\epsilon(\omega) = (1 + 2 \rho)/(1 - \rho)\). Also, it is useful to point out that the response function \((\epsilon(\omega) - 1)/(\epsilon(\omega) + 1)\), whose imaginary part enters the integrand in Eq. (17a), can be reproduced as follows,

\[ \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1} = \frac{3 \rho(\omega)}{\rho(\omega) + 2}. \]  

Formula (21) leads to a satisfactory representation of the data for both infrared and ultraviolet absorption bands of SiO\(_2\).

In order to model the dielectric response function of gold (Au), we proceed in two steps. First, we employ a Drude model,

\[ \epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i \gamma_p)} + \Delta \epsilon(\omega) \]

with \(\omega_p = 0.3330 \, E_h/h\) and \(\gamma_p = 1.164 \times 10^{-3} \, E_h/h\) (the specification in terms of \(E_h/h\) is equivalent to the use of atomic units). For the remainder function \(\Delta \epsilon(\omega)\), we find the following representation,

\[ \frac{\Delta \epsilon(\omega) - 1}{\Delta \epsilon(\omega) + 2} = \Delta \rho(\omega) \approx 1 - a + \frac{a \omega_0^2}{\omega_0^2 - i \gamma_0 \omega - \omega^2} \]

with \(a = 1.5373\), \(\omega_0 = 1.462 \, E_h/h\), and \(\gamma_0 = 4.550 \, E_h/h\). In view of the asymptotics,

\[ \Delta \rho(\omega) = 1 + \frac{i a \gamma_0}{\omega_0^2} \omega, \quad \omega \to 0, \]

the functional form (24) ensures that the dielectric permittivity of gold, as modeled by the leading Drude model.
term (23), for \( \omega \to 0 \), retains its form of a leading term, equal to unity, plus an imaginary part which models the (nearly perfect) conductivity of gold for small driving frequencies.

Our discussion of atomic units provides us with an excellent opportunity to discuss the natural unit of the normalized friction coefficient \( \eta \). In order to convert \( \eta \) from atomic to SI mksA units, one needs to examine the functional relationship \( F_e = -\eta v_x \), where \( v_x \) is the particle’s velocity. The atomic unit of velocity is \( \alpha c \), while the atomic unit of force is equal to the force experienced by two elementary charges, which are apart from each other by a Bohr radius. Denoting the atomic unit of force, for which we have not found a commonly accepted symbol by a Bohr radius. Denoting the atomic unit of force, for which we have not found a commonly accepted symbol by a Bohr radius. Denoting the atomic unit of force, for which we have not found a commonly accepted symbol by a Bohr radius.

For completeness, we also note the atomic units \( \omega_{\text{a.u.}} \) and \( v_{\text{a.u.}} \) of angular frequency and the cycles per second, respectively,

\[
\omega_{\text{a.u.}} = \frac{E_h}{\hbar} = 4.13414 \times 10^{16} \text{ rad/s}, \quad (28)
\]

\[
v_{\text{a.u.}} = \frac{E_h}{\hbar} = 6.57968 \times 10^{15} \text{ Hz}. \quad (29)
\]

The data published in the reference volume of Palik [23] for the optical properties of solids relate to measurements at room temperature. The integral (17a) carries an explicit temperature dependence in view of the Boltzmann factor, which appears in disguised form (hyperbolic sine function in the denominator), but there is also an implicit temperature dependence of the dielectric response function \( [\varepsilon(\omega) - 1]/[\varepsilon(\omega) + 1] \), which has been analyzed (for CaF\(_2\)) in Refs. [27–29].

For the SiO\(_2\), gold and CaF\(_2\) interactions investigated here, we perform the calculations for temperatures around room temperature, i.e., within the range 273 K ≤ \( T \) ≤ 300 K. We use the spectroscopic data from Tables I—II, and employ the formula for the imaginary part of the polarizability given in Eq. (18), and the representation of the dielectric response function in Eq. (21). Because of the narrow temperature range under study, this procedure is sufficient for \( \alpha\text{-quartz} \) and CaF\(_2\). For gold, we take into account the Drude model, as given in Eq. (23). The uncertainty of our theoretical predictions should be estimated to be on the level of 10% to 20%, in view of the necessarily somewhat incomplete character of any global fit to discrete data on the dielectric constant and dielectric response function, which persists even if care is taken to harvest all available data from [23].

A priori, the data in Palik’s book [23] pertain to room temperature. For CaF\(_2\), we may enhance the theoretical treatment somewhat because the temperature dependence of the dielectric response function has been studied in Refs. [25, 26, 28, 29]. The dominant effect on the temperature dependence of the dielectric response function of CaF\(_2\) is due to the shift of the large-amplitude vibrational excitation at \( \omega_1 = 1.74 \times 10^{-3} \text{ a.u.} \) given in Table II. We find that the temperature-dependent data for the response function \( [\varepsilon(\omega) - 1]/[\varepsilon(\omega) + 1] \) given in Fig. 10 of Ref. [29] can be fitted satisfactorily by introducing a single temperature-dependent parameter in our fit function, namely, a temperature-dependent width. The replacement in terms of the parameters listed in Table II is

\[
\gamma_1 \to \gamma_1 + a (T - T_0), \quad a = 4.97 \times 10^{-7} \frac{E_h}{h K}, \quad (30)
\]

(4.97 × 10\(^{-7}\) a.u./K), where \( T_0 = 300 \text{ K} \) is the room-temperature reference point.

We finally obtain the friction coefficients given in Tables III—V. The normalized friction coefficient \( \eta_0 \) given in Tables III—V is indicated in atomic units, for a distance of one Bohr radius from the surface. The \( Z_\alpha \) dependence and the conversion to SI mksA units is accomplished as follows: One takes the respective entry for \( \eta_0 \) from Tables III—V, multiplies it by the atomic unit of the friction coefficient given in Eq. (27) and corrects for the \( 1/Z^5 \) and \( 1/Z^8 \) dependences,

\[
\eta^{(1)} = \eta_0^{(1)} a_{\text{a.u.}} \frac{(a_0 Z)^5}{Z_\alpha} 3.76594 \times 10^{-14} \frac{\text{kg}}{\text{s}}, \quad (31a)
\]

\[
\eta^{(2)} = \eta_0^{(2)} a_{\text{a.u.}} \frac{(a_0 Z)^8}{Z_\alpha} 3.76594 \times 10^{-14} \frac{\text{kg}}{\text{s}}. \quad (31b)
\]

TABLE V. Same as Table III, but for the hydrogen and helium interactions with CaF\(_2\).

| \( T [\text{K}] \) | \( \eta_0^{(1)} \) | \( \eta_0^{(2)} \) | \( \eta_0^{(1)} \) | \( \eta_0^{(2)} \) | \( \eta_0^{(1)} \) | \( \eta_0^{(2)} \) |
|---|---|---|---|---|---|---|
| 273 | \( 3.12 \times 10^{-25} \) | \( 4.79 \times 10^{-1} \) | \( 8.34 \times 10^{-16} \) | \( 4.53 \times 10^{-2} \) | \( 1.54 \times 10^{-11} \) | \( 2.37 \times 10^{3} \) |
| 298 | \( 3.61 \times 10^{-15} \) | \( 5.09 \times 10^{-1} \) | \( 8.85 \times 10^{-16} \) | \( 4.81 \times 10^{-2} \) | \( 1.78 \times 10^{-11} \) | \( 2.52 \times 10^{3} \) |
| 300 | \( 3.65 \times 10^{-15} \) | \( 5.11 \times 10^{-1} \) | \( 8.88 \times 10^{-16} \) | \( 4.83 \times 10^{-2} \) | \( 1.80 \times 10^{-11} \) | \( 2.53 \times 10^{3} \) |
This consideration should be supplemented by an example. The backaction friction coefficients $\eta^{(2)}$ given in Tables III—V are found to be numerically larger than the coefficients $\eta^{(1)}$ by several orders of magnitude, but they are suppressed, for larger atom-wall distances, by the functional form of the effect (1/2$^3$ versus 1/2$^5$). Let us consider the case of a helium atom (mass $m_{\text{He}} = 6.695 \times 10^{-27}$ kg), at a distance

$$Z_{20} = 20 a_0,$$

away from the $\alpha$-quartz surface (extraordinary axis). We employ the normalized friction coefficients $\eta^{(1)}_0 = 8.81 \times 10^{-16}$ and $\eta^{(2)}_0 = 4.80 \times 10^{-2}$ from Table III, for a temperature $T = 298$ K. With

$$u_0 = 3.76594 \times 10^{-14} \text{kg s}^{-1},$$

being the atomic units of the friction coefficient, the attenuation equation $F_x = -\eta \nu_x$ is solved by

$$\frac{d\nu_x}{dt} = -\gamma \nu_x, \quad \nu_x(t) = \nu_x(0) \exp(-\gamma t),$$

for ground-state helium atoms. This corresponds to an attenuation time of $\tau = 0.0948$ s, in the functional relationship $d\nu_x/dt = \nu_x/\tau$.

IV. CONCLUSIONS

In this paper, we have performed the analysis of the direct and backaction friction coefficients in Sec. II, to arrive at a unified formula for the quantization friction coefficient of a neutral atom, in Eqs. (17a) and (17b). The numerical evaluation for the interactions of atomic hydrogen and helium with $\alpha$-quartz and calcium difluorite are described in Sec. III. The results in Tables III—V are indicated in atomic units, i.e., in terms of the atomic unit of the friction coefficient, which is equal to the atomic force unit (electrostatic force on two elementary charges a Bohr radius apart), divided by the atomic unit of velocity [equal to the speed of light multiplied by the fine-structure constant, see Eq. (27)]. The conversion of the entries given in Tables III—V to SI units is governed by Eq. (31a). The friction coefficients indicated in Table IV for gold are smaller by several orders of magnitude than those for SiO$_2$ (Table III) and CaF$_2$ (Table V).

Finally, in Appendix A, we illustrate the result on the basis of a calculation of the Maxwell stress tensor, and verify that the zero-temperature contribution to the quantum friction is suppressed in comparison to the main term given in Eq. (17a). In Appendix A, we refer to the zero-point/quantum fluctuations as opposed to the thermal fluctuations of the electromagnetic field.

For a discussion of experimental possibilities to study the calculated effects discussed here, we refer to Ref. [12]. An alternative experimental possibility would involve a laser interferometer [39]. An interferometric apparatus has recently been proposed for the study of gravitational interactions of anti-hydrogen atoms (see Refs. [40, 41]); the tiny gravitational shift of the interference pattern from atoms, after passing through a grating, should enable a test of Einstein’s equivalence principle for antimatter (this is the main conceptual idea of the AGE Collaboration, see Ref. [41]). Adapted to a conceivable quantum friction measurement, one might envisage the installation of a hot single crystal in one arm of a laser atomic beam interferometer, with a variable distance from the beam, in order to measure the predicted $Z^{-8}$ scaling of the effect.

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Appendix A: Quantum Friction for $T = 0$

We start from the zero-temperature result for the quantum friction of two semi-infinite solids, which is derived independently in Ref. [42]. Indeed, from Eqs. (15), (25) and (54) of Ref. [42], we have

$$F_x = \frac{\hbar S}{\pi^3} \int_0^\infty dk_\parallel k_\parallel \int_0^\infty dk_\perp e^{-2k_\parallel Z}$$

$$\times \int_0^{\nu_x k_\parallel} d\omega \text{Im} \left[ \epsilon_1(\omega) - 1 \right] \text{Im} \left[ \epsilon_2(k_\parallel \nu_x - \omega) - 1 \right] \left[ \epsilon_2(k_\parallel \nu_x - \omega) + 1 \right].$$

(A1)

The quantum friction force for an atom can be obtained from the above formula by a matching procedure. Namely, for a dilute gas of atoms, which we assume to model the slab with subscript 1, the relative permittivity can be written as follows,

$$\epsilon_1(\omega) = 1 + \frac{N_V}{\epsilon_0} \alpha(\omega),$$

(A2)

where $\alpha(\omega)$ is the (dipole) polarizability, and $N_V$ is the (volume) density of atoms. Here, $\epsilon_1(\omega)$ is assumed to deviate from unity only slightly. We can then substitute

$$\frac{\epsilon_1(\omega) - 1}{\epsilon_1(\omega) + 1} \approx \frac{N_V}{2\epsilon_0} \alpha(\omega).$$

(A3)
Here, \( N_V = S^{-1} dN/dz \) is equal to the increase \( dN \) in the number of atoms as we shift one of the plates by a distance \( dz \) from the other. The factor \( dN/dz \) can then be brought to the left-hand side where it reads as \( F_0(v)dz/dN \). Differentiating with respect to \( dz \), one obtains \( (dF_0(v)/dz)(dz/dN) = dF_0(v)/dN \), i.e., the force on the added atom. The net result is that we have to differentiate \( F_0 \) over \( z \), and divide the result by \( S N_V \), to obtain the force on the atom,

\[
F_x = -\frac{\hbar}{\pi^3 \epsilon_0} \int_0^\infty dk_{\parallel} k \int_{-\infty}^\infty dk_\perp k e^{-2k z} \times \int_0^\infty d\omega \, \text{Im} [\alpha(\omega)] \, \text{Im} \left[ \frac{\epsilon(k_{\parallel} v_x - \omega) - 1}{\epsilon(k_{\parallel} v_x - \omega) + 1} \right]. \tag{A4}
\]

In the limit of small velocities, i.e., \( v_x \ll Z \omega_0 \), where \( \omega_0 \) is the first resonance frequency of either the atom \( \alpha(\omega) \), we can replace both the polarizability of the atom as well as the dielectric function of the solid by their limiting forms for small argument, i.e., small \( \omega \) and small \( \omega' = k_{\parallel} v_x - \omega \), can be replaced by their low-frequency limits. We assume an atomic polarizability of the functional form

\[
\alpha(\omega) = \sum_n \frac{f_{n0}}{E_{n0}^2 - i \Gamma_n} \frac{1}{(\hbar \omega)^2 - (\hbar \omega)^2} , \tag{A5}
\]

where the oscillator strengths are denoted as \( f_{n0} \) and the \( E_{n0} \) are the excitation frequencies of the atom. For the zero-temperature quantum friction, the relevant limit is the limit of small angular frequency \( \omega \ll E_{10}/\hbar \), and we assume that the first resonance dominates, with \( \Gamma_1 \ll E_{10} \). Under these assumptions, we can approximate

\[
\text{Im} [\alpha(\omega)] = \sum_n \frac{f_{n0}}{E_{n0}^2} \Gamma_n \hbar \omega \approx \frac{\Gamma_1 (\hbar \omega)}{E_{10}^2} \alpha_0 . \tag{A6}
\]

We have written \( \alpha_0 = \alpha(0) \) for the static polarizability, and we assume that the sum is dominated by the lowest resonance corresponding to the first excited state with \( n = 1 \). If the assumptions are not fulfilled, then the relationship

\[
\alpha_0 = \frac{E_{10}^2}{\Gamma_1} \sum_n \frac{f_{n0}}{E_{n0}^2} \Gamma_n \tag{A7}
\]

may serve as the definition of the quantity \( \alpha_0 \). For the solid, we assume the functional form of a dielectric constant of a conductor, which contains a term with zero resonance frequency in the decomposition of the dielectric function. We have (see also Ref. [31]),

\[
\epsilon(\omega) \sim 1 - \frac{\omega_p^2}{\omega(\omega + i \gamma)} , \tag{A8a}
\]

\[
\text{Im} \left[ \frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 1} \right] \sim \frac{2 \omega_0 \gamma}{\omega_p^2} = \frac{2 \omega_0 \epsilon_0}{\sigma_T(0)} , \tag{A8b}
\]

where \( \sigma_T(0) \) is the temperature-dependent direct-current conductivity (for zero frequency). Substituting the results obtained in Eqs. (A6) and (A8)) in Eq. (A1) gives

\[
F_x = -\frac{\hbar}{\pi^3 \epsilon_0} \frac{\Gamma_1 \alpha_0}{E_{10}^2} \frac{2 \gamma}{\omega_p^2} \int_0^\infty dk_{\parallel} k \times \int_{-\infty}^\infty dk_\perp k e^{-2k z} \int_0^{v_x} d\omega' \omega (k_{\parallel} v_x - \omega' )
\]

\[
= -\frac{45 \hbar}{20 \pi^3 \epsilon_0} \frac{\Gamma_1 \alpha_0}{E_{10}^2} \frac{v_3^2}{\omega_p^2} z^2 \approx -\frac{45 \hbar}{20 \pi^3 \epsilon_0} \frac{\Gamma_1 \alpha_0}{E_{10}^2} \frac{v_3^2}{\omega_p^2} Z \sigma_T(0) , \tag{A9}
\]

with a \( Z^{-7} \) dependence. The \( \epsilon_0 \) factors cancel between the polarizability and the conductivity. The result vanishes in the limit \( \sigma_T(0) \rightarrow \infty \), where many materials become superconducting \( [\sigma(0) = \sigma_T(0) \rightarrow \infty \text{ for } T \rightarrow 0] \).

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