Comments on the Interaction Energy of a Quantum Oscillator in the Blackbody Radiation Field

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Recent results on the interaction energy of a quantum oscillator in a radiation field are critically reviewed and compared with the directly calculated thermal expectation values. The proper thermodynamic definition of the interaction energy is given.

The model Hamiltonian describes a linear charged oscillator in the blackbody radiation field (in the minimal coupling Hamiltonian the A^2-term is neglected; dipol-approximation; see formula (1) in [1], which corresponds to the one dimensional version of formula (1) in [2]; see also [3]):

$$\hat{H} = \frac{1}{2}(P^2 + \omega_0^2 Q^2) + \sum_k \left(\frac{4\pi e^2 \omega_0^2}{m V \omega_k^2}\right)^{1/2} \omega_k q_k Q + \frac{1}{2}\sum_k (p_k^2 + \omega_k^2 q_k^2). \tag{1}$$

In (1) the generalized canonical variables P and Q are related with the original variables p and x of the oscillator by the canonical transformation $p = -(m\omega_0^2)^{1/2} Q$, $x = (m\omega_0^2)^{-1/2} P$; p_k and q_k denote the canonical variables of the field.

The averages $\langle\rangle_{\hat{H}}$ are taken on the assumption that the Hamiltonian (1) is in thermal equilibrium (i.e. the density matrix ϱ is given by $\varrho \sim e^{-\hat{H}/k_B T}$). E.g., the internal energy of the oscillator is defined by the difference

$$\hat{U} = \langle \hat{H} \rangle_{\hat{H}} - \langle H_B \rangle_{H_B}, \tag{2}$$

where $H_B = \frac{1}{2}\sum_k (p_k^2 + \omega_k^2 q_k^2)$, and where $\langle\rangle_{H_B}$ denotes the thermal average with respect to the undisturbed field ($\varrho_B \sim e^{-H_B/k_B T}$).

By functional integration techniques (Feynman Vernon theory; an effective action leads to the partition function; the field oscillators are averaged out) Castrigiano [2] calculated the internal energy $\hat{U}$ of the oscillator and the moments $\langle P^2 \rangle_{\hat{H}}$ and $\langle Q^2 \rangle_{\hat{H}}$. In order to get finite values for $\hat{U}$, $\langle Q^2 \rangle_{\hat{H}}$ and $\langle P^2 \rangle_{\hat{H}}$, in [2] a twofold renormalization had to be performed. The main point in [2] was the calculation of the finite and temperature independent difference (we refer to the one dimensional version):

$$\hat{\Delta} = \hat{U} - \left[\frac{1}{2}\langle P^2 \rangle_{\hat{H}} + \frac{\omega_0^2}{2}\langle Q^2 \rangle_{\hat{H}}\right] \tag{3}$$

with the result

$$\hat{\Delta} = \frac{1}{3\pi}\hbar\omega_0 \varepsilon, \tag{4}$$

where ε denotes the small coupling parameter:

$$\varepsilon = \frac{e^2}{\hbar c}\frac{\omega_0}{m c^2/\hbar}. \tag{5}$$

It was claimed that (3) represents the interaction energy of the oscillator with the radiation field, and that (3) takes the value (4).

In our opinion, and in contrast with (3) the thermodynamic interaction energy should alternatively be defined by the expression

$$\hat{\delta} = \hat{U} - \hbar\omega_0 \left\{\left[\exp\frac{\hbar\omega_0}{k_B T} - 1\right]^{-1} + \frac{1}{2}\right\} \tag{6}$$

Equation (6) represents the difference of the internal energies of a system (oscillator and field) in a heatbath after and before there is a coupling between the two subsystems.

In this letter I calculate the different contributions to (6) seperately and give the corresponding high- and low-temperature expansions. My calculations indicate that the result (4) is due to an inconsistency in [2].

In order to make the Hamiltonian (1) integrable one can introduce a Debye-like ($\sum_k \to \sum_k \theta(\gamma - \omega_k)$) or Drude-like ($\sum_k \to \sum_k \gamma(\gamma^2 + \omega_k^2)^{-1/2}$) regularisation in

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the interaction Hamiltonian. The limit $\gamma \to \infty$ ('Markovian limit') requires a renormalization of the frequency and (1) has to be replaced by

$$H = \hat{H} + \frac{1}{3}\omega_0 \varepsilon \gamma Q^2. \tag{7}$$

The added term causes the just mentioned renormalization of a divergent frequency. This frequency $\Omega^2 = \omega_0^2 - 2\omega_0 \varepsilon \gamma/3$ is the centre of the corresponding susceptibility $\chi(\omega) = [-\omega^2 + \Omega^2 - i\omega(2\omega_0 \varepsilon)]^{-1}$ by which the relevant contributions can be expressed [4]. This centre is shifted to ω_0^2 by the renormalization procedure (7) [5]. Accordingly, the results in [2] have to be compared with the results which are based on (7) and in the above formulas (especially (2), (3) and (6)) $\hat{H}$ has to be replaced by H. The Hamiltonian (7) corresponds to Ullersma's model [4], which can exactly be diagonalized. The exact solutions for $P(t)$, $Q(t)$, $p_k(t)$ are linearily related with the normal modes of (7). My considerations are based on the knowledge of these solutions [4, 6].

The transition to a continuum of field oscillators demands the introduction of the density of states:

$$\sum_k \to \frac{V}{3\pi^2 c^3} \int_0^\infty \omega_k^2 \, \mathrm{d}\omega_k.$$

For the averaged interaction Hamiltonian we find the exact result (in (2.26) in [6] ω_0^2 has to be replaced by $\omega_0^2 - \frac{2}{3}\omega_0 \varepsilon \gamma$ because we have to refer to (7) and not to (1)):

$$\langle H_{\mathrm{int}} \rangle_H = \sum_k \left[\frac{4\pi e^2 \omega_0^2}{m V \omega_k^2} \frac{\gamma^2}{\omega_k^2 + \gamma^2} \right]^{1/2} \omega_k \langle q_k Q \rangle_H \tag{8}$$

$$= 2\left[\frac{1}{2}\langle P^2 \rangle_H - \frac{1}{2}\omega_0^2 \langle Q^2 \rangle_H - \frac{1}{3}\omega_0 \varepsilon \gamma \langle Q^2 \rangle_H \right].$$

The expression (8) is negative and illustrates the attractive character of the interaction in Ullersma's model. The finite solutions for $\frac{1}{2}\langle P^2 \rangle_H$ and $\frac{\omega_0^2}{2}\langle Q^2 \rangle_H$ are given by (10) and (11) in [1], respectively. This formulas exactly correspond to (11) and (13) in [2].

A rather involved calculation yields the difference [7]:

$$\langle H_{\mathrm{B}} \rangle_H - \langle H_{\mathrm{B}} \rangle_{H_{\mathrm{B}}} = -\langle H_{\mathrm{int}} \rangle_H - \omega_0 \varepsilon \gamma/3 \langle Q^2 \rangle_H + O(\varepsilon/\gamma). \tag{9}$$

In (9) the transition to the continuous spectrum is to be made after the difference of the discrete version was formed. To begin with, the difference (9) is written as a contour integral in the complex plane. Secondly, the proper transition from the discrete poles to a out on the real axis can be made (see the similar considerations in [4]).

As an important result we find that the thermodynamic quantites are well defined in the limit $\gamma \to \infty$ (the terms which are proportional to γ cancel) and can be written in terms of the moments $\langle P^2 \rangle_H$ and $\langle Q^2 \rangle_H$:

$$U = \langle H \rangle_H - \langle H_{\mathrm{B}} \rangle_{H_{\mathrm{B}}} = \frac{1}{2}\langle P^2 \rangle_H + \frac{\omega_0^2}{2}\langle Q^2 \rangle_H$$

$$= \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \hbar \left[\langle n_\omega \rangle + \frac{1}{2} \right] \tag{10}$$

$$\cdot (\omega^2 + \omega_0^2) \, \mathrm{Im}[-\omega^2 + \omega_0^2 - i\omega(2\varepsilon\omega_0/3]^{-1},$$

$$\Delta = U - \left[\frac{1}{2}\langle P^2 \rangle_H + \frac{\omega_0^2}{2}\langle Q^2 \rangle_H \right] = 0. \tag{11}$$

In contrast to the thermal part of (10) (the $T = 0$ contributions are subtracted; $\langle \ldots \rangle^{\mathrm{th}} = \langle \ldots \rangle - \langle \ldots \rangle^{T=0}$), $\langle H_{\mathrm{int}} \rangle_H^{\mathrm{th}}$ does not exist in the limit $\gamma \to \infty$. In the high-and-low-temperature approximation we find the results (we only consider the leading terms; see also the results in [3] which coincide with my results):

$$U^{\mathrm{th}} \xrightarrow[k_{\mathrm{B}} T \gg \hbar\omega_0]{} \hbar\omega_0 \left[\exp \frac{\hbar\omega_0}{k_{\mathrm{B}} T} - 1 \right]^{-1} - \frac{1}{3\pi} \varepsilon \hbar \omega_0 \ln \frac{2\pi k_{\mathrm{B}} T}{\hbar \omega_0}, \tag{12}$$

$$U^{\mathrm{th}} \xrightarrow[k_{\mathrm{B}} T \ll \hbar\omega_0]{} \hbar\omega_0 \left[\exp \frac{\hbar\omega_0}{k_{\mathrm{B}} T} - 1 \right]^{-1} + \frac{\pi}{9} \varepsilon \frac{(k_{\mathrm{B}} T)^2}{\hbar \omega_0}. \tag{13}$$

With respect to the Ullersma model one can define the 'kinetic' and 'potential' energies, $\frac{1}{2}\langle P^2 \rangle_H$ and $\frac{1}{2}\omega_0^2 \langle Q^2 \rangle_H$, respectively (the term which was added to $\hat{H}$ is not included in the so defined potential energy). We see that U is exactly the sum of 'kinetic' and 'potential' energy as it was assumed in [1]. In contrast to the result (4), Δ vanishes. The temperature independent part of $\frac{1}{2}\langle P^2 \rangle_H$ (and of U) is divergent. A proper renormalization could be interpreted as a finite shift of the zero point of energy. E.g., we find

$$\lim_{\gamma \to \infty} \left[\frac{1}{2}\langle P^2 \rangle_H^{T=0} - \frac{\hbar\omega_0 \varepsilon}{3\pi} \ln \frac{\gamma}{\omega_0} \right] = \frac{1}{4}\hbar\omega_0 \left(1 - \frac{2\varepsilon}{3\pi} \right). \tag{14}$$

I assume that the finite result for Λ in [2] is due to an inconsistent renormalization procedure with respect to U on the one hand and $\langle P^2\rangle_H/2$ on the other hand (of course, in [2, 3] also a twofold renormalization had to be performed, which essentially corresponds to (7) and (14)).

It should be noted that the omission of the $\boldsymbol{A}^2$-term destroys the original gauge invariance of the minimal coupling Hamiltonian. This shortcoming had to be repaired by the regularization (7) [7]. With respect to the original minimal coupling Hamiltonian (including the $\boldsymbol{A}^2$-term) we must distinguish between canonical and kinetic momentum. Therefore, the kinetic energy is given by the expression $\frac{1}{2m}\left\langle\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}\right)^2\right\rangle$ $\left(\dot{\boldsymbol{x}}=\frac{1}{m}\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}\right)\right)$, and the expression $\frac{1}{2m}\langle p^2\rangle^{\text{th}}$ $=\omega_0^2/2\langle Q^2\rangle^{\text{th}}$ can in principle not be interpreted as the kinetic energy of the electron.

The thermal part of the interaction energy (6) leads in the high- and low-temperature regime to the second term in (12) and (13), respectively.

At last I emphasize that due to the neglection of the $\boldsymbol{A}^2$-term the model (7), which was considered in [1–3], cannot reveal the well known T^2-dependent energy shift in the high temperature regime ($k_B T \gg h\omega_0$) [8]. The inclusion of the $\boldsymbol{A}^2$-term in (1) would cause the additional term $\eta=\frac{1}{9}\pi\varepsilon h\omega_0$ $(k_B T/h\omega_0)^2$ in U^{th}. Consequently, the low-temperature T^2-shifts in (13) cancel out whereas in the high-temperature regime η represents the most important correction to the free oscillator result.

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