Comment on the exact calculation of the partition function for a quantum oscillator interacting with the radiation field

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In their recent paper [Phys. Rev. A 35, 4122 (1987)] Castrigiano and Kokiantonis claim to present an exact calculation of the partition function for a quantum oscillator interacting with the blackbody radiation field. In this Comment it is shown that their result is in fact wrong, due essentially to their neglect at the outset of the  $A^2$  term in the Hamiltonian. It is further shown how their error can be repaired to give the correct result given by us in an earlier publication [Phys. Rev. Lett. 55, 2273 (1985)].

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In their paper,<sup>1</sup> Castrigiano and Kokiantonis claim to present an exact calculation of the partition function and, hence, the free energy of a quantum harmonic oscillator interacting with the radiation field. We wish to point out here that their calculation is wrong and that when the error is repaired a calculation such as theirs gives the correct result.<sup>2</sup>

The point is this. They begin with the correct Hamiltonian for a three dimensional charged oscillator of (bare) mass m and spring constant K interacting via dipole coupling with the radiation field:

$$H = \frac{1}{2m} \left( \vec{p} - \frac{e}{c} \vec{A} \right)^{2} + \frac{1}{2} K \vec{r}^{2} + H_{rad} , \qquad (1)$$

where the vector potential in dipole approximation is

$$\vec{A} = \sum_{\vec{k},\sigma} \left( \frac{2\pi\hbar^2}{\omega V} \right)^{\frac{1}{2}} \hat{e}_{\vec{k},\sigma} \left( a_{\vec{k},\sigma} + a_{\vec{k},\sigma}^* \right) , \qquad (2)$$

and the radiation field Hamiltonian is

$$H_{rad} = \sum_{\vec{k},\sigma} \hbar\omega \left( a_{\vec{k},\sigma}^* a_{\vec{k},\sigma} + \frac{1}{2} \right) .$$
(3)

But at the outset they drop the term:

$$e^{2}A^{2}/2mc^{2}$$
 (4)

Then, at a later stage, they add a term (the "counter term" appearing in the text following Eq.(10)) that, when expressed in terms of the variables of the original Hamiltonian (1), takes the form:

$$\frac{2\pi e^2}{m^2 V} \sum_{\vec{k},\sigma} \left( \frac{\hat{e}_{\vec{k},\sigma} \cdot \vec{p}}{\omega} \right)^2.$$
(5)

Finally they interchange the meaning of coordinate and momentum with the canonical transformation:  $\vec{r} \rightarrow \vec{p}$ ,  $\vec{p} \rightarrow -\vec{r}$ . The result is

the Hamiltonian:

$$H^{*} = \frac{1}{2}K_{p}^{\dagger 2} + \frac{1}{2m}\vec{r}^{2}$$
$$+ \sum_{\vec{k},\sigma} h\omega \left\{ \left[ a_{\vec{k},\sigma}^{*} + \left( \frac{2\pi e^{2}}{\hbar\omega^{3} V} \right)^{\frac{1}{2}} \hat{e}_{\vec{k},\sigma} \cdot \frac{\vec{r}}{m} \right] \left[ a_{\vec{k},\sigma}^{*} + \left( \frac{2\pi e^{2}}{\hbar\omega^{3} V} \right)^{\frac{1}{2}} \hat{e}_{\vec{k},\sigma} \cdot \frac{\vec{r}}{m} \right] + \frac{1}{2} \right\} .$$
(6)

This Hamiltonian does not correspond to the oscillator coupled to the radiation field. In fact it corresponds to a Drude model with a frequency-independent friction constant equal to  $2\text{Ke}^2/3\text{mc}^3$ . This, then, is their error: they calculate from the outset with the wrong Hamiltonian.

Indeed, the "main result" of Castrigiano and Kokiantonis, their Eq.(11), is equivalent with the expression for the free energy for such a Drude model given in Ref.2, Eq.(25). Thus their path integral calculation is correct; it is their physics which is wrong. Here we should perhaps emphasize that their wrong starting point leads them to completely miss the well known  $T^2$  dependence of the free energy of an atom interacting with *high temperature* blackbody radiation They are incorrect when they say this is a low temperature result.

The importance of retaining the A<sup>2</sup> term in order to obtain physically consistent results was pointed out in the well known work of Power and Zienau.<sup>3,4</sup> There, too, one finds (Ref. 4 p.104) the unitary transformation:

$$U = \exp\left\{\frac{ie}{\hbar c} \vec{r} \cdot \vec{A}\right\}, \qquad (7)$$

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which brings the Hamiltonian (1) to the form:

$$H = \frac{1}{2m} \dot{p}^{2} + \frac{1}{2} K \dot{r}^{2} + \frac{1}{2} K \dot{r}^{2} + \sum_{\substack{k,\sigma \\ \vec{k},\sigma}} \hbar \omega \left\{ \left[ a_{\vec{k},\sigma}^{*} - i \left( \frac{2\pi e^{2}}{\hbar \omega V} \right)^{\frac{1}{2}} \hat{e}_{\vec{k},\sigma} \cdot \dot{r} \right] \left[ a_{\vec{k},\sigma} + i \left( \frac{2\pi e^{2}}{\hbar \omega V} \right)^{\frac{1}{2}} \hat{e}_{\vec{k},\sigma} \cdot \dot{r} \right] + \frac{1}{2} \right\}.$$

$$(8)$$

This Hamiltonian is equivalent to the original Hamiltonian (1), with no terms added and no terms dropped, and it is of the form desired by Castrigiano and Kokiantonis for their path integration method. With it they will find the exact result for the free energy obtained in Ref.2 by a rigorous and, we believe, far simpler method.

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