Quantum oscillator in a non-self-interacting radiation field: Exact calculation of the partition function

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With the use of functional integration, an exact analytic expression valid for the whole temperature range is derived for the partition function of a charged quantum oscillator coupled to a non-self-interacting (with the A^2 term neglected) radiation field. To derive this result, special care is taken with renormalization which is carried out at two stages. The temperature-dependent free-energy shift due to blackbody radiation is studied and compared with recent work. It is shown that the ground state is the only stable state and that the higher states have a finite lifetime.

I. INTRODUCTION

This paper is concerned with an exactly solvable three-dimensional model of a harmonically bound electron in a radiation field. The model arises from minimal coupling of the electron to the free-electromagnetic field by (i) retaining only the dipole interaction and (ii) neglecting the self-interaction term of the field (see Sec. II). One recognizes the simplified system as the special case of the fully coupled oscillator model where the oscillator couples uniformly to the noninteracting field oscillators. Such a model has universal character and has often been considered mainly in statistical mechanics, see, e.g., Refs. 1—6. It yields a commonly used description of a harmonically bound particle in a heat bath with linear coupling. Furthermore, it often gives a good approximation to more complicated systems, as, e.g., the polaron, where variational methods are used to calculate the free energy of the system. For other systems, as, e.g., Rydberg atoms, one may expect the oscillator model to be a good approximation, as suggested in Ref. 7 (cf. also the remarks below). Concerning our main interest here we shall see that the model is able to give detailed answers to questions about the influence of the radiation field. Exact formulas for the thermodynamical potentials and their dependence on the temperature $T=\hbar(k\beta)^{-1}$ and the coupling strength $\alpha=e^2(\hbar c)^{-1}$ can be derived.

Let us elucidate our results. Because of the quadratic form of the action of the oscillator model, the path integrational method is well suited and allows a nonperturbative *ab initio* computation. Following Feynman's method we average out the variables of the field oscillators which includes the division by the partition function of the free-field oscillators. The result is an effective action, see Eq. (9), where the coupling to the field oscillators is replaced by a memory potential for the oscillator. Before evaluating the remaining path integral, two renormalizations have to be performed: (i) a renormalization of the kinetic energy (mass renormalization) and (ii) a redefinition of the zero mark of the energy by an infinite shift.

Our main result is the exact analytic expression (12), which we believe is new, for the partition function Z_α of the oscillator subjected to the radiation field. It incorporates the influence of the radiation field on the oscillator. There is no restriction on the size of the coupling constant α. The expression (12) for Z_α is valid for the whole temperature range.

From Z_α one gets exact expressions for the closely related thermodynamical potentials. We discuss the asymptotic behavior of the free energy, see (13) and (15). The question, which recently has generated some interest, is the low-temperature behavior of the shift $\Delta F(\beta)$ in free energy. Up to higher-order corrections, we get

$$\Delta F(\beta)=-\pi\alpha k^2T^2(3mc^2)^{-1} \tag{1}$$

[which is approximately $-0.17\ T^2\ (\mathrm{s\,K}^2)^{-1}$ for the electron]. Ford *et al.*[7] obtain for the low-temperature shift in free energy the same absolute value but the opposite sign to (1). We postpone our criticism of the result of Ref. 7 until the end of this section.

The question arises if (1) is in accord with the recent experiments[8] (cf. Ref. 7 for Ref. 8—13) on the shift of Rydberg energy levels induced by blackbody radiation, which are consistent with a T^2 dependence of the shift.

As a tentative answer, let us make the following considerations: First (i), the shift (1) is global and it is not attributed to individual energy levels. (ii) the energy spectrum (state density) of the oscillator subjected to the radiation field is obtained as the inverse Laplace transform of the partition function with respect to β. Hence the energy levels do not depend on the temperature. However (iii), this is no longer true if one had to deal with thermal inequilibrium and the radiation field had to be regarded as an external field, so that the radiation temperature T_R may be different from that of the ensemble of atoms T. In that case one can consult previous calculations[9—13] based on temperature-dependent perturbative QED performed for the Coulomb potential. There, indeed, the level shifts depend on the radiation temperature (dynamic Stark shifts). As detailed calculations in Ref. 12 indicate, in general they depend also on the specific kind of atoms under consideration. For temperatures $T_R \ll \alpha^2 mc^2/k$ ($\sim 2\times 10^5$ K for the electron), second-order nonrelativistic perturbation theory combined with the dipole sum rule (Thomas-Reiche-Kuhn sum rule) yields a universal state-independent energy-level shift which coincides (casually?), including sign, with Eq. (1) but with T being replaced by T_R. For the oscillator potential this is the correct result even without the restriction on the temperature, see Eq. (14). It is concluded in Ref. 13 that the dominant thermal QED effects are the same for all levels, and thus not seen in transitions. However, it should be stressed that for real atoms this conclusion is true as long as it refers to transitions between Rydberg levels, but in general it fails to hold for transitions to more tightly bound levels which will suffer relatively small dynamic Stark shifts. As a fourth point (iv), one notes that there is common agreement on the absolute value of the dominant thermal shift but that there is discrepancy on its sign, cf., e.g., Refs. 11 and 13. Finally (v), in this context it is pointed out in Ref. 7 that because of the thermodynamic relation $U=F-T(\partial F/\partial T)$, a term proportional to T^2 has the same absolute value but has opposite sign in internal energy U and free energy F, and it is argued in Ref. 7 that the measurement of Ref. 8 measures the shift in free energy and not in internal energy.

Mainly because of the temperature dependence of the shifts, we may conclude from the above considerations that the experimental situation in Ref. 8 is met at best by the description mentioned in (iii). So one has to deal with a partial equilibrium which is not investigated in this paper [only Eq. (14) refers to it]. In this situation initially the radiation field is decoupled from the atoms and is in thermal equilibrium corresponding to a temperature T_R (blackbody radiation). The atoms are imagined to be prepared separately. Then, brought into contact with the radiation field, the atomic levels are shifted according to a dynamical Stark effect. Obviously the shifts depend on the temperature T_R which, however, has nothing to do with the temperature T of a statistical ensemble of the atoms. The shifts of Rydberg levels measured in Ref. 8 correspond to differences in the energy between Rydberg levels, for which the present oscillator model should be reasonably valid, and more tightly bound levels which, as already mentioned, will suffer smaller shifts. To get an estimate of the shifts in free and internal energy in the following considerations, let us nevertheless assume, in accord with the mentioned perturbative calculations [see Eq. (14) and Ref. 13], that the value ε of the shift of an energy-level is approximately the same for all levels and coincides with the right side of Eq. (1) where T is replaced by T_R. Within the simplifications made so far we may suppose that ε does not depend on the temperature T of the atomic system (in contrast is that of the radiation field T_R). Now, the partition function of the atomic system in contact with the radiation field is given by $\sum_n \exp[-\beta(E_n+\varepsilon)]$, where E_n denotes the unperturbed energy levels and $\beta=\hbar(kT)^{-1}$. It follows immediately that the shift in free energy is equal to ε. Since ε is independent of T (not of T_R), the thermodynamic relation recalled in (v) above yields the same shift in internal energy. Concerning the experiments[8] we conclude that the effect of blackbody radiation on atoms is a shift (depending on the temperature of the radiation T_R as discussed) of the energy levels (measured for highly excited, i.e., Rydberg states, with respect to tightly bound states) which for a statistical ensemble of atoms in thermal equilibrium gives rise to approximately the same shift, including its sign, in free energy and internal energy.

Returning now to our harmonic oscillator model in complete thermal equilibrium, the limit of $\Delta F(\beta)$ for $\beta\to\infty$ yields the renormalization-dependent negative-ground-energy shift

$$3\hbar\eta(\cos\varphi+\varphi\sin\varphi)/\pi-3\hbar\eta/2\ , \tag{2}$$

where η is the oscillator frequency and $\cos\varphi\equiv\alpha\eta(3\omega_{\rm CF})^{-1}$ with $\omega_{\rm CF}\equiv mc^2/\hbar$ the Compton frequency corresponding to the oscillator mass m. The shift is of second order in α, namely $-(\frac{3}{4})\hbar\eta\cos^2\varphi$.

Let us, at this point, mention a peculiarity of the partition function (12). It depends on only two dimensionless quantities, $p=\beta\eta/(2\pi)$ and $\cos\varphi$. The latter is fundamental for the system. In particular, the damping constant for a classical dipole is given by

$$\gamma=2\eta\cos\varphi=2e^2\eta^2/(3mc^3)\ . \tag{3}$$

For a quantum oscillator, γ is the natural linewidth of the first excited state. The linewidth of the higher states should be multiples of γ. In the formalism of Ref. 6 the limiting classical equation of motion $\ddot q+\gamma\dot q+\eta^2 q=0$ of the oscillator follows on the assumption that the effective spectral density is proportional to the frequency.

For a rough illustration of the magnitude of (3) for atomic levels, let us approximate the Coulomb potential $-Z\alpha\hbar c/r$ at the Bohr radius $r_B=n^2c/(Z\alpha\omega_{\rm CF})$ of the nth eigenstate by an oscillator potential $m\eta^2r^2/2-b$. It follows $\eta=Z^2\alpha^2\omega_{\rm CF}/n^3$ and $\cos\varphi=Z^2\alpha^3/(3n^3)$. This yields $\gamma=2Z^4\alpha^5\omega_{\rm CF}/(3n^6)$ corresponding to a lifetime $1/\gamma=(n^6/Z^4)10^{-10}$ s.

For high temperatures the free-energy shift tends to $-\infty$ logarithmically (15). As a consequence of this the mean density of the states at high frequencies is the same as for the free oscillator. Physically this is clear since the effect of the coupling to the electromagnetic field is a perturbation of the free case.

A most interesting aspect regarding the formula (12) for the partition function is the possibility to get detailed information about the state density f_α which is available from Z_α through the inverse Laplace transformation. We show analytically (see the Appendix) several nontrivial facts being most satisfactorily in agreement with physics: (i) Z_α is indeed the Laplace transform of a function f_α, (ii) f_α is nonnegative, (iii) f_α vanishes for all frequencies less than $\omega_\alpha=3\eta\ (\cos\varphi+\varphi\sin\varphi)/\pi$ corresponding to the ground energy, (iv) f_α starts with a δ peak at ω_α, and (v) f_α is continuous at all frequencies larger than ω_α. The physical interpretation is obvious. In particular, it shows the existence of a ground state and it shows that the ground state is the only stable state of the perturbed oscillator.

We should remark on the case of very strong coupling. It is present if $\cos\varphi=\alpha\eta/(3\omega_{\rm CF})=e^2\eta/(3mc^3)$ exceeds the value 1. Then the angle φ becomes imaginary or, equivalently, $\cos\varphi$ has to be replaced by $\cosh\varphi$. The formulas remain valid, but we do not study this case here.

As mentioned we disagree with Ref. 7 about the correct expression for the free energy of the oscillator model. The expression derived in Ref. 7 is, for one dimension,

$$F_0(\beta)=\hbar A\beta^{-2}+\int_0^\infty f(\omega,\beta)L(\omega)d\omega \ ,$$

where

$$f(\omega,\beta)=\hbar\beta^{-1}\ln[1-\exp(-\beta\omega)]$$

and

$$L(\omega)=(\gamma/\pi)(\omega^2+\eta^2)[(\omega^2-\eta^2)^2+\gamma^2\omega^2]^{-1}$$

and

$$A=\pi\alpha\hbar/(9mc^2) \ .$$

In order to formulate our objections to F_0 we first discuss its temperature dependence. Obviously $F_0(\beta)\leqq\hbar A\beta^{-2}$ since $f<0$ and $L>0$. Then one notes that L is bounded and that L is p integrable for any $p\geq 0$. The latter is also true for $\omega\to f(\omega,\beta)$, denoted by $f(\cdots,\beta)$, since it tends logarithmically to $-\infty$ for $0<\omega\to 0$ and vanishes exponentially for $\omega\to\infty$. Hence we may apply the Hölder inequality and get $\hbar A\beta^{-2}-F_0(\beta)\leq\|f(\cdots,\beta)\|_p\|L\|_q$. By the change $x=\beta\omega$ of variables $\|f(\cdots,\beta)\|_p$ becomes $\hbar\beta^{-1-1/p}\|g\|_p$, where $g(x)\equiv-\ln[1-\exp(-x)]$, so that $F_0(\beta)\geqq\hbar A\beta^{-2}-\hbar B_p\beta^{-1-1/p}$, where $B_p\equiv\|g\|_p\|L\|_q>0$. Passing to the partition function $Z(\beta)=\exp[-\beta F_0(\beta)/\hbar]$ we get

$$\exp(-A\beta^{-1})\leq Z(\beta)\leq\exp(-A\beta^{-1}+B_p\beta^{-1/p}) \tag{4}$$

for all $\beta>0$ and where p is any number greater than or equal to 1. This displays some unreasonable features of Z.

(i) Because of the smallness of the coupling constant α, one knows from QED that one may regard the interaction with the radiation field as a *perturbation* of the free oscillator. Indeed, the calculations of, e.g., the transition probabilities based on perturbation theory in QED are in good agreement with observation. Due to the perturbative character of the electromagnetic coupling to the radiation field the properties of the oscillator do not change drastically in the presence of a radiation field. This means that the weak coupling limit $\alpha\to 0(\alpha\neq 0)$ yields the free oscillator.

Now a simple test, which rules out the expression F_0 of Ref. 7 as a correct formula of the free energy of the perturbed oscillator (and which confirms our formula), consists in looking at the total number of states of the oscillator. This number is given by the value of the partition function at $\beta=0$. From (4) one easily infers $Z(\beta=0)=0$. Thus F_0 gives rise to a total number of states equal to zero instead to infinity, even in the weak coupling limit. This is unphysical.

(ii) By the same reason, i.e., $Z(\beta=0)=0$, Eq. (4) implies that Z is not decreasing and hence not the Laplace transform of a positive function, the state density, as it should.

So far (i) and (ii) prove that F_0 is not the right expression for the free energy. It fails to be correct for any positive coupling strength. Now, one would like to know if there is a region of approximate validity of F_0. Let us add some remarks on the inverse question. Since L approaches a δ function in η in the limit of vanishing coupling, $Z(\beta)$ tends for any $\beta>0$ to the value of the partition function of the free case which is infinite at $\beta=0$, however not in a uniform manner, since $Z(\beta=0)$ persists to be zero for all positive coupling strengths. From (4) it follows that Z tends to 1 as $\beta\to\infty$. Hence, for weak coupling, Z has a peak. Thus for temperatures beyond that peak Z is definitively wrong. Moreover, for strong coupling this peak does not even exist, the maximum of Z is equal to 1 and lies at $\beta=\infty$. Indeed, for $\cos\varphi\geqq\sqrt{3}/2$ or, equivalently, $\gamma^2/\eta^2\geqq 3$ one gets $B_1=A$ and hence, from (4), $Z\leqq 1$. Thus Z fails in the strong coupling case for the whole temperature range.

In a forthcoming paper we will present numerical and analytic computations on the state density f_α which shows the expected pattern of the natural line structure of a charged quantum oscillator coupling to the surrounding electromagnetic vacuum.

II. DIPOLE INTERACTION AND NON-SELF-INTERACTING RADIATION FIELD

A charged oscillator minimally coupled to an electromagnetic field is described by the Hamiltonian

$$H=\frac{1}{2m}[p-eA(x)]^2+\frac{m}{2}\eta^2x^2 +\tfrac{1}{2}\int[E(y)^2+B(y)^2]d^3y \ , \tag{5}$$

where m, η, and e are the mass, the frequency, and the charge of the oscillator, respectively. Expressed in terms of creation and destruction operators the vector potential is

$$A(x)=\sum_{k,\sigma}\left[\frac{2\pi\hbar}{\Omega\omega_k}\right]^{1/2}u_{k\sigma}(a_{k\sigma}e^{ikx}+a_{k\sigma}^*e^{-ikx}) \tag{6}$$

where $u_{k\sigma}$, $\sigma=1,2$, are orthonormal polarization vectors perpendicular to the momentum k, and where Ω is a normalizing volume in momentum space. To achieve a simplified version of (5) we retain only the dipole interaction, i.e., we replace $A(x)$ by $A\equiv A(0)$, and neglect the self-interaction of the field by dropping the quadratic term $e^2A^2/2m$. The resulting Hamiltonian

$$H'=H_{\rm osc}+H_{\rm rad}-\frac{e}{m}pA \ , \tag{7}$$

where $H_{\rm rad}=\frac{1}{2}\sum_{k,\sigma}\hbar\omega_k(a_{k\sigma}a_{k\sigma}^*+a_{k\sigma}^*a_{k\sigma})$, now has to be transformed equivalently for a path integrational treatment. For this purpose, position and momentum variables for the field are introduced,

$$x_{k\sigma}\equiv(2\mu\omega_k/\hbar)^{-1/2}(a_{k\sigma}^*+a_{k\sigma})$$

and

$$p_{k\sigma} \equiv i(\hbar\mu\omega_k/2)^{1/2}(a^*_{k\sigma} - ak\sigma) ,$$

where μ is a mass. Then except for the interaction term $-epA/m$, in all other terms momentum variables are separated from position variables. Full separation is achieved by passing to the momentum-space representation of the oscillator. Thus we end up with the Hamiltonian

$$H'' = \left[\frac{m}{2}\eta^2 p^2 + \frac{1}{2\mu}\sum_{k,\sigma} p_{k\sigma}^2 \right] + \left[\frac{1}{2m}x^2 + \frac{\mu}{2}\sum_{k,\sigma}\omega_k^2 x_{k\sigma}^2 + \frac{e}{m}\left[\frac{4\pi\mu}{\Omega}\right]^{1/2} x \sum_{k,\sigma} u_{k\sigma}x_{k\sigma} \right] . \tag{8}$$

III. PATH INTEGRATION, RENORMALIZATION

The partition function Z_α ascribed to the oscillator coupled to the radiation field is the partition function of the whole system (8) divided (normalized) by the partition function of the radiation field in absence of the oscillator. The latter is $\prod_k [2\sinh(\beta\omega_k/2)]^{-2}$ so that $Z_\alpha(\beta) = \oint \mathscr{D}q \exp(-S_{\text{eff}}[q]/\hbar)$ with [cf. Ref. 14, Eq. (14)]

$$S_{\text{eff}}[q] = \int_0^\beta \left[\frac{1}{2m\eta^2}\dot{q}^2 + \frac{1}{2m}q^2 \right] dt - \frac{2\alpha}{3\pi}\frac{1}{m\omega_{\text{CF}}}\int_0^\beta\int_0^\beta \left[\int_0^{\omega_c} \frac{\omega\cosh\left[\omega\left[|t-s| - \frac{\beta}{2}\right]\right]}{2\sinh(\beta\omega/2)} \right] q(t)q(s)\,dt\,ds , \tag{9}$$

where we replaced $\sum_{k,\sigma}$ by

$$\frac{\Omega}{(2\pi c)^3}\sum_\sigma \int \sin\vartheta\, d\vartheta\, d\varphi \int_0^{\omega_c} \omega^2 d\omega$$

introducing a frequency cutoff ω_c. We shall get rid of ω_c after renormalization.

Expanding the closed path $q(t) = \sum_{n=-\infty}^{\infty} a_n \exp(i\nu_n t)$, $\nu_n = 2\pi\eta/\beta$, $a_{-n} = a_n^*$, in a Fourier series, one gets

$$S_{\text{eff}}[q] = \frac{\beta}{2m}\sum_n |a_n|^2 f_n ,$$

where

$$f_n \equiv 1 - \frac{4\alpha}{3\pi}\frac{1}{\omega_{\text{CF}}}\left[\omega_c - \nu_n \arctan\left[\frac{\omega_c}{\nu_n}\right]\right] + \nu_n^2/\eta^2 ,$$

$$f_0 = 1 - \frac{4\alpha}{3\pi}\frac{\omega_c}{\omega_{\text{CF}}} .$$

Hence, for $y \equiv q(0) = q(\beta)$ fixed, the action is minimized at

$$S_{\text{eff}}^{\min}(y) = \frac{\beta}{2m}y^2\left[\sum_n 1/f_n\right]^{-1} .$$

Since the action is quadratic, $Z_\alpha(\beta)$ splits into two factors, one of them being $\int \exp[-S_{\text{eff}}^{\min}(y)/\hbar]d^3y$. The other is expressed by the coefficients $K_n \equiv f_n - \nu_n^2/\eta^2$ being the Fourier coefficients $\int_0^\beta K(t)\exp(-i\nu_n t)dt$ of the kernel

$$K(t) = \delta(t) - \frac{2\alpha}{3\pi}\frac{1}{\omega_{\text{CF}}}\int_0^{\omega_c}\frac{\omega\cosh[\omega(t-\beta/2)]}{\sinh(\beta\omega/2)}d\omega ,$$

cf. Ref. 15, Eqs. (34) and (55). One gets

$$Z_\alpha(\beta) = \left[\eta\beta\prod_{n=1}^{\infty}\left[1 + \frac{\eta^2}{\nu_n^2}K_n\right]\right]^{-3} . \tag{10}$$

Let us discuss the dependence of (10) on the cutoff. The term

$$\eta^2\left[1 - \frac{4\alpha}{3\pi}\frac{\omega_c}{\omega_{\text{CF}}}\right]$$

is well known, e.g., from the theory of the natural linewidth, and gives rise to a *renormalization of the kinetic energy,* see, e.g., Ref. 16, Sec. 5.3. According to it, the f_n are replaced by new

$$f_n = 1 + \frac{4\alpha}{3\pi}\frac{\nu_n}{\omega_{\text{CF}}}\arctan\left[\frac{\omega_c}{\nu_n}\right] + \nu_n^2/\eta^2 , \quad f_0 = 1 .$$

Indeed, the new coefficients f_n and K_n correspond to the memory term

$$+\frac{\alpha}{6\pi}\frac{1}{m\omega_{\text{CF}}}\int_0^\beta\int_0^\beta\left[\int_0^{\omega_c}\frac{\omega\cosh[\omega(|t-s|-\beta/2)]}{\sinh(\beta\omega/2)}d\omega\right][q(t)-q(s)]^2 dt\,ds ,$$

added to (9) the kinetic energy term

$$\left[\frac{\alpha}{3\pi}\frac{1}{m\omega_{\rm CF}}\int_0^\beta\int_0^{\omega_c}\frac{\omega\cosh[\omega(\,|t-s\,|-\beta/2)]}{\sinh(\beta\omega/2)}d\omega\,ds\right]q^2 = \frac{2\alpha}{3\pi}\frac{\omega_c}{m\omega_{\rm CF}}q^2 .$$

[We recall that q has the dimension of momentum since in (8) we passed to the momentum-space representation.] This term proportional to the cutoff can be generated from the beginning adding to (8) the counter term

$$\frac{2\pi}{\Omega}\frac{e^2}{m^2}\sum_{k,\sigma}\left[\frac{xu_{k\sigma}}{\omega_k}\right]^2 .$$

Terms like the latter have been discussed in connection with the generation of a dissipative term in the corresponding classical equation of motion (Ref. 17, Sec. 3). Here it is a consequence of renormalization.

At this stage one should look at the limit $\omega_c\to\infty$: the memory term becomes

$$+\frac{\alpha\pi}{6}\frac{\beta^{-2}}{m\omega_{\rm CF}}\int_0^\beta\int_0^\beta\frac{[q(t)-q(s)]^2}{\sin^2[\pi(t-s)/\beta]}dt\,ds ,$$

where the singularities at $t=s$ are removed. However, those at $t=\beta$, $s=0$ and $s=\beta$, $t=0$ still are present. They are likely to be responsible for the term proportional to ν_n in

$$K_n(\omega_c=\infty)=1+\frac{2\alpha}{3}\frac{\nu_n}{\omega_{\rm CF}}$$

making the partition function Eq. (10) divergent. In order to reveal the nature of this divergence we retain the finite cutoff and expand the shift in free energy $\Delta F=-(\hbar/\beta)\ln(Z_\alpha/Z_0)$ in a power series in α, thus

$$\Delta F=3\frac{\hbar}{\beta}\sum_{k=1}^{\infty}\left[\frac{4\alpha}{3\pi}\right]^k\left[\frac{(-1)^{k+1}}{k}\sum_{n=1}^{\infty}(h_n)^k\right]$$

with

$$h_n\equiv\frac{\eta^2/\nu_n^2}{1+\eta^2/\nu_n^2}\frac{\nu_n}{\omega_{\rm CF}}\arctan\left[\frac{\omega_c}{\nu_n}\right],$$

which converges for $\omega_c\le\omega_{\rm CF}$. The first-order term reads, after some algebraic manipulations,

$$\frac{\hbar\alpha}{\pi}\frac{\eta^2}{\omega_{\rm CF}}\int_0^{\omega_c}\frac{\omega\coth(\beta\omega/2)-\eta\coth(\beta\eta/2)}{\omega^2-\eta^2}d\omega .$$

From this the divergent part $(\hbar\alpha/\pi)(\eta^2/\omega_{\rm CF})\ln(1+\omega_c/\eta)$ is extracted; the remainder becomes

$$\frac{\hbar\alpha}{\pi}\frac{\eta^2}{\omega_{\rm CF}}⨍_0^\infty\frac{2\omega}{\omega^2-\eta^2}\frac{d\omega}{e^{\beta\omega}-1}=\frac{\hbar\alpha}{\pi}\frac{\eta^2}{\omega_{\rm CF}}[\,\ln p-\mathrm{Re}\psi(ip)],$$

where $p=(\eta\beta/2\pi)$ and ψ denotes the digamma function. Moreover, all higher-order terms converge for $\omega_c\to\infty$ in a dominated manner, so that the sum converges absolutely. Therefore, we are led to regard the (unique) divergent term $(\hbar\alpha/\pi)(\eta^2/\omega_{\rm CF})\ln(1+\omega_c/\eta)$, being independent of the temperature, as normalizable just by *redefining the zero mark of the energy*. Thus we drop this term and keep and expression of ΔF independent of the cutoff.

Rearranging the terms, we get

$$\Delta F=\frac{\hbar\alpha}{\pi}\frac{\eta^2}{\omega_{\rm CF}}[\,\ln p-\mathrm{Re}\psi(ip)] +\frac{3\hbar}{\beta}\sum_{n=1}^{\infty}\left[\ln\left[1+\frac{2\alpha}{3}\frac{\eta^2}{\omega_{\rm CF}}\frac{\nu_n}{\nu_n^2+\eta^2}\right]-\frac{2\alpha}{3}\frac{\eta^2}{\omega_{\rm CF}}\frac{\nu_n}{\nu_n^2+\eta^2}\right].$$

This can be summed up and we find

$$\Delta F(\beta)=\frac{3\hbar}{\pi}\eta\left[\cos\varphi\ln p-\frac{1}{p}\ln\left|\frac{\Gamma(pe^{i\varphi})}{\Gamma(ip)}\right|\right], \tag{11}$$

and hence

$$Z_\alpha(\beta)=\left[\frac{p}{2\pi}e^{-(2\cos\varphi)p\ln p}\left|\Gamma(pe^{i\varphi})\right|^2\right]^3 , \tag{12}$$

where

$$p=\frac{\beta\eta}{2\pi}=\frac{\hbar}{2\pi k}\frac{\eta}{T},\quad \cos\varphi=\frac{\alpha\eta}{3\omega_{\rm CF}}=\frac{\hbar\alpha}{3}\frac{\eta}{mc^2} .$$

IV. DISCUSSION

Of course, in the limit of vanishing coupling $\alpha\to0$, or equivalently $\varphi\to\pi/2$, the partition function (12) becomes that of the free oscillator $Z_0(\beta)=[2\sinh(\pi p)]^{-3}$ and the free-energy shift vanishes. In the limit of low temperatures Stirling's formula yields

$$\Delta F(\beta)=-\frac{3\hbar}{\pi}\eta\left[\frac{\pi}{2}-\cos\varphi-\varphi\sin\varphi+\frac{\cos\varphi}{12p^2}-\frac{\cos3\varphi}{360p^4}+\frac{\cos5\varphi}{1260p^6}-\cdots\right]\quad\text{for } T\to0 . \tag{13}$$

The temperature-independent term is the ground-energy shift (2) and the next term is the well-known free-energy shift (1) depending quadratically on the temperature. It is the leading term of the first order of the α expansion of ΔF, namely

$$\frac{\hbar\alpha}{\pi}\frac{\eta^2}{\omega_{\rm CF}}⨍_0^\infty\frac{2\omega}{\omega^2-\eta^2}\frac{d\omega}{e^{\beta\omega}-1} .$$

Just for comparison, in the case of partial equilibrium (see the Introduction) the second-order contribution of nonrelativistic perturbation theory

$$\Delta E_n(\beta)=\frac{2\hbar\alpha}{3\pi c^2}\sum_{n'\neq n}\int_0^{\omega_c}\left[\frac{1}{\omega_n-\omega_{n'}-\omega}+\frac{1}{\omega_n-\omega_{n'}+\omega}\right]\times|\langle n\,|P/m\,|n'\rangle|^2\frac{\omega d\omega}{e^{\beta\omega}-1} , \tag{14}$$

where this time $\beta=\hbar(kT_R)^{-1}$ refers to the radiation temperature T_R, produces exactly this term, since

$$|\langle \kappa,\lambda,\nu|P/m\,|\kappa',\lambda',\nu'\rangle|^2=\frac{\hbar\eta}{m}\{\delta_{\lambda\lambda'}\delta_{\nu\nu'}N_\kappa^{-2}[(\kappa+1)^2N_{\kappa+1}^2\delta_{\kappa+1,\kappa'}+\tfrac{1}{4}N_{\kappa-1}^2\delta_{\kappa-1,\kappa'}]+\cdots\}$$

where the ellipse represents cyclic permutations with $N_\kappa^{-2}=2^\kappa\kappa!(\pi\hbar/m\eta)^{1/2}$. It is independent of the state $|n\rangle=|\kappa,\lambda,\nu\rangle$.

For the high-temperature limit we get from (11)

$$\Delta F(\beta)=(3\hbar/\pi)\eta\cos\varphi(\gamma+\ln p)\quad\text{for } T\to\infty \tag{15}$$

(γ being Euler's constant), which tends to $-\infty$ only logarithmically. Hence $Z_\alpha/Z_0\to1$ for $\beta\to0$ independently of α. This implies the expected result that the mean density of the states at high frequencies is the same for the perturbed and unperturbed oscillator.

From Eq. (12) one gets the state density f_α by inverse Laplace transformation. In other words $Z_\alpha(\beta)=\int_0^\infty e^{-\beta\omega}f_\alpha(\omega)d\omega$. For the unperturbed oscillator one has

$$f_0(\omega)=\sum_{n=0}^{\infty}\tfrac{1}{2}(n+1)(n+2)\delta(\omega-\eta_n),\quad \eta_n=(n+\tfrac{3}{2})\eta\ .$$

The effects of the coupling to radiation on f_α are a broadening of the lines (δ peaks) and a shift of their position. (Of course, as already mentioned earlier, they do not depend on the temperature.)

In the Appendix we prove a theorem on the structure of f_α. The essence of that theorem is that the ground state, shifted down to $\hbar\omega_\alpha=(3\hbar\eta/\pi)(\cos\varphi+\varphi\sin\varphi)$, see Eq. (2), remains stable, a property which is expected from rather general considerations, and that all other states become unstable. For the position of the lines and for the linewidths, which are closely related to the lifetimes, more details about the inverse Laplace transform of Z_α are needed.

A numerical analysis of the one-dimensional case shows that f_α is very well approximated by the sum of Lorentz profiles

$$\frac{\Gamma_n/\pi}{(\omega-\omega_n)^2+\Gamma_n^2}$$

centered around $\omega_n=2(n+\frac{1}{2})\omega_\alpha$ with widths $2\Gamma_n=2\eta n\cos\varphi$ and heights $(\pi\Gamma_n)^{-1}$. In particular this shows an increasing of the negative shifts and of the linewidths proportional to n. Since $\Gamma_1=e^2\eta^2(3mc^3)^{-1}$, we have reproduced the formulas for the transition probabilities from the nth eigenstate to the $(n-1)$th eigenstate found by perturbative quantum electrodynamics, which give the natural linewidths. A detailed presentation of these results will be the subject of a forthcoming paper.

APPENDIX

Theorem. Let $\alpha>0$ (more precisely $0<\varphi<\pi/2$) and $\omega_\alpha\equiv(3/\pi)\eta(\cos\varphi+\varphi\sin\varphi)$. Then (i) $f_\alpha(\omega)\geq0$ for all $\omega\geq0$, (ii)

$$f_\alpha(\omega)=\delta(\omega-\omega_\alpha)+\frac{\pi}{\eta}\cos\varphi\,\Theta(\omega-\omega_\alpha)+r_\alpha(\omega)\ ,$$

where r_α is a continuous function with $r_\alpha(\omega)=0$, for all $\omega\leq\omega_\alpha$, and $\lim_{\omega\to\infty}e^{-\sigma\omega}r_\alpha(\omega)=0$, for any $\sigma>0$.

Proof. It suffices to prove the analogous assertions for the inverse Laplace transform $f(x)$ of

$$z(p)\equiv\frac{p}{2\pi}\exp[-(2\cos\varphi)p\ln p]\,|\Gamma(pe^{i\varphi})|^2\ .$$

According to Stirling's formula the asymptotic expansion

$$z(p)=e^{-x_\alpha p}\left[1+\frac{\cos\varphi}{6p}+\frac{\cos^2\varphi}{72p^2}+\cdots\right],$$

$$x_\alpha\equiv2(\cos\varphi+\varphi\sin\varphi)\ ,$$

holds for $|p|\to\infty$, $|\arg(p)|\leq\pi/2$. Hence

$$z_1(p)\equiv z(p)-e^{-x_\alpha p}\left[1+\frac{\cos\varphi}{6p}\right]$$

is analytic in the open right half-plane, vanishes there as $|p|\to\infty$, and $\int_{-\infty}^{\infty}|z_1(\sigma+i\rho)|d\rho<\infty$ for any $\sigma>0$. The latter follows from

$$|z_1(\sigma+i\rho)|\leq M_\sigma\,|e^{-x_\alpha(\sigma+i\rho)}|\,|\sigma+i\rho|^{-2}$$

with some constant M_σ. According to Ref. 18, Sec. 5, theorem 11.2, there is a function f_1 satisfying $z_1(p)=\int_0^\infty e^{-px}f_1(x)dx$. Moreover,

$$f_1(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{(\sigma+i\rho)x}z_1(\sigma+i\rho)d\rho\ ,$$

and hence, by the Riemann-Lebesgue lemma $e^{-\sigma x}f_1(x)$ is continuous and vanishes for $|x|\to\infty$. To accomplish (ii), it remains to show $f(x)=0$ for all $x<x_\alpha$. Consider

$$z_2(p)\equiv z(p)-e^{-x_\alpha p}\left[1+\frac{1}{2\pi p}\right].$$

We like to apply Ref. 19, theorem 9.6. Indeed, $\sigma\mapsto z_2(-i\sigma)$ is the pointwise limit of $z_2(\rho-i\sigma)$ for $\rho\downarrow0$, which is analytic in the upper half-plane. Since $z_2(p)=-(\cos\varphi/\pi)\ln p+O(p^0)$ for $p\to0$ and $z_2(-i\sigma)=O(\sigma^{-1})$ for $|\sigma|\to\infty$,

$$\int_{-\infty}^{\infty}|z_2(-i\sigma)|^2d\sigma<\infty\ .$$

Finally, from Stirling's formula it follows that

$$|z_2(\rho-i\sigma)|^2\leq\exp(-2x_\alpha\rho)\frac{M}{\sigma^2+\rho^2}$$

with some constant M for all ρ sufficiently large.

We turn to (i). By Bernstein's theorem (Ref. 18, Sec. 6.7), an equivalent property is that $z(p)/p$ is completely monotonic. We apply the following simple fact. Let g be a real infinitely differentiable function such that $-g'$ is completely monotonic. Then $h\equiv\exp(g)$ is completely monotonic, too. This is proved by induction: Clearly, $h>0$ and, since $h'=hg'$,

$$(-1)^{n+1}h^{(n+1)} = \sum_{k=0}^{n} \binom{n}{k}(-1)^k h^{(k)}(-1)^{(n+1-k)}g^{(n+1-k)} \geq 0 \ .$$

In the present case, where $h(p)=z(p)/p$, we have

$$-g'(p)=2(\cos\varphi)(1+\ln p) - e^{i\varphi}\psi(pe^{i\varphi})-e^{-i\varphi}\psi(pe^{-ip}) \ .$$

Using Binet's expression

$$\psi(z)=\ln z+\int_0^\infty [x^{-1}-(1-e^{-x})^{-1}]e^{-xz}dx \ ,$$

one can show that

$$-g'(p)=x_\alpha+2\int_0^\infty \mathrm{Re}\{[1-\exp(-xe^{i\varphi})]^{-1} - (xe^{i\varphi})^{-1}\}e^{-xp}dx \ .$$

Since Re{ } ≥ 0, the assertion follows by once more applying Bernstein's theorem.

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