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Connection of the classical electromagnetic zero-point radiation spectrum to quantum mechanics for dipole harmonic oscillators

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(Received 14 February 1992)

Recently the classical electrodynamic zero-point spectrum was derived as being the appropriate spectrum for the thermodynamic definition of absolute-zero temperature to hold for classical, electric dipole harmonic oscillators [Cole, Phys. Rev. A **42**, 1847 (1990)]. This analysis involved the lengthy calculation of nonperturbative, retarded van der Waals thermodynamic functions. Here this derivation is shown to hold for the much simpler unretarded, resonance situation. The connection to quantum mechanics is then more immediate.

PACS number(s): 05.90.+m, 05.40.+j, 05.70.−a, 34.30.+h

The theory of stochastic electrodynamics (SED) considers the behavior of classical electromagnetic fields and classical charged particles to obey (i) Maxwell's equations and (ii) the relativistic generalization of Newton's second law of motion. Where this theory differs from traditional classical physics is that the assumption is *not* also imposed that electromagnetic thermal radiation must reduce to zero at absolute zero temperature. Instead, the $T=0$ spectrum is taken to be the classical electromagnetic zero-point (ZP) radiation spectrum, which assigns an energy of $\hbar\omega/2$ to each mode in the spectrum. Surprisingly, this simple change has enabled quantum physical properties to be deduced for a number of physical systems. References [1–6] review this work. Some very interesting results have been obtained to date. Nevertheless, presently the full range of strengths and shortcomings of this theory for describing nature is not fully known, particularly for nonlinear, realistic systems in nature, such as the hydrogen atom.

A recent result obtained in SED will be extended further here. In Ref. [7] the functional form of the classical electromagnetic ZP radiation spectrum was deduced as the appropriate spectrum to be in equilibrium at temperature $T=0$ with a set of nonrelativistic electric dipole simple harmonic oscillators, if the system is to obey the fundamental thermodynamic definition of absolute-zero temperature. If SED is a fundamental theory of nature, then this same result should apply to more complicated, and more physically realistic, systems. Indeed, Ref. [8] showed that this property also holds for blackbody radiation between conducting parallel plates, or within conducting rectangular cavities.

The calculations in Ref. [7] were quite involved (e.g., see the Appendix), largely because the full unretarded fields were treated. Since heat flow $\langle \mathcal{Q} \rangle$, due to electromagnetic thermal radiation, is largely a result of the radiation fields from atoms, I originally assumed it was necessary to retain these terms when calculating $\langle \mathcal{Q} \rangle$ during a quasistatic thermodynamic operation. However, the present analysis shows that retaining these terms is *not* necessary. If one directly calculates the heat radiated via the use of the Poynting vector [as in Eqs. (23) and (28a)–(28d) in Ref. [6]], then yes, one must include the radiation fields. However, $\langle \mathcal{Q} \rangle$ in Ref. [7] was calculated not directly with the Poynting vector, but rather by finding the ensemble average of the change in internal energy of the system $\langle \Delta\mathcal{U}_{\rm int} \rangle$ and the work done $\langle \mathcal{W} \rangle$ upon displacing one or more dipole oscillators,

$$\langle \mathcal{Q} \rangle = \langle \Delta\mathcal{U}_{\rm int} \rangle - \langle \mathcal{W} \rangle \; . \qquad (1)$$

(These terms are described in detail in Ref. [6].) For $\langle \Delta\mathcal{U}_{\rm int} \rangle$ and $\langle \mathcal{W} \rangle$, the radiation terms add only correction terms and are not essential, provided the oscillators are sufficiently close to each other that they satisfy $\omega_0 R/c \ll 1$, where R is the maximum distance between oscillators and ω_0 is the approximate resonant frequency of each oscillator.

The resulting derivation for the ZP spectrum is considerably shorter, and the connection with quantum mechanics more immediate. Of course, the fact that the ZP spectrum was deduced when *all* the radiation terms was retained is indeed physically significant, and certainly more significant than not retaining them; however, retaining them is not necessary if the purpose of the derivation is to simply examine the essential physical content of the reasoning.

To begin our analysis, the kinetic (KE), potential (PE), and electromagnetic (EM) energies for N dipole oscillators in Ref. [7] are given by

$$U_{\rm PE}\equiv\sum_{A=1}^{N}\left\langle\frac{m\omega_0^2}{2}|\delta z_A|^2\right\rangle$$
$$=\pi\int_0^\infty d\omega\, h_{\rm in}^2\,{\rm Im}\left[\frac{1}{C}\sum_{A=1}^{N}\sum_{i=1}^{3}(\underline{M}^{-1})_{Ai;Ai}\frac{\omega_0^2}{\omega}\right], \quad (2)$$

$$U_{\rm KE}\equiv\sum_{A=1}^{N}\left\langle\frac{m}{2}|\delta\dot z_A|^2\right\rangle$$
$$=\pi\int_0^\infty d\omega\, h_{\rm in}^2\,{\rm Im}\left[\frac{1}{C}\sum_{A=1}^{N}\sum_{i=1}^{3}(\underline{M}^{-1})_{Ai;Al}\omega\right], \quad (3)$$

and by $U_{{\rm EM},\mathcal{D}a\text{-}\mathcal{D}a}$, $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$, and $U_{{\rm EM},\mathcal{D}\text{-in}}$, which represent volume integrals over the electromagnetic energy cross terms due to the acceleration fields of each individual oscillator, the dipole-dipole fields, and the dipole-incident fields, respectively. The notation here follows Ref. [7]. In particular,

$$C(\omega)=-\omega^2+\omega_0^2-i\Gamma\omega^3\ , \quad (4)$$

$$M_{Ai;Bj}=\delta_{AB}\delta_{ij}-(1-\delta_{AB})\frac{e^2}{m}\frac{\eta_{ij}^{\mathcal{D}}(Z_A-Z_B,\omega)}{C(\omega)}\ , \quad (5)$$

$$\eta_{ij}^{\mathcal{D}}(x-\mathbf{Z}_A,\omega)=(\nabla_i\nabla_j+k^2\delta_{ij})\frac{e^{ik|\mathbf{x}-\mathbf{Z}_A|}}{|\mathbf{x}-\mathbf{Z}_A|}\ , \quad (6)$$

where $\eta_{ij}^{\mathcal{D}}(\mathbf{x}-\mathbf{Z}_A,\omega)$ occurs in the electric-field expression for an electric dipole $\mathbf{p}_A(t)$ at position $\mathbf{Z}_A$ (Eq. (38) in Ref. [7]).

The calculations for the energies $U_{\rm PE}$, $U_{\rm KE}$, and $U_{{\rm EM},\mathcal{D}a\text{-}\mathcal{D}a}$ were relatively short, while the ones for $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$ and $U_{{\rm EM},\mathcal{D}\text{-in}}$ were quite lengthy [9]. Moreover, $U_{{\rm EM},\mathcal{D}a\text{-}\mathcal{D}a}$, $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$ and $U_{{\rm EM},\mathcal{D}\text{-in}}$ all depend on the shape and size of the volume $\mathcal{V}$ enclosing the N particles; their magnitudes can be quite large, as they increase with $\mathcal{V}$. Nevertheless, for large $\mathcal{V}$, the sum of these three terms, denoted by $U_{\rm EM|in}$, is independent of $\mathcal{V}$.

In the unretarded (ur) case of $\omega_0 R/c \ll 1$, $\eta_{ij}^{\mathcal{D}}(\mathbf{R},\omega_0)$ is approximately given by

$$\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{R},\omega_0)=\nabla_i\nabla_j\left[\frac{1}{R}\right]+i\tfrac{2}{3}k_0^3\delta_{ij}$$
$$\underset{(R\neq 0)}{=}\frac{(-\delta_{ij}+3R_iR_j/R^2)}{R^3}+i\tfrac{2}{3}k_0^3\delta_{ij} \quad (7)$$

the real part of which is independent of ω_0. Under this condition, and also when $\Gamma\equiv e^2/mc^3\ll 1/\omega_0$, our energy expressions become integrals over strongly peaked integrands near $\omega\approx\omega_0$, as will be shown. Substituting Eq. (7) into the terms in brackets in Eq. (55) in Ref. [7],

$$U_{\rm EM|in}\approx\pi\int_0^\infty d\omega\, h_{\rm in}^2\,{\rm Im}\left\{\frac{1}{C}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}(\underline{M}^{-1})_{Ai;Bj}\left[\delta_{ij}2i\Gamma\omega_0^2-(1-\delta_{AB})\frac{e^2}{m\omega}{\rm Re}\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{Z}_A-\mathbf{Z}_B)\right]\right\}. \quad (8)$$

As we will verify shortly [after Eq. (19)], only the real part of the quantity in square brackets contributes in the resonance approximation. Neglecting the $2i\Gamma\omega_0^2$ term, Eq. (8) can then be shown to be precisely equal to the "electrostatic" energy of interaction between electric dipoles, computed using only the unretarded ($\omega R/c\ll 1$) electric dipole fields [10],

$$U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}^{\rm ur}\equiv\sum_{\substack{A,B=1\\A\neq B}}^{N}\frac{1}{8\pi}\int_{\mathcal{V}}d^3x\,\langle\mathbf{E}_{\mathcal{D},A}^{\rm ur}\cdot\mathbf{E}_{\mathcal{D},B}^{\rm ur}\rangle=-\tfrac{1}{2}\sum_{A\neq B,i,j}{\rm Re}[\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{Z}_A-\mathbf{Z}_B)]\langle p_{Ai}(t)p_{Bj}(t)\rangle\ , \quad (9)$$

where

$$[\mathbf{E}_{\mathcal{D},A}^{\rm ur}(\mathbf{x},t)]_i=\sum_{j=1}^{3}{\rm Re}[\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{x}-\mathbf{Z}_A)]p_{Aj}(t)\ , \quad (10)$$

and $\mathbf{p}_A(t)=e\delta\mathbf{z}_A(t)$.

We have now explicitly justified using only the energies $U_{\rm PE}$, $U_{\rm KE}$, and $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}^{\rm ur}$ when calculating the total energy in the unretarded van der Waals situation. We obtained this result despite the fact that $U_{{\rm EM},\mathcal{D}a\text{-}\mathcal{D}a}$, $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$, and $U_{{\rm EM},\mathcal{D}\text{-in}}$ are each not at all negligible, since they increase with $\mathcal{V}$. The calculations for $U_{\rm PE}$, $U_{\rm KE}$, and $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}^{\rm ur}$ are enormously simpler than these other terms. Moreover, we have the welcome connection that $U_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}^{\rm ur}$ is precisely the electrostatic energy of interaction used in quantum mechanics when calculating the unretarded van der Waals force between electric dipoles [11,12]. The quantity $U_{\rm EM|in}$ in Ref. [7] contains the remaining radiative contributions to the total energy.

Turning to the resonance method for explicitly evaluating the integrals in the energy terms, we can make use of the diagonalization procedure by Blanco, Franca, and Santos in Ref. [13]. Let

$$\underline{L}\equiv\underline{M}mC(\omega)\approx\underline{\overline{K}}+i\,{\rm Im}\underline{R}-m\omega^2\underline{I}\ , \quad (11)$$

where

$$(\underline{\overline{K}})_{Ai;Bj}\equiv m\omega_0^2\delta_{AB}\delta_{ij}-(1-\delta_{AB})e^2{\rm Re}\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{Z}_A-\mathbf{Z}_B)\ , \quad (12)$$

$${\rm Im}(\underline{R})_{Ai;Bj}\equiv-\Gamma m\omega^3\delta_{AB}\delta_{ij}-(1-\delta_{AB})e^2{\rm Im}\eta_{ij}^{\mathcal{D}\rm ur}(\mathbf{Z}_A-\mathbf{Z}_B,\omega)\ . \quad (13)$$

Since $\underline{\overline{K}}$ is symmetric, there exists an orthogonal matrix $\underline{A}$ that transforms and diagonalizes $\underline{\overline{K}}$,

$$(\underline{\tilde{A}\overline{K}A})_{Ai;Bj}\equiv(\underline{\overline{K}}')_{Ai;Bj}=\delta_{AB}\delta_{ij}m\varpi_{Ai}^2\ . \quad (14)$$

A subsequent transformation due to $\underline{I}+\underline{C}$, where $\underline{C}=O(e^2)$, as discussed in Ref. [13], then enables $\underline{L}$ to be diagonalized up to order $O(e^4)$ in the charge:

$$(\underline{L}'')_{Ai;Bj}=\delta_{AB}\delta_{ij}[m(\tilde{\omega}_{Ai}^2-\omega^2)+i\,\mathrm{Im}R'_{Ai;Ai}(\omega)]+O(e^4)\,. \tag{15}$$

To calculate $U_{\rm PE}$, $U_{\rm KE}$, and $U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$, as well as show that $U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}\approx U_{\rm EM|in}$, we need to make use of (i) $\mathrm{Tr}(\underline{L}^{-1}\underline{B})=\mathrm{Tr}(\underline{L}''^{-1}\underline{B}'')$ and (ii) the resonance integral evaluation described in a number of other places, such as Refs. [13] and [14]. Consider the following:

$$\begin{aligned}\int_0^\infty d\omega\,\mathrm{Im}\{\mathrm{Tr}[\underline{L}^{-1}(\omega)\underline{B}(\omega)]\}&\approx\int_0^\infty d\omega\,\mathrm{Im}\left\{\sum_{A=1}^{N}\sum_{i=1}^{3}\left[\frac{B''_{Ai;Ai}}{m(\tilde{\omega}_{Ai}^2-\omega^2)+i\,\mathrm{Im}R'_{Ai;Ai}}\right]\right\}+O(e^4)\\&\approx\sum_{A,i}\int_0^\infty d\omega\frac{\mathrm{Re}(B''_{Ai;Ai})(-\mathrm{Im}R'_{Ai;Ai})+\mathrm{Im}(B''_{Ai;Ai})m(\omega_{Ai}^2-\omega^2)}{m^2(\tilde{\omega}_{Ai}^2-\omega^2)^2+[\mathrm{Im}R'_{Ai;Ai}]^2}\\&\approx\sum_{A,i}\frac{\pi\,\mathrm{Re}[B''_{Ai;Ai}(\tilde{\omega}_{Ai})]}{2m\tilde{\omega}_{Ai}}\,.\end{aligned}\tag{16}$$

Here, we used the fact that $\mathrm{Im}R_{Ai;Ai}<0$. To evaluate $U_{\rm PE}$, let

$\underline{B}=\underline{I}m\pi h_{\rm in}^2(\omega)(\omega_0^2/\omega)$;

for $U_{\rm KE}$, $\underline{B}=\underline{I}m\pi h_{\rm in}^2(\omega)\omega$. In both cases, $\underline{B}=\underline{B}''$, and we obtain

$$U_{\rm PE}\approx\sum_{A=1}^{N}\sum_{i=1}^{3}\frac{\pi^2}{2}h_{\rm in}^2(\tilde{\omega}_{Ai})\frac{\omega_0^2}{\tilde{\omega}_{Ai}^2}\,, \tag{17}$$

$$U_{\rm KE}\approx\sum_{A=1}^{N}\sum_{i=1}^{3}\frac{\pi^2}{2}h_{\rm in}^2(\tilde{\omega}_{Ai})\,. \tag{18}$$

As for $U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$, $\underline{B}(\omega)=m\pi h_{\rm in}^2(\omega)\underline{Q}(\omega)$, where

$$Q_{Ai;Bj}\equiv-(1-\delta_{AB})\frac{e^2}{m\omega}\mathrm{Re}\eta_{ij}^{\mathcal{D}\,\rm ur}(\mathbf{Z}_A-\mathbf{Z}_B)\,. \tag{19}$$

For $U_{\rm EM|in}$, one would add the imaginary term $\delta_{ij}2i\Gamma\omega_0^2$ in square brackets in Eq. (8) to $Q_{Ai;Bj}$. Since $\underline{B}'=\underline{\tilde{A}}\underline{B}\underline{A}$, and here $\underline{B}=O(e^2)$, while $A_{Ai;Bj}$ contains terms of order $O(e^2)$, then $\underline{B}'=O(e^2)$ as well. Hence, $\underline{B}''=(\underline{I}+\underline{C})^{-1}\underline{B}'(\underline{I}+\underline{C})\approx\underline{B}'+O(e^4)$, since $\underline{C}=O(e^2)$. Moreover, $\mathrm{Re}\underline{B}''\approx\mathrm{Re}\underline{B}'=\underline{\tilde{A}}\,\mathrm{Re}(\underline{B})\underline{A}$, since $\underline{A}$ is real. Thus, $\mathrm{Re}\underline{B}''$ is identical, except for terms of order $O(e^4)$, for both cases of $U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$ and $U_{\rm EM|in}$. From Eqs. (12) and (14),

$$Q'_{Ai;Bj}=\frac{1}{m\omega}\delta_{AB}\delta_{ij}m(\tilde{\omega}_{Ai}^2-\omega_0^2)\,. \tag{20}$$

Hence, $U_{\rm EM|in}\approx U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}$ and

$$U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}\approx\sum_{A,i}\frac{\pi^2}{2}h_{\rm in}^2(\tilde{\omega}_{Ai})\frac{\tilde{\omega}_{Ai}^2-\omega_0^2}{\tilde{\omega}_{Ai}^2}\,, \tag{21}$$

yielding $U_{\rm PE}+U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}=U_{\rm KE}$, and

$$U_{\rm PE}+U_{\rm KE}+U^{\rm ur}_{{\rm EM},\mathcal{D}\text{-}\mathcal{D}}\approx\sum_{A,i}\pi^2h_{\rm in}^2(\tilde{\omega}_{Ai})\,. \tag{22}$$

Turning to the work $\langle\mathcal{W}\rangle$ done in slowly displacing the dipoles from positions $\mathbf{Z}_{A,\rm I}$ to $\mathbf{Z}_{A,\rm II}$, Sec. V in Ref. [7] showed how $\langle\mathcal{W}\rangle$ was related to

$$\langle F_{{\rm Lor},A}(t)\rangle=\left\langle\mathbf{p}_A\cdot\nabla_{\mathbf{Z}_A}\mathbf{E}_{{\rm tot}|A}(Z_A,t)+\frac{1}{c}\dot{\mathbf{p}}_A\times\mathbf{B}_{{\rm tot}|A}(Z_A,t)\right\rangle\,, \tag{23}$$

which represents the Lorentz force acting on electric dipole A due to the total (tot) sum of the thermal radiation fields plus the fields of the other $(B\neq A)$ oscillators. The following point will just be noted here. With some difficulty, and using the analysis in Sec. III of Ref. [15], one can show that in the unretarded, resonant condition, the calculation of $\langle\mathbf{F}_{{\rm Lor},A}\rangle$ using Eq. (23) is equivalent to lowest order in e^2 to the same quantity, but where $\mathbf{E}_{{\rm tot}|A}$ and $\mathbf{B}_{{\rm tot}|A}$ in Eq. (23) are replaced by only the sum over the $B\neq A$ *unretarded* dipole fields, and the thermal fields are excluded.

From Sec. V of Ref. [7], and using $\det(\underline{L})=\det(\underline{L}'')$,

$$\begin{aligned}\langle\mathcal{W}\rangle&=\pi\int_0^\infty d\omega\frac{h_{\rm in}^2}{\omega}\mathrm{Im}[\ln\det\underline{M}]\Big|_{\mathbf{Z}_{\rm I}}^{\mathbf{Z}_{\rm II}}\\&=\pi\sum_{B,j}\int_{Z_{Bj,\rm I}}^{Z_{Bj,\rm II}}dZ_{Bj}\int_0^\infty d\omega\frac{h_{\rm in}^2}{\omega}\mathrm{Im}\frac{\partial}{\partial Z_{Bj}}\ln\left[\frac{\det(\underline{L})}{(mC)^{3N}}\right]\\&=\pi\sum_{B,j}\int_{Z_{Bj,\rm I}}^{Z_{Bj,\rm II}}dZ_{Bj}\int_0^\infty d\omega\frac{h_{\rm in}^2}{\omega}\sum_{A,i}\mathrm{Im}\left\{\frac{\frac{\partial}{\partial Z_{Bj}}[m(\tilde{\omega}_{Ai}^2-\omega^2)+i\,\mathrm{Im}R'_{Ai;Ai}]}{m(\tilde{\omega}_{Ai}^2-\omega^2)+i\,\mathrm{Im}R'_{Ai;Ai}}\right\}\\&\approx\pi\sum_{B,j}\int_{Z_{Bj,\rm I}}^{Z_{Bj,\rm II}}dZ_{Bj}\sum_{A,i}\frac{h_{\rm in}^2(\tilde{\omega}_{Ai})}{\tilde{\omega}_{Ai}}\frac{\pi\frac{\partial}{\partial Z_{Bj}}[m\tilde{\omega}_{Ai}^2]}{2m\tilde{\omega}_{Ai}}=\sum_{A,i}\int_{\tilde{\omega}_{A,\rm I}}^{\tilde{\omega}_{Ai,\rm II}}d\tilde{\omega}_{Ai}\pi^2\frac{h_{\rm in}^2(\tilde{\omega}_{Ai})}{\tilde{\omega}_{Ai}}\,.\end{aligned}\tag{24}$$

From Eqs. (1), (22), and (24), we can now deduce that for no heat to flow during a slow displacement operation, as required by the thermodynamic definition of $T=0$, then

$$\frac{h_{\mathrm{in}}^2(\omega)}{\omega}=\frac{\partial h_{\mathrm{in}}^2(\omega)}{\partial \omega} . \tag{25}$$

Hence, $h_{\mathrm{in}}^2=\kappa\omega$, which yields the spectral form for classical electromagnetic ZP radiation.

In conclusion, besides deducing the form of classical electromagnetic ZP spectrum, we also explicitly obtained that at $T=0$ (i) the kinetic plus "electrostatic" energy of a set of classical electric dipole harmonic oscillators equals a constant times the sum of the normal frequencies of oscillators [Eq. (22) with $h_{\mathrm{in}}^2=\kappa\omega$], and (ii) the work done in displacing these dipoles equals the difference in this sum of frequencies [Eq. (24) with $h_{\mathrm{in}}^2=\kappa\omega$]. The same result occurs in quantum mechanics at $T=0$, although in quantum mechanics one does not make a distinction in the methods for calculating these two quantities at $T=0$. In classical physics the methods are quite different: one method involves the ensemble average of kinetic and potential energies, while the other entails the average of the Lorentz force. As shown here, these two methods become equivalent for harmonic oscillators when the thermal radiation spectrum has the ZP spectral form.

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