Towards quantum contact friction

Rasoul Kheiri
Skolkovo Institute of Science and Technology, Moscow, Russia
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A thermal model of kinetic friction is assigned to a classical loaded particle moving on a fluctuating smooth surface. A sinusoidal wave approximates surface fluctuations with a relaxation time. The Hamiltonian is approximated to the mean energy of the wave describing a system of Harmonic oscillators. The quantization of amplitudes yields in terms of annihilation and creation operators multiplied by a quantum phase. Further, we consider acoustic dispersion relation and evaluate the friction coefficient from the force autocorrelation function. The model results in the temperature dependence of the friction coefficient. It follows an asymptotic value for higher temperatures and suppresses at low temperatures. Moreover, a correspondence between quantum and classical views gives rise to a relation between the maximum amplitudes of the surface fluctuations and temperature.

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I. INTRODUCTION

According to the genuine antique results by Leonardo da Vinci, friction is independent of the contact area and proportional to the weight. Posterior, the first model of dry friction proposed by Coulomb explaining the proportionality of friction force on the normal load that is recognized as Amontons’ law [1]. The coulomb model provides a simple geometrical description for the friction coefficient, and further, it can be applied to show the independence of this coefficient from the contact area. The autonomy of friction force on surface roughnesses, however, was bestowed via novel experimental evidence in the last few decades [2]. The correctness of Coulomb law stems from the fact that the actual contact area could roughly be proportional to the normal load. In other words, the more normal load will bring more real contact areas.

As a significant improvement, classical contact mechanics is beholden to Heinrich Hertz, who studied elastic deformations published in 1882 via the problem of elastic curved surfaces in contact. For instance, surfaces that deform purely elastically like diamond or carbon coating planes are described by Hertzian force. A century later [3, 4], a similar theory for adhesive contact was proposed by Johnson, Kendall, and Roberts (JKR-Theory), which reduces to Hertz’ theory in the case of zero adhesion.

Experimentally, using atomic force microscopy (AFM) mainly [5], and other apparatus in general, people have accounted elastic properties such as Young’s modulus of different materials from graphene [6, 7] to other substances, including mica [8], and polymers [10]. Such surfaces are suitable as substrates to study the elastic properties like the proportionality of normal load and Hertzian compression effects [11, 12]. Notably, a graphene monolayer is known as one of the stiffest substrates ever seen [6]. By adding more layers, it has been reported that friction monotonically increases as the number of layers decreases [13, 14]. It follows that elastic distortions like wrinkles and similar deformations add friction with fewer atomic layers. Yet, the difference between the electron-phonon coupling of one layer and two layers is declared as another reason for reduced friction in one layer in comparison with bilayer graphene [15, 16]. Since then, molecular dynamics simulations have also investigated more the experimentally observed phenomenon [17, 18].

Indeed, friction is more complicated than elastic contacts because of plastic deformations, adhesion, cold-welding in metals [19], electric charges in the contact area, serrated deformations, etc. Remarkably, however, the Coulomb friction coefficient can still be independent of the normal load. Moreover, for plastic deformations of the surface, there are classifications for calculating the friction coefficient in terms of penetration hardness and tangential stress [20]. Taking this into account ambitiously, a theory of quantum contact friction might go beyond elasticity. For one thing, plastic deformations are to be explained quantum mechanically in part [21, 22]. From this perspective, in addition to a linear dispersion for acoustic phonons, a quadratic dispersion relation is approximated for plastic deformations. It could be interesting that an analogy between such localized plasticity and superfluidity regime is maintained. Likewise, in the case of low-temperature serrated deformations [23], a quantum mechanism for dislocation motion is suggested for deformation stress dependency on temperature. In particular, loading effects on the deformation observed for Aluminum samples experimentally at 1.4 K. Consequently, the future of quantum contact friction may include elastic and plastic deformations, serrated surfaces, and maybe beyond.

Additionally, there are inherently quantum phenomena like superconductivity, superfluidity, and vacuum field at absolute zero temperature. Especially, in the absence of static friction in incommensurate crystals [24–26], phononic friction for atomically flat dielectrics is temperature-dependent. As a consequence, quantum su-
perslipperiness occurs at low temperatures [29]. These pioneer results are quite inspiring to do more studies in regard to phononic sliding friction [30].

Macroscopically, the "dry friction" between solid surfaces is a force $F_{fr}$ that is linearly dependent on the normal load $F_N$ acting on the bulk ($F_{fr} = \mu F_N$). For a body moving through a viscous fluid with viscosity $\eta$, on the other hand, the dissipative mechanism is a function of the object’s velocity $v$, to be linear $F_{fr} = \eta v$ at relatively low speeds. One main difference between the dry friction and viscous friction is that in the former, there is static friction ($\mu_s > \mu_k$), which is absent in the latter. In addition, the Coulomb law emphasizes that the dry friction is independent of the object’s velocity for ordinary sliding faces that are opposed to that of viscous friction.

Nevertheless, the micro-scale situations are often more detailed and more complicated. For example, regarding a thin film, there might be no constant and net normal force on it. In this case, surface friction can be close to a viscous fluid regime in the absence of any classical fluid [31]. On the atomic scale, while surface asperities are a certain cause for the surface friction, the friction coefficient can remain non-zero or even relatively high in the absence of wear, and plowing effects [32]. Equally important, one may find a superlubricity regime for such surfaces as a quantum effect when approaching absolute zero temperature [29]. These two thresholds are of fundamental importance for phononic models.

A first-principle model of lattice vibrations was introduced by Prandtl (known as Prandtl-Tomlinson model) [33, 34]. The model contains a point particle moving in a combination of a periodic potential and a harmonic oscillator potential as conservative forces. The particle is also subjected to a viscous damping force, which is non-conservative. Interestingly, the coefficient of periodic force determines the static friction, and the damping force is related to sliding friction. Tabor [35] inspired by Tomlinson’s work [36], suggested that in the cases where friction is dependent on speed or temperature, the strain energy of shear distortions is lost in the form of vibrations (phonons) [37]. Besides, the model can be extended from one particle to a system of particles. A significant extension of the Prandtl-Tomlinson image is called the Frenkel-Kontorova (FK) model [38, 39]. It is a chain of classical particles coupled harmonically with their nearest neighbors and subjected to a substrate periodic potential [40]. In this connection, the damping mechanism as the source of sliding friction can emerge from the absorption of kinetic energy by phonons [41]. Neglecting the kinetic energy, otherwise, is referred to as static FK model [42]. In addition, the structural superlubricity comes from the incommensurability of the system [43], which is observed experimentally for graphite [44]. Furthermore, nonlinear phenomena can also be described based on FK models [45].

In effect, phonons might be counted on transversal or longitudinal excitations [45]. For instance, a transverse-based study [46], show a connection between the natural frequency of the vibrational surface and the dissipated kinetic energy. In another study, longitudinal vibrations are considered as a two-dimensional FK model [42].

Above all, the first experiments, as evidence of phononic friction, utilized Quartz Crystal Microbalance (QCM) to probe sliding friction for an absorbed monolayer on metal surfaces [24] followed by [47, 48]. Further, in detailed simulations [49], an anharmonic coupling is suggested as the dissipation mechanism.

In the current study, an atomically smooth plane is supposed on which the surface phonons are the origin of kinetic friction [50]. On the surface, we consider an elastically deformed particle [51] undergoing a normal load described by the Hertzian force. By this model, we consider thermal fluctuations on a surface around a constant temperature for calculating the friction coefficient. Our work steps are as the following. In Section II we elaborate a classical thermal contact model of friction for a compressed particle on a fluctuating surface. A sinusoidal function approximates the surface fluctuations for evaluating the friction force. Further, the friction coefficient will be assessed via the fluctuation-dissipation theorem for the resistance force autocorrelation in a canonical averaging. Next in Section III on a quantum level, surface fluctuations are described by raising and lowering operators together with a phase operator [52]. As a result, the temperature-dependent friction coefficient will be evaluated and illustrated. It follows that both classical and quantum theories have an identical asymptotic value. In addition, correspondence between classical and quantum evaluations, in Section IV makes the maximum amplitudes of the surface fluctuations be a non-trivial function of temperature. Finally, appendix A expands the phase operator properties as used in the article.

II. A CONTACT MODEL OF KINETIC FRICTION

A. Friction force

Figure 1 is an outline of an ideal flat surface without any other asperities but some sinusoidal vibrations as the only bulges of the surface. In this picture, a particle is being pushed by the normal load $F_s$ while moving on the surface with the velocity of $v$. To begin with, the current height of the surface at point $r$ and time $t$ is determined by the amplitude and phase of the surface phonons at this point, i.e.

$$z_k(r, t) = A_k \cos(k \cdot r - \omega_k t + \phi_k) e^{-t/\tau_{ph}},$$  \hspace{1cm} (1)

where $k$ is a given wavenumber ($k = 2\pi/\lambda$), and $\tau_{ph}$ stands for the relaxation time of phonons. In one dimension, the exponential decomposition of Eq. 1 at $t = 0$ is
\[ z_k(x, 0) = \frac{A_k}{2} [e^{i\Phi_k} + e^{-i\Phi_k}], \quad \Phi_k = kx + \phi_k. \quad (2) \]

It turns out that, the first approximation for a non-flat surface comes from small phases, \( \Phi_k \), to the extent that:

\[ e^{i\Phi_k} \approx 1 + i\Phi_k + \frac{i^2\Phi_k^2}{2}, \quad (3) \]

from which

\[ z_k(x, 0) \approx A_k[1 - \frac{\Phi_k^2}{2}] = A_k[1 - \frac{1}{2}(kx + \phi_k)^2]. \quad (4) \]

Alternatively, the inclination of the surface makes an angle, say \( \alpha \), for a particle on it. Since the particle is pushing down with a normal load, a horizontal resistant force of \( F_N \sin \alpha \) applies to the compressed particle with slight deformation of \( \xi \) on the surface. Therefore, the height \( z_p \) of a squeezed particle in an inclined surface will be shifted by

\[ z_p(x) = R_p - \sqrt{R_p^2 - x^2} - \xi, \]

where \( R_p \) stands for the radius of the particle. Thus, for small deformations of \( \xi \ll R_p \),

\[ z_p(x) \simeq \frac{1}{2R_p}x^2 - \xi. \quad (5) \]

Therewith, the quadratic equation of

\[ z_k(x) = z_p(x), \quad \rightarrow \quad ax^2 + bx + c = 0, \quad (6) \]

gives rise to the solution points \( x_1, x_2 \) for the contact line between the surface and the deformed particle on it. Therefore, having the center of the contact line as \( x_m = (x_1 + x_2)/2 = -b/2a \), an estimation for the inclination angle is

\[ \sin \alpha \simeq \tan \alpha = \frac{x_m}{R_p} = -\frac{1}{2R_p} \frac{b}{a} \simeq -A_k k \phi_k. \quad (7) \]

where, we omitted the term including \( A_k^2 \) in the denominator by virtue of the small-amplitude assumption \( |\xi| \ll 1 \).

Consequently, the horizontal force against the particle movement reads

\[ F_k = F_N \sin \alpha \approx -(A_k k \phi_k) F_N. \quad (8) \]

This is the kinetic friction, \( F_{fr} \equiv F_k \), when a particle traverses such a fluctuating surface undergoing a normal load \( F_N \). The normal load is assumed to impose small deformations \( \xi \) to the particle, and the surface fluctuations approximated to the small phases \( \Phi_k \) according to Eq. 3.

**FIG. 1:** A particle on a fluctuating surface is squeezed by a normal load \( F_z \) while moving with the velocity of \( v \). The fluctuations are described by a cosine wave function and approximated further to the first two terms.

### B. Fluctuation-dissipation theorem

From the velocity of the classical particle, we can define the thermal frictional coefficient via the fluctuation-dissipation theorem \([50, 54]\).

\[ F_{sol.fr}(t) = \sum_k F_k(t) = -\int_0^t \tilde{\gamma}_{sol.fr}(t - \tau) v(\tau) d\tau + \zeta(t), \]

where \( v \) stands for the velocity of the particle, and \( \tilde{\gamma}_{sol.fr}(t) \) is the memory function. Accordingly, the microscopic random forces \( \zeta(t) \) make the macroscopic friction coefficient of the solid friction force \( F_{sol.fr} \). Namely,

\[ \langle \zeta(t') \cdot \zeta(t) \rangle = 2k_B T \tilde{\gamma}_{sol.fr}(t - t'), \quad \langle \zeta(t) \rangle = 0, \]

where \( k_B \) and \( T \) are Boltzmann constant and temperature, respectively. For non-correlated random forces, \( \tilde{\gamma}_{sol.fr}(t - t') = 4 \gamma_{sol.fr} \delta(t - t') \), the two-dimensional friction coefficient will be evaluated by

\[ \gamma_{sol.fr} = \frac{1}{2k_B T} \int_0^\infty \sum_{k_1, k_2} \langle F_{k_1}(0) F_{k_2}(t) \rangle dt. \]

To calculate the time correlation function, averaging takes place with respect to the canonical (Boltzmann-Gibbs) distribution of

\[ \exp(-\beta \mathcal{H})/Z, \]

which implies that the system with Hamiltonian \( \mathcal{H} \) is in a thermal equilibrium. Here \( Z \) stands for the partition function and \( \beta = 1/k_B T \). In addition, assuming isotropic directions for wavenumbers, the friction coefficient reduces to

\[ \gamma_{sol.fr} = \frac{1}{2k_B T} \int_0^\infty \sum_k \langle F_k(0) F_k(t) \rangle dt, \quad (9) \]
where, the wavevector $k$ in the summation refers to the number of wavenumbers $k$ on a two-dimensional surface.

The thermal friction coefficient assumes to satisfy the fluctuation-dissipation theorem with a zero mean when a Langevin equation describes the motion of a particle, including a random thermal force \[. In our case, $F_k$ is approximated by Eq. \[\text{in each directions}. In brief, the thermal frictional force $-\gamma_{\text{sol.fr.}}\mathbf{v}$ is acting against the velocity $\mathbf{v}$ of the squeezed particle. It has a different nature other than the Coulomb friction force, which is athermal and does not depend on particle velocity. The diffusion coefficient, in turn, is obtainable via the corresponding Langevin equation \[\text{.}

\[\text{C. Mean energy}

For a sinusoidal wave in two dimension

\[z_k(r, t) = A_k \cos(kr - \omega t + \phi_k) \tag{10}\]

the wave mean energy might be obtained from $E_k = \rho_s S/((\partial z/\partial t)^2)$ \[\text{, from which}

\[E_k = \frac{1}{2} \rho_s \omega_k^2 A_k^2. \tag{11}\]

Therefore, considering a system of non-interacting lattice excitations, the mean energy obtains form

\[E = \frac{1}{2} \rho_s \sum_{k=1}^{k_D} \omega_k^2 A_k^2. \tag{12}\]

We use the mean energy for the classical averaging. By quantization, we show that the mean energy corresponds to the Hamiltonian of a system of Harmonic oscillators.

\[\text{D. Classical friction coefficient}

Substitution of Eq. \[\text{in Eq. \[\text{gives rise to}

\[\gamma_{\text{sol.fr.}} = \frac{F_N^2}{2k_B T} \int_0^\infty dt \sum_k k^2 \langle A_k(0) A_k(t) \rangle \langle \phi_k(0) \phi_k(t) \rangle. \tag{13}\]

On the surface of $S$ \[\text{,}

\[\sum_k f(k) = \frac{S}{2\pi} \int_0^{k_D} f(k) k dk, \tag{14}\]

where $k_D$ is the maximum wavenumber. Moreover, the time dependency is a relaxation for the amplitudes, $A_k(t) = A_k(0) e^{-t/\tau_{ph}}$, and a shift for the phases $\phi_k(t) = \phi_k(0) - \omega_k t$, according to Eq. \[\text{. Thereupon,}

\[\langle A_k(0) A_k(t) \rangle = \langle A_k^2 \rangle e^{-t/\tau_{ph}}, \tag{15}\]

and in a symmetric interval

\[\langle \phi_k(0) \phi_k(t) \rangle = \langle \phi_k^2(0) \rangle. \tag{16}\]

We take averaging in a thermal equilibrium supposing thermal fluctuations of the surface around a constant temperature. Thereby, an average on the amplitudes $A_k$ makes true in regard to $\mathcal{H}_k$ of the surface fluctuations. Having

\[\mathcal{E}_k = \frac{1}{2} \rho_s \omega_k^2 A_k^2, \tag{17}\]

\[\alpha_k^2 = \rho_s \omega_k^2/2k_BT, \tag{18}\]

then

\[\langle A_k^2 \rangle = \frac{\int_0^{A_k^{\text{max}}} A_k^2 \exp(-\beta \mathcal{E}_k) dA_k}{\int_0^{A_k^{\text{max}}} \exp(-\beta \mathcal{E}_k) dA_k} \tag{19}\]

For a significant $A_k^{\text{max}}$, the integral is Gaussian. Otherwise, $\langle A_k^2 \rangle$ depends on $A_k^{\text{max}}$. In the more general case,\n
\[\langle A_k^2 \rangle = \frac{1}{2\alpha_k^2} \langle \phi_k^2 \rangle A_k^2, \tag{20}\]

where $\alpha_k A_k$ is a dimensionless variable. Furthermore, the mean energy $\mathcal{E}_k$ is independent of phases. Thereupon, for averaging on phases $\phi_k$

\[\langle \phi_k(0) \phi_k(t) \rangle = \langle \phi_k^2(0) \rangle = \frac{\int_0^{\pi} \phi_k^2(t) d\phi_k}{\int_0^{\pi} d\phi_k} = \frac{\pi^2}{3}, \tag{21}\]

It is noted that $\Phi_k = kx + \phi_k$ is small, but $\phi_k \in [-\pi, \pi]$ for which $\langle \phi_k \rangle = 0$. Additionally, in the linear approximation of acoustic branch $\omega_k = c_k$, phase velocity is equal to the speed of sound. Eventually, substituting Eq. \[ and Eq. \[ in Eq. \[ gives rise to the classical friction coefficient $\gamma_{\text{cd}}$, viz.,

\[\frac{\gamma_{\text{cd}}}{\Gamma} = (2\alpha_k^2 \langle A_k^2 \rangle), \quad \Gamma = \frac{\pi}{24} \frac{F_N^2 \tau_{ph} k_D^2}{\rho_s c_s^2}, \tag{22}\]

where $\Gamma$ is the asymptotic value. One can rewrite the asymptotic friction coefficient in terms of Debye temperature $\Theta_D$. That is,
might be more tangible than the
shows that a significant maximum for the am-
in effect of a random force
one. In the current thermal model, we have counted the
surface may have higher or lower fluctuations than a hot
particles, temperature, etc. As a tangible example, a cold
action potentials, the viscosity of the surface, mass of the
mechanism for small fluctuations relates to the inter-
trivial. Fortunately, the dependence between
more temperature adds more energy to the surface fluc-
to calculate the friction coefficient. It is expected that
Figure 2 shows that a significant maximum for the am-
plitude of the surface fluctuations $A_k^{\text{max}}$ gives rise to a
stable friction coefficient $\Gamma$. Alternatively, the friction
coefficient goes to zero when $A_k^{\text{max}} \to 0$.
Indeed, for a surface consisting of interacting particles,
the mechanism for small fluctuations relates to the inter-
action potentials, the viscosity of the surface, mass of the
particles, temperature, etc. As a tangible example, a cold
surface may have higher or lower fluctuations than a hot
one. In the current thermal model, we have counted the
effect of a random force $\zeta(t)$ and a relaxation time $\tau_{\text{ph}}$
to calculate the friction coefficient. It is expected that
more temperature adds more energy to the surface fluct-
uations. However, this temperature dependency is not
trivial. Fortunately, the dependence between $\alpha_k A_k^{\text{max}}$
and temperature $T$ will be revealed later in Section IV in
comparing classical and quantum models.
Before that, we calculate the corresponding quantum
friction coefficient utilizing a quantized force as the fol-
III. FORCE QUANTIZATION AND FRICTION
COEFFICIENT
At the atomic level, kinetic energy is transforming
into thermal energy [31]. Therefore, a quantum ther-
mal model for kinetic friction becomes sensible, especially
when neglecting the athermal asperities. Even in an ideal
case of the thermal model, there could be more than one
source of friction, including electronic and phononic fric-
tion mechanisms. However, phonons’ contribution looks
significant in the case of smooth insulators (dielectrics).
The simplicity of (non-magnetic) insulators as a sub-
strate to be compared to solid metals, for example, is due
to phonons being the only source of transport processes
[29, 59]. In this regard, one may assume an ideal surface
without any source of friction but thermal phonons.

A. Quantum amplitudes

For amplitude quantization, it is essential to have sur-
faced excitations in correspondence with the classical cos-
ine function of Eq. (1). Otherwise, we might miss some-
thing in our derivations or have some additional terms
and add non-sense assumptions to justify the results. For
this purpose, one may use rising and lowering operators
as well as quantum phase operators to build a quantized
form of Eq. (1). The phase operator method has firstly
been in optics for electromagnetic fields [60, 61]. Here,
we suggest a similar theory for phonon excitations on
condensed matter.
Assume surface excitations as
$$
\hat{\zeta}(r, t) = \sum_k \sqrt{\frac{\hbar}{m \omega_k}} \left[ \hat{a}_k e^{i(k x - \omega t)} + \hat{a}^\dagger_k e^{-i(k x - \omega t)} \right],
$$
we show that such excitations correspond to the classical
wave of Eq. (1). For a single excitation, and in the one-
dimensional case at $t = 0$
$$
\hat{\zeta}(x, 0) = \sqrt{\frac{\hbar}{m \omega_k}} [\hat{a}_k e^{ik x} + \hat{a}^\dagger_k e^{-ik x}],
$$
Now, let’s check the classical correspondence with $\hat{a}^\dagger_k \rightarrow a^*_k$. Introducing the real $A_k$ such that
$$
a_k = R_k e^{i\phi_k}, \quad a^*_k = R_k e^{-i\phi_k}
$$
then, classically
$$
z(x, 0) = \sqrt{\frac{\hbar}{m \omega_k}} R_k [e^{i(k x + \phi_k)} + e^{-(i k x + \phi_k)}],
$$
which is precisely in correspondence with the cosine function of
$$
z(x, 0) = A_k \cos(k x + \phi_k), \quad A_k = R_k \sqrt{\frac{\hbar}{m \omega_k}}
$$
Thereupon, we rewrite the equation (26) for quantum am-
plitudes. Namely,
\[ \hat{R}_k = \hat{a}_k e^{-i\hat{\phi}_k}, \quad \text{or} \quad \hat{R}_k = \hat{a}_k^\dagger e^{i\hat{\phi}_k}, \quad (27) \]

where \( \hat{\phi}_k \) is a Hermitian quantum phase operator detailed in Appendix A. Because of commutation, one notes that these two alternatives for the operator \( \hat{R}_k \) are not equivalent, in contrast with the classical case. Therefore, we should count for both possibilities in Eq. (27). That is to say,

\[ \hat{A}_{k,1} = \sqrt{\frac{\hbar}{m\omega_k}} \hat{a}_k e^{-i\hat{\phi}_k}, \quad \text{and} \quad \hat{A}_{k,2} = \sqrt{\frac{\hbar}{m\omega_k}} \hat{a}_k^\dagger e^{i\hat{\phi}_k}. \quad (28) \]

Hence, the quantization of amplitudes as a vertical displacement of the surface yields in terms of annihilation \( \hat{a}_k \) and creation \( \hat{a}_k^\dagger \) operators multiplied by a quantum phase \( e^{\pm i\hat{\phi}_k} \) in correspondence with the classical model.

### B. Approximated Hamiltonian

Having Eq. (28), one can take the averages of amplitudes in a given state \( |n_k\rangle \). For \( \hat{A}_{k,1} \)

\[ \langle n_k|\hat{A}_{k,1}\hat{A}_{k,1}|n_k\rangle = \frac{2\hbar}{m\omega_k} \langle n_k|\hat{a}_k e^{-i\hat{\phi}_k} \hat{a}_k e^{-i\hat{\phi}_k}|n_k\rangle, \quad (29) \]

we can use the Hermitian property of the amplitude as

\[ \hat{a}_k e^{-i\hat{\phi}_k} = e^{i\hat{\phi}_k} \hat{a}_k^\dagger, \quad (30) \]

which reads

\[ \langle n_k|\hat{a}_k e^{-i\hat{\phi}_k} e^{i\hat{\phi}_k} \hat{a}_k^\dagger|n_k\rangle = \langle n_k|\hat{a}_k \hat{a}_k^\dagger|n_k\rangle = \langle n_k|N + 1|n_k\rangle \]

or

\[ \langle n_k|\hat{A}_{k,1}\hat{A}_{k,1}|n_k\rangle = \frac{\hbar}{m\omega_k} (n_k + 1). \]

In a similar way for another possible amplitude,

\[ \hat{A}_{k,2} = \sqrt{\frac{\hbar}{m\omega_k}} \hat{a}_k e^{i\hat{\phi}_k}, \]

the average in a given \( |n_k\rangle \) derives from

\[ \langle n_k|\hat{a}_k^\dagger e^{i\hat{\phi}_k} \hat{a}_k e^{i\hat{\phi}_k}|n_k\rangle = \langle n_k|\hat{a}_k^\dagger \hat{a}_k|n_k\rangle = n_k. \]

To consider both kinds of amplitudes in the energy,

\[ \langle n_k|\hat{A}_{k,1} \hat{A}_{k,1} \rangle + \hat{A}_{k,2} \hat{A}_{k,2}|n_k\rangle = \frac{2\hbar}{m\omega_k} n_k. \quad (31) \]

where we omitted the constant factor on the right-hand side belonging to the vacuum state that is canceled by changing the reference frame \[62\]. Accordingly, the energy of the states reads \( E_{n_k} = n_k \hbar \omega_k \). Eventually, having the classical mean energy, \( E_k = (1/2) m\omega_k^2 A_k^2 \), the mean energy of the wave describes the Hamiltonian of a system of independent harmonic oscillators.

\[ \hat{H} = \sum_{k=1}^{k_D} \hbar \omega(k) \hat{a}_k^\dagger \hat{a}_k. \quad (32) \]

### Time evaluation and relaxation time

The time-evolution of a quantum operator follows from \( \hat{A}_k(t) = \hat{U}^\dagger \hat{A}_k(0) \hat{U} \), where in a time-independent potential, the propagator is simply a shift as \( \hat{U} = \exp(-i\hat{H}t/\hbar) \). Therefore, regarding the Hamiltonian of Eq. (32) the time-dependent phase operator follows (see Eq. (A4) in Appendix A2)

\[ \hat{\phi}_k(t) = \hat{\phi}_k - \omega_k t. \quad (33) \]

Furthermore, the amplitudes in Eq. (28) are time-invariant operators. For example,

\[ \hat{U}^\dagger \hat{a}_k e^{-i\hat{\phi}_k} \hat{U} = \hat{U}^\dagger \hat{a}_k \hat{U} \hat{U}^\dagger e^{-i\hat{\phi}_k} \hat{U}, \]

and

\[ \hat{a}_k(t) e^{-i\hat{\phi}_k(t)} = \hat{a}_k e^{-i\omega_k t} e^{-i\hat{\phi}_k - \omega_k t} = \hat{a}_k e^{-i\hat{\phi}_k}. \]

Then, for the time-independent Hamiltonian of Eq. (32) phonon amplitudes are time-invariant.

Yet, a quantum excited state can not remain exited forever \[63\]. Ergo, the relaxation time is supposable by considering \( \omega_k \rightarrow \omega_k \pm i(t/\tau_{ph}) \) only for the argument of \( e^{\pm i\hat{\phi}_k} \) respectively, where \( \tau_{ph} \) refers to the relaxation time of phonons. This argument agrees with the response theory, where a phase shift corresponds to the imaginary part of the frequency response function. Consequently,

\[ \hat{A}_k(t) = \hat{A}_k(0) e^{-t/\tau_{ph}}, \quad (34) \]

for both \( \hat{A}_{k,1} \), and \( \hat{A}_{k,2} \). Otherwise, for a first principle relaxation, one needs a time-dependent Hamiltonian \( \hat{H}(t) \), which we have not followed here. On this account, the Hamiltonian in \( t = 0 \) is approximated by Eq. (32). However, it would be different for \( t > 0 \) so that the phase...
\( \hat{\phi}_k \) of a phonon’s amplitude has an imaginary part for relaxation. Equation (34) corresponds to the classical relaxation in Eq. (1) for a two-dimensional surface. The existence of an effective relaxation time implies that the thermal fluctuations are not quantum adiabatic. It means that moving the particle on the surface is not faster than surface changes. Namely, the surface is dynamic during an experiment.

C. Quantum time-correlation function

Having the Hamiltonian of Eq. (32) the aim is to derive the force correlation function and evaluate Eq. (9) in the quantized form. Time-correlation, \( C_{A,A}(t,t') \), for the function \( A \), is an average over an equilibrium ensemble \( \langle \ldots \rangle_{eq} \). Namely,

\[
C_{A_k A_k}(t,t') = \langle A_k(t) A_k(0) \rangle_{eq}.
\]

In quantum regime, the corresponding average of an operator \( A \) in its matrix representation can be obtained by taking a trace weighted by a density operator in equilibrium \( \rho_{eq} \). That is

\[
\langle \hat{A} \rangle = \text{Tr}(\rho_{eq} \hat{A}), \quad \mathcal{Z}_k = \text{Tr}(e^{-\beta \hat{H}_k}).
\]

Thereby, \( \langle \hat{A}_k \rangle = \sum_{n_k=0}^{\infty} e^{-\beta E_{nk}} / \mathcal{Z}_k \langle n_k | \hat{A}_k | n_k \rangle \), and

\[
C_{A_k A_k}(t) = \frac{\sum_{n_k=0}^{\infty} e^{-\beta E_{nk}} \langle n_k | \hat{A}_k(t) \hat{A}_k(0) | n_k \rangle}{\sum_{n_k=0}^{\infty} e^{-\beta E_{nk}}}. \tag{35}
\]

As a consequence, regarding a Hermitian quantum force \( \hat{F}^1 = \hat{F} \), the quantized form of Eq. (9) by \( |F| \equiv F \) will be

\[
\gamma_{\text{sol.fr.}} = \frac{1}{2k_B T} \int_0^\infty \sum_k \left| \frac{\hat{F}_k(0) \hat{F}_k(t) + \hat{F}_k(t) \hat{F}_k(0)}{2} \right| dt. \tag{36}
\]

In what follows, we are about to quantize the force of Eq. (8) to evaluate the quantum friction coefficient in the thermal equilibrium.

1. Quantized force

For elastic Hertzian deformation \( \xi \), the normal load \( F_N = K \xi^{3/2} \) remains classical with the assumption of \( A_k \ll \xi \). To put it another way, one could say that we quantized the surface but not the particle moving on it. Thereupon, a quantum force corresponding to Eq. (8) is

\[
\hat{F}_k \simeq -(\hat{A}_k k \hat{\phi}_k) F_N. \tag{37}
\]

Further, the autocorrelation function for a quantized force is derived in Appendix \( \text{III C} \). Regarding Eq. (34),

\[
[\hat{A}_k, \hat{A}_k(t)] = 0.
\]

As a result, the quantized force commute at different times, and the friction coefficient of Eq. (38) reduces to

\[
\gamma = \frac{1}{2k_B T} \int_0^\infty \sum_k \langle \hat{F}_k(0) \hat{F}_k(t) \rangle dt. \tag{38}
\]

Substituting Eq. (37) to Eq. (38) gives rise to the friction coefficient for the quantized force.

\[
\gamma = \frac{F^2}{2k_B T} \int_0^\infty \sum_k k^2 \langle \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) \rangle dt, \tag{39}
\]

where \( \hat{A}_k(t) = \hat{A}_k(0) e^{-t/\tau_{ph}} \), and \( \hat{\phi}_k(t) = \hat{\phi}_k - \omega_k t \). Following the discussion in Appendix \( \text{A} \), for \( \langle \hat{\phi}_k \rangle = 0 \),

\[
\langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) | n_k \rangle = \frac{\pi^2 h)e^{-t/\tau_{ph}}}{3 \omega_k} \left( 1 - \frac{\Psi(1, n_k + 1)}{\pi^2/3} \right). \tag{40}
\]

where \( \Psi(m, x) \) is the polygamma function of order \( m \), that is the \( (m+1) \)th derivative of the logarithm of the gamma function \( (\frac{d^{m+1}}{dx^{m+1}} \ln \Gamma(x)) \).

In the thermal equilibrium,

\[
\sum_{n_k} e^{-\epsilon n_k} \langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) | n_k \rangle ,
\]

where \( \epsilon = \beta \omega_k \), and the averages on a given state \( |n_k \rangle \) derived by Eq. (40).

2. Friction coefficient

To have a close analytic form, we note that the term \( \Psi(1, n_k + 1)/(\pi^2/3) \) in Eq. (40) will rapidly vanish. Then, an approximation comes true when one let

\[
\langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) | n_k \rangle = \frac{\pi^2 h)e^{-t/\tau_{ph}}}{3 \omega_k} n_k, \tag{41}
\]

from which the thermal average of the amplitudes obtains simply by

\[
\langle \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) \rangle = \frac{\pi^2 h)e^{-t/\tau_{ph}}}{3 \omega_k} \sum n_k e^{-\beta E_{nk} n_k} \sum n_k e^{-\beta E_{nk}} = \frac{\pi^2 h)e^{-t/\tau_{ph}}}{3 \omega_k} \frac{1}{e^{\beta \omega} - 1}. \tag{42}
\]
Further, substituting Eq. 12 into Eq. 39 gives rise to
\[
\gamma = \frac{\pi^2}{3} \frac{F_N^2 \tau_{ph}}{2m} \sum_k \frac{k^2}{\omega_k^2} \frac{\beta \hbar \omega_k}{e^{\beta \hbar \omega_k} - 1}.
\]
For acoustic phonons \(\omega_k = c_s k\),
\[
\gamma = \frac{\pi^2}{3} \frac{F_N^2 \tau_{ph}}{2mc_s^2} \sum_k \frac{\beta \hbar c_s k}{e^{\beta \hbar c_s k} - 1}.
\]
On the surface of \(S\) \[\sum_k f(k) = \frac{S}{2\pi} \int_0^{k_D} f(k) \, k \, dk\], thus
\[
\gamma = \frac{\pi}{12} \frac{F_N^2 \tau_{ph}}{\rho_s c_s^2} \int_0^{k_D} \frac{\beta \hbar c_s k^2}{e^{\beta \hbar c_s k} - 1} \, dk,
\]
where \(\rho_s = m/S\) is the surface density. Considering the Debye temperature
\[
k_B \Theta_D = \hbar \omega_D = \hbar c_s k_D,
\]
one can define
\[
\epsilon = \beta \hbar c_s k, \quad \frac{\Theta_D}{T} = \beta \hbar c_s k_D, \quad x = \Theta_D/T,
\]
whence the approximated friction coefficient simplifies to the second Debye function:
\[
\gamma = \frac{\pi}{24} \frac{F_N^2 \tau_{ph} k_D^2}{\rho_s c_s^2} \frac{2}{x^2} \int_0^x \frac{\epsilon^2}{e^\epsilon - 1} \, d\epsilon.
\]
Remembering the asymptotic friction coefficient \(\Gamma\), Eqs. 22 & 23 in the classical derivations and Debye functions
\[
D_n(x) = \frac{n}{x^n} \int_0^x \frac{\epsilon^n}{e^\epsilon - 1} \, d\epsilon,
\]
the friction coefficient reads
\[
\frac{\gamma}{\Gamma} = D_2(x).
\]
Equation 43 is an approximation for the friction coefficient with quantized amplitudes based on the analytic approximation of Eq. 12. One sees that the exclusion of the vacuum state avoids having infinities in the friction coefficient.

FIG. 3: Friction coefficient as a function of temperature for the quantized force of Eq. 37. The asymptotic value \(\Gamma\) is identical to the classical case. Moreover, the friction coefficient vanishes for lower temperatures \(T \to 0\). The dashed line refers to \(D_2(x)\); an approximation by the quantized amplitudes but classical phases. The blue line \(Dp_{21}(x)\) has counted both quantized amplitudes and phases.

Nevertheless, taking into account the term \(\Psi(1, n_k + 1)/(\pi^2/3)\) in Eq. 40, it will change the thermal equilibrium of Eq. 12 to
\[
\langle \hat{A}_k \hat{\phi}_k \hat{A}_k(t) \hat{\phi}_k(t) \rangle = \frac{\pi^2}{3} \frac{\hbar e^{-t/\tau_{ph}}}{m \omega_k} \sum_e e^{-\beta E_{n_k}} n_k \left[ 1 - \frac{\Psi(1, n_k + 1)}{\pi^2/3} \right] \sum_{n_k} e^{-\beta E_{n_k}} \frac{1 - \Psi(1, n_k + 1)}{\pi^2/3}.
\]
so that the friction coefficient is modified as
\[
\frac{\gamma}{\Gamma} = \frac{2}{x^2} \int_0^x \frac{\epsilon^2}{e^\epsilon - 1} \, d\epsilon \sum_{n_k} e^{-\epsilon_{n_k}} n_k \left[ 1 - \frac{\Psi(1, n_k + 1)}{\pi^2/3} \right] \sum_{n_k} e^{-\epsilon_{n_k}} \frac{1 - \Psi(1, n_k + 1)}{\pi^2/3}.
\]
We may call the right-hand side of Eq. 44 as \(Dp_{21}(x)\) due to changing \(D_2(x)\) by quantum phase average in Eq. 20. Accordingly, with this correction
\[
\frac{\gamma}{\Gamma} = Dp_{21}(x).
\]
To sum up, Eq. 43 was the first derivation for the friction coefficient by the second Debye function \(D_2(x)\). Then, we added quantum average of the phases (Eq. 20) resulted in Eq. 46. Figure 3 illustrates \(Dp_{21}(x)\) in blue. In addition, the second Debye function, \(D_2(x)\), is depicted in a black dashed line. The horizontal axis in Fig. 3 is temperature scaled in the Debye temperatures. In the case of \(D_2(x)\), the phase average remains identical to the classical phase \((\pi^2/3)\). For \(Dp_{21}(x)\), the classical \(\pi^2/3\) is replaced by the quantum phase average of Eq. 20. A comparison between \(D_2(x)\) and \(Dp_{21}(x)\) in Fig. 3 shows that the quantum phase average of Eq. 20 decreases the friction coefficient slightly at the middle temperatures.
IV. CORRESPONDENCE BETWEEN CLASSICAL AND QUANTUM MODELS

According to the quantum theory, the friction coefficient is a function of temperature; $T/\Theta_D$. The classical dependency of friction coefficient, on the other hand, is $\alpha_k A_k^{\text{max}}$ where $A_k^{\text{max}}$ is the maximum amplitude that appears on the surface. To have a correspondence between classical and quantum results, $\alpha_k A_k^{\text{max}} \propto T/\Theta_D$. Further, letting this proportionality be an equation (we don’t have any reason for otherwise), then

$$\alpha_k A_k^{\text{max}} = \frac{T}{\Theta_D}. \quad (47)$$

Thereupon, one can make a comparison between classical and quantum friction coefficients. To point out, Debye temperature is a finite temperature typically around $(10^2-10^3)^\circ K$. Thus, a finite temperature quantum effect could be reported if some experimental measurements on friction coefficient agree more with a quantum theory.

Nevertheless, one notes that the harmonic assumption might not be a satisfactory theory when approaching the melting point. Finally, the quantum theory predicts a super slippery for $T \to 0$ consistent with $A_k^{\text{max}} \to 0$ in the classical evaluation. Yet, quantum uncertainty or virtual particles at $T = 0$ demand a vanishing but non-zero friction coefficient in the quantum realm, which needs to be figured out by future works.

V. CONCLUSION

In this paper, we followed a model of kinetic friction regarding a thermal-fluctuating surface and a particle moving on it. The particle is deformed elastically by exerting a normal load on it. We considered (acoustic) transversal phonons on the surface where a sinusoidal function with a relaxation time describes the amplitudes. The theory neglects electric charges making the surface more similar to a non-magnetic insulator. In addition, any chemical capacity for particle-surface bonds is not included. The surface is assumed to be atomically clean without other surface asperities but phonons. Accordingly, the source of surface fluctuations is temperature.

In the classical picture, a loaded nano-particle is moving on a molecularly smooth surface where the amplitudes of the transversal phonons make the surface inclined. This inclination, in turn, produces a resistance force against the particle’s velocity, which is the origin of sliding friction. The friction coefficient is then calculated via the fluctuation-dissipation theorem, where a force autocorrelation function is averaged in a canonical ensemble. The averaging is approximated regarding the mean energy of the waves that corresponds to a system of Harmonic oscillators. Besides, the resistance force is approximated upon small phases, small amplitudes, and lattice wavenumbers multiplied by the normal load on the particle. On this account, the friction coefficient derived as a function of maximum amplitude of thermal waves $A_k^{\text{max}}$ appearing on the surface.

For a quantum theory, we quantized the resistance force through phonons’ quantum amplitudes and phases. At the same time, the Hertzian normal load remained classical due to the classical deformations of the particle. That is, we quantized the surface but not the particle moving on it. Accordingly, the quantum amplitudes were built by the raising and lowering operators multiplied by a quantum phase operator, $\exp(\pm i\phi_k)$. For the quantization of the phases, we postulated $\langle \phi_k \rangle = 0$ from a statistical point of view, which is consistent with the classical statistics of phases $\langle \phi_k \rangle = 0$ about the wavenumbers $k$. We argue that even if the quantum mechanical phase can be questionable in the ground state, the quantum statistical phase could be sensible.

At first, we took an approximation for the friction coefficient as the second Debye function from which the asymptotic value of the friction coefficient is consistent with the classical theory. Next, we added a modification by quantum phase averaging. The resulting friction coefficient is slightly lower but with the same asymptotic value, referring to not all phases allowed in the quantization.

In $T = 0$, both classical and quantized theories bring about a vanishing friction coefficient. However, one notes that the quantum uncertainty, virtual phonons, or vacuum state are differences between classical and quantum realms in $T = 0$. Upon this, a non-zero friction coefficient at $T = 0$ is imaginable and needs to be worked out separately.

Finally, we suggest computer simulations for classical molecular dynamics to understand better and confirm the present theory. Having other parameters in asymptotic value of Eq. (23) for a particular surface, an objective of the simulations could be the derivation of asymptotic friction coefficient as a function of normal load $\Gamma \propto F^2$. Under these circumstances, an agreement between the theoretically estimated friction coefficient (a quadratic curve) and simulated points can support the present model. Furthermore, computer simulations provide more complicated scenarios like rolling friction or adhesion described by JKR theory or by product phonons, which can be worked out in turn.

Comparison with other studies

Byproduct phonons The velocity-dependent friction forces in nanoscale might be classified as adhesion, deformation, and stick-slip forces. In the case of atomic stick-slip, the stored energy releases (dissipates) as phonons. However, phonons are not the cause of friction in such studies but a side effect to dissipate the stored energy. In the current article, on the other hand, the sliding friction arises from the existence of thermal phonons on the surface. Accordingly, in the present
model, phonons cause friction and are not a byproduct.

Non-contact friction The term "quantum friction" coined in non-contact earlier studies [67, 68] followed by [69, 70] considering a fluctuating electromagnetic field near a surface when an object in intimacy is moving along the surface. Further studies are inspired mainly by the Casimir effect [71, 72] in a dynamic scenario. Yet, there are other considerations like exchanging virtual photons with a Doppler shift. It turns out that there is a separation between the moving object, say a particle, and the surface in these works. Thereby, the existing literature for quantum friction addresses non-contact dynamic models utilizing quantum field theory. There are two limitations in this sense. For one thing, it could be challenging to think of classical counterparts for such systems and seek a correspondence between microscopic derivation and classical observations. Accordingly, the quantum source of classical friction will remain under question. As another reason, the non-contact friction force is experimentally elusive and negligibly much smaller than the contact friction force. As for an example, utilizing AFM cantilever as a pendulum [80], an oscillating tip over an elastic surface could excite acoustic phonons parallel to the surface [81]. Consequently, although the non-contact friction, including quantum friction, is absolutely essential for understanding and possible applications, the non-contact dissipation is minor compared to the effect of contact observations.

Quantum adiabaticity One reason for studying friction is diminishing it to reduce energy consumption. For instance, a normal oscillating load exerting upon a particle that is moving on a corrugated surface could reduce the friction [20]. In the quantum regime, in particular, the question is how to suppress friction using quantum adiabaticity [82]. A quantum adiabatic process means that the process is happening fast enough so that other conditions like the propagation of probability functions can be assumed constant. In contrast with our study, the existence of an effective relaxation time implies that the thermal fluctuations are not quantum adiabatic. That is, the process of moving the particle on the surface is not faster than surface changes. Namely, the loaded particle is moving on a dynamic surface.

Other possibilities for future studies

Random forces in the fluctuation-dissipation theorem might be considered quantum operators [83]. Moreover, any connection with thermal quantum field theory could be interesting and might open new ideas in the scope. Explicitly, one may think of operators such as $\hat{a}(k, \phi) = \hat{a}_k e^{-i\phi}$. Bogoliubov transformation, states like $|n_k\rangle \rightarrow |n_{k}(k, \phi)\rangle$ or thermal states as discussed in [84, 85]. Alternatively, a path integral approach could change the partition function.

Eventually, a significant turning point is providing quantum theories for more complicated classical friction models. With this intention, any quantum description of plastic deformations can support the idea that quantum contact friction goes beyond elasticity [21, 22]. Remarkably, a quadratic dispersion is approximated for plastic deformations. Furthermore, quantum description of fractures in solids [86], and low-temperature serrated deformation [23] could have paved more possibilities for quantum contact friction. Yet, quantizations for the Prandtl-Tomlinson model (and the generalizations) might be taken into account. Indeed, the 1928 Prandtl model was introduced for plastic deformations in a crystal.

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Appendix A: Quantum phase operator

A quantization for a sinusoidal wave gives rise to the problem of phase operator. The application has been in optic [87] regarding the quantization of an electrical plain field [61]. The paradoxical difficulty of the problem is about the ground state $|n = 0\rangle$ in quantum mechanics. However, for quantum field states $|n_k\rangle$, the ground state is already excluded in the Hamiltonian to avoid infinities. In this regard, utilizing the quantum phase operator in quantum statistics could be plausible.

In literature, one may refer to the matrix representation [88], a critical review paper [60], some physics and history of the problem [89], and a review book [90].

1. Matrix representation

Regarding a quantized phase operator $\hat{\phi}_k$, the representation in terms of raising and lowering operators are

$$\exp(i\hat{\phi}_k) = \hat{a}_k \hat{N}_k^{-1/2} = \frac{\hat{a}_k}{\sqrt{\hat{a}_k^\dagger \hat{a}_k}}.$$ 

One immediate question is about the effect of the phase operator on the states $|n_k\rangle$:

$$\exp(ik\hat{b}_k) |n_k\rangle = ?$$

Having $e^{i\hat{\phi}_k} \hat{N}_k^{1/2} = \hat{a}_k$,

$$\langle n_k | e^{i\hat{\phi}_k} \hat{N}_k^{-1/2} | m_k \rangle = \sqrt{m_k} \langle n_k | m_k - 1 \rangle,$$

and
\[ \langle n_k | e^{i\hat{\phi}} | m_k \rangle = \langle n_k | m_k - 1 \rangle = \delta_{n_k, m_k - 1}. \]

Therefore, the phase operator is unitary except for the ground state \( n_k = 0 \). Hence, one can write

\[ \exp(i\hat{\phi}_k) = \sum_{n_k} |n_k\rangle \langle n_k + 1|. \quad (A1) \]

Additionally,

\[ [e^{i\hat{\phi}}, \hat{N}_k] = \sum_{n_k} |n_k\rangle \langle n_k + 1| \hat{N}_k - \sum_{n_k} \hat{N}_k |n_k\rangle \langle n_k + 1| = \sum_{n_k} |n_k\rangle \langle n_k + 1| \langle n_k + 1|, \quad (A2) \]

that is

\[ [e^{i\hat{\phi}}, \hat{N}_k] = \sum_{n_k} |n_k\rangle \langle n_k + 1| = e^{i\hat{\phi}_k}. \]

In this representation, we can easily find the dagger operator, as

\[ \exp(-i\hat{\phi}_k) = \sum_{n_k} |n_k + 1\rangle \langle n_k|. \]

Further,

\[ e^{i\hat{\phi}_k} |n_k + 1\rangle = |n_k\rangle \quad \rightarrow \quad e^{i\hat{\phi}_k} |n_k\rangle = |n_k - 1\rangle. \]

and

\[ e^{-i\hat{\phi}_k} |n_k\rangle = |n_k + 1\rangle. \]

In our context,

\[ \begin{cases} \exp(i k \hat{b}_k) |n_k\rangle = |n_k - 1\rangle, \\ \exp(-i k \hat{b}_k) |n_k\rangle = |n_k + 1\rangle. \end{cases} \quad (A3) \]

2. Time evolution

For a quantum phase operator \( \hat{\phi}_k = k \hat{b}_k \),

\[ [\exp(i\hat{\phi}), \hat{N}_k] = \exp(i\hat{\phi}_k) \quad \rightarrow \quad [\hat{N}_k, \hat{\phi}_k] = i. \]

Remembering the Hamiltonian, Eq. 32

\[ \hat{H} = \hbar \sum_j \omega_j \hat{a}_j^\dagger \hat{a}_j = \hbar \sum_j \omega_j \hat{N}_j, \]

one can evaluate the time evolution of phase operator,

\[ \hat{\phi}_k(t) = \exp(i \hat{H} t / \hbar) \hat{\phi}_k \exp(-i \hat{H} t / \hbar). \]

Using Baker-Hausdorff relation

\[ \hat{\phi}_k(t) = \hat{\phi}_k(0) - \omega_k t, \quad (A4) \]

which is in agreement with the classical phase interval, and statistics. We need to find

\[ \langle \phi_k(0) | \phi_k(t) \rangle = \langle \phi_k^2(0) \rangle = \frac{\int_\pi^{-\pi} \phi_k^2 d\phi_k}{\int_{-\pi}^{\pi} d\phi_k} = \frac{\pi^2}{3}. \quad (A5) \]

In quantum realm, for the commutator \([\hat{N}, \hat{\phi}] = i\), the phase element of \( \langle n | \hat{\phi} | n \rangle \) can be undefined or related to a reference frame in general. However, in the interval of \( \phi_k \in [-\pi, \pi] \), and for a statistical \( k \) that is regarding \( \phi_k, |n_k\rangle \), but not given \( \phi, |n\rangle \), the reference can be statistical too. For this we use \( \langle \hat{\phi}_k \rangle = 0 \), corresponding to the classical phase interval, and statistics. We need to find

\[ \langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k^\dagger \hat{\phi}_k | n_k \rangle, \quad (A6) \]

with either

\[ \hat{A}_{k,1} = \sqrt{\frac{\hbar}{2m\omega_k}} \hat{a}_k e^{-i\hat{\phi}_k}, \quad \text{and} \quad \hat{A}_{k,2} = \sqrt{\frac{\hbar}{2m\omega_k}} \hat{a}^\dagger_k e^{i\hat{\phi}_k}. \]

Let’s consider \( \hat{A}_{k,1} \), then

\[ \langle n_k | \hat{A}_{k,1} \hat{\phi}_k \hat{A}_{k,1}^\dagger \hat{\phi}_k | n_k \rangle = \frac{\hbar}{2m\omega_k} \langle n_k | \hat{a}_k e^{-i\hat{\phi}_k} \hat{\phi}_k \hat{a}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle. \quad (A7) \]
and, \( \hat{a}_k = e^{i\hat{\phi}_k} \hat{N}^{1/2} \). Subsequently,

\[
\langle n_k | \hat{A}_{k,1} \hat{\phi}_k \hat{A}_{k,1} \hat{\phi}_k | n_k \rangle = \frac{\hbar}{2m\omega_k} \langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k e^{i\hat{\phi}_k} \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle = \frac{\hbar}{2m\omega_k} \langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle
\]

(A8)

from the zero commutator of phase and its exponential function. In the next step, we use

\[
[\hat{N}_k, \hat{\phi}_k] = i, \quad [\hat{N}^{1/2}_k, \hat{\phi}_k] = \frac{i}{2} \hat{N}^{-1/2}_k,
\]

(A9)

or

\[
\hat{N}^{1/2}_k \hat{\phi}_k - \frac{i}{2} \hat{N}^{-1/2}_k = \hat{\phi}_k \hat{N}^{1/2}_k
\]

\[
\langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle = \langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \left( \hat{N}^{1/2}_k \hat{\phi}_k - \frac{i}{2} \hat{N}^{-1/2}_k \right) e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle
\]

\[
= \langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle - \frac{i}{2} \langle n_k | \hat{\phi}_k | n_k \rangle
\]

\[
\langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle = \langle n_k | e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} \hat{\phi}_k | n_k \rangle,
\]

(A10)

for \( \langle \hat{\phi}_k \rangle = 0 \). In addition, we note that,

\[
\hat{A}_{k,1} \hat{A}_{k,1} = \frac{\hbar}{2m\omega_k} \hat{\phi}_k e^{-i\hat{\phi}_k} \hat{\phi}_k e^{-i\hat{\phi}_k}
\]

\[
e^{i\hat{\phi}_k} \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} e^{i\hat{\phi}_k} \hat{N}^{1/2}_k e^{-i\hat{\phi}_k} = e^{i\hat{\phi}_k} \hat{N}^{1/2}_k \hat{\phi}_k \hat{N}^{1/2}_k e^{-i\hat{\phi}_k}.
\]

(A11)

Therefore,

\[
\langle n_k | \hat{A}_{k,1} \hat{\phi}_k \hat{A}_{k,1} \hat{\phi}_k | n_k \rangle = \langle n_k | \hat{A}_{k,1} \hat{\phi}_k \hat{\phi}_k | n_k \rangle.
\]

(A12)

One can follow a similar argument for \( \hat{A}_{k,2} \), and reaches the same result. Thereupon,

\[
\langle n_k | \hat{A} \hat{\phi}_k \hat{A} \hat{\phi}_k | n_k \rangle = \langle n_k | \hat{A} \hat{\phi}_k | n_k \rangle
\]

(A13)

with \( \langle \hat{\phi}_k \rangle = 0 \), either for \( \hat{A}_{k,1} \) or \( \hat{A}_{k,2} \). For the next step,

\[
\langle n_k | \hat{A}_k \hat{\phi}_k (t) \hat{\phi}_k (t) | n_k \rangle = \sum_{n'} \langle n_k | \hat{A}_k \hat{\phi}_k (t) | n' \rangle \langle n' | \hat{\phi}_k (t) \hat{\phi}_k (t) | n_k \rangle,
\]

\[
\langle n_k | \hat{A}_k \hat{\phi}_k (t) | n_k \rangle = \delta_{nn'} \langle n_k | \hat{A}_k \hat{\phi}_k (t) | n_k \rangle,
\]

\[
\langle n' | \hat{\phi}_k (t) \hat{\phi}_k (t) | n_k \rangle = \langle n' | \hat{\phi}_k \hat{\phi}_k | n_k \rangle.
\]

Consequently,

\[
\langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k \hat{\phi}_k (t) | n_k \rangle = \langle n_k | \hat{A}_k \hat{\phi}_k (t) | n_k \rangle \langle n_k | \hat{\phi}_k \hat{\phi}_k | n_k \rangle.
\]

(A14)

Additionally, in the general case of quantum phase \[ \theta_k \] 

\[
\langle n_k | \hat{\phi}_k^2 | n_k \rangle = \langle n_k | \hat{\phi}_k | n_k \rangle^2 = \frac{\pi^2}{6} + \sum_{l=1}^{\infty} \frac{1}{l^2} = \frac{\pi^2}{3} - \sum_{l=n_k+1}^{\infty} \frac{1}{l^2},
\]

(A15)

which reads

\[
\langle n_k | \hat{\phi}_k^2 | n_k \rangle = \frac{\pi^2}{6} + \sum_{l=1}^{n_k} \frac{1}{l^2} = \frac{\pi^2}{3} - \sum_{l=n_k+1}^{\infty} \frac{1}{l^2},
\]

for \( \langle \hat{\phi}_k \rangle = 0 \). Furthermore,

\[
\sum_{l=1}^{n_k} \frac{1}{l^2} = \frac{\pi^2}{6} - \Psi(1, n_k + 1),
\]

(A17)

where \( \Psi(m,x) \) is the polygamma function of order \( m \), that is the \( (m+1) \)th derivative of the logarithm of the gamma function \( (\frac{d^{m+1}}{dx^{m+1}} \ln \Gamma(x)) \). As a result,

\[
\langle n_k | \hat{\phi}_k^2 | n_k \rangle = \frac{\pi^2}{3} - \Psi(1, n_k + 1).
\]

(A18)

In the classical limit

\[
\lim_{n_k \to \infty} \langle n_k | \hat{\phi}_k (0) \hat{\phi}_k (t) | n_k \rangle = \frac{\pi^2}{3}
\]

(A19)

which corresponds to Eq. Rewriting Eq. we have

\[
\langle n_k | \hat{\phi}_k (0) \hat{\phi}_k (t) | n_k \rangle = \frac{\pi^2}{3} \left[ 1 - \frac{\Psi(1, n_k + 1)}{\pi^2/3} \right].
\]

(A20)

Finally,

\[
\langle n_k | \hat{A}_k \hat{\phi}_k \hat{A}_k (t) \hat{\phi}_k (t) | n_k \rangle = \frac{\pi^2}{3} \frac{e^{-t/\tau_m}}{m\omega_k} \left[ 1 - \frac{\Psi(1, n_k + 1)}{\pi^2/3} \right].
\]

(A21)
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