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Dispersion self-energy of an electron in a dielectric

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The self-energy of an electron in a dielectric medium is calculated using the dispersion-energy approach. The approach that gave a qualitative value for the self-energy in an earlier publication is now improved to produce the quantitative result.

The interaction between an electron and the polar vibrations of an ionic crystal is widely studied in the literature using the Fröhlich Hamiltonian. The purpose of this paper is to show that the interaction between a free (or a bound) electron and its surrounding dielectric medium can also be obtained using the dispersion-self-energy theory. In an earlier paper,[1] referred to hereafter as I, the theory was applied to yield a qualitative estimate for the interaction, but it is shown in this communication that by a simple extension of I, the value for the interaction energy, which agrees exactly with the earlier theories,[2] can be derived. Thus dispersion theory provides a valid alternative to Fröhlich's theory[3] in the study of the electron-lattice interaction.

The dispersion-energy formalism utilizes the idea that the magnitude of the electron-medium interaction is equal to the change the interaction produces in the zero-point energy of the radiation field. The change is obtained by using the dielectric response of the medium through its frequency-dependent dielectric constant $\epsilon(\omega)$ and by considering the excitations of the electron from its stationary state. The electronic excitations caused by its interaction with the medium can be described as dipolar and other multipolar excitations, as the case may be. In I, only dipolar excitations were considered on the assumption that others would not contribute to the interaction. In this comment, a simple procedure is developed to include all the multipolar excitations of the electron in calculating the electron-medium interaction. The result is then seen to be in agreement with the earlier theories.

A sketch of the general procedure for calculating electron-medium interaction is described using the dispersion self-energy formalism. For simplicity and for the sake of comparison with other work, we shall take the medium to be an ionic crystal with a single vibrational frequency ω_0 although the generalization is straightforward. We shall also assume that the electron is free.

Consider an electric field $\vec{E}(\vec{r},\omega)$ with a frequency ω at a point $\vec{r}$ in the medium. The field causes virtual excitations of the electron from its stationary state, which is denoted by its wave vector $\vec{k}_0$. These excitations in turn generate an electric field with frequency ω. If the generating and the generated electric fields are identical, then they are due to the self-excitations of the electron. Thus,

$$\vec{E}(\vec{r},\omega)=\int \vec{\vec{F}}(\vec{r},\vec{r}\,',\omega)\cdot\vec{E}(\vec{r}\,',\omega)\,d^3r' , \tag{1}$$

where the tensor $\vec{\vec{F}}$ depends on the stationary electron state and on the dielectric properties of the medium. For convenience we rewrite (1) in terms of its Fourier components

$$\vec{E}(\vec{k},\omega)=\sum_{\vec{k}'}\vec{\vec{F}}(\vec{k},\vec{k}',\omega)\cdot\vec{E}(\vec{k}',\omega) . \tag{2}$$

For nontrivial solutions for $\vec{E}$ to exist, the secular equation

$$D(\omega)=|\hat{I}-\hat{F}(\vec{k},\vec{k}',\omega)|=0 \tag{3}$$

must be satisfied. $\hat{F}(\vec{k},\vec{k}',\omega)$ is an infinite matrix with 3×3 submatrices. The natural frequencies of the medium with the free electron present in it are obtained from the poles of the function $1/D(\omega)$. At zero temperature the dispersion self-energy E_s of the electron is given, following Mahanty and Ninham,[4] by

$$E_s=\frac{\hbar}{4\pi i}\oint d\omega\ \mathrm{Tr}\sum_l\frac{[\hat{F}(\vec{k},\vec{k}',\omega)]^l}{l} , \tag{4}$$

where the contour encloses the positive real axis and l takes positive integral values.

In I, Eq. (4) is used to derive the dispersion energy by assuming that

$$\vec{\vec{F}}(\vec{r},\vec{r}\,',\omega)=\vec{\vec{G}}(\vec{r},\vec{r}\,',\omega)\alpha(r') , \tag{5}$$

where $\alpha(r')$ is the space-dependent polarizability of the electron, and $\vec{\vec{G}}(\vec{r},\vec{r}\,',\omega)$ is the well-known Green's function that gives the electric field at $\vec{r}$ due to a dipole at $\vec{r}\,'$—the dipole moment in our case being $\alpha(r')\vec{E}(\vec{r}')$. Since α, the polarizability, contains only the dipolar excitations of the electron, the above assumption is far too restrictive and can give only a qualitative estimate of the dispersion energy.

The use of this assumption creates additional difficulties which are dealt with in I by making further assumptions. In this paper we calculate $\vec{F}(\vec{k},\vec{k}'\omega)$ exactly but within linear-response theory. In this theory the change in the average value $\Delta\bar{O}(\omega)$ of the operator O can be obtained for a system in state $|k_0\rangle$ under the influence of a time-dependent perturbation $-e\phi(r,\omega)$ in the following form:

$$\Delta\bar{O}(\omega)=\frac{1}{\hbar}\sum_{\vec{k}''}\left(\frac{\langle\vec{k}_0|0|\vec{k}''\rangle\langle\vec{k}''|e\phi(\vec{r},\omega)|\vec{k}_0\rangle}{\omega_{k''k_0}-\omega}+\frac{\langle\vec{k}_0|e\phi(\vec{r},\omega)|\vec{k}''\rangle\langle\vec{k}''|0|\vec{k}_0\rangle}{\omega_{k''k_0}+\omega}\right), \qquad (6)$$

where $\hbar\omega_{k''k_0}$ is the difference between the energy of an electron in state $|\vec{k}''\rangle$ and its energy in state $|\vec{k}_0\rangle$. If the operator

$$O=\nabla_{r'}[e/|\vec{r}-\vec{r}|\epsilon(\omega)] \qquad (7)$$

is the electric field in the medium at $\vec{r}'$ due to the charge $-e$ at $\vec{r}$, then $\Delta\bar{O}(\omega)$ would be the field produced by the electronic excitation due to the perturbation $-e\phi(r,\omega)$. To write Eq. (6) in terms of its Fourier coefficients we use the following relations:

$$\frac{1}{|\vec{r}-\vec{r}'|}=-\frac{1}{2\pi^2}\int\frac{\exp[i\vec{k}'\cdot(\vec{r}-\vec{r}')]}{k'^2}d^3k\,, \qquad (8)$$

$$\phi(\vec{r},\omega)=\sum_{\vec{k}}\phi(\vec{k},\omega)e^{i\vec{k}\cdot\vec{r}}\,, \qquad (9)$$

$$\frac{i\vec{k}\cdot\vec{E}(\vec{k},\omega)}{k^2}=\phi(\vec{k},\omega), \qquad (10)$$

and the transformation

$$\sum_{k}=\frac{V}{8\pi^3}\int d^3k\,, \qquad (11)$$

where V is the volume of the dielectric.

Further, in view of (7) we identify $\Delta O\langle(\vec{r},\omega)\rangle=\vec{E}(\vec{r},\omega)$ and rewrite $\vec{F}(\vec{k},\vec{k}',\omega)$ in Eq. (2) using Eq. (6) as

$$\overleftrightarrow{F}(\vec{k},\vec{k}',\omega)=\frac{-4\pi e^2}{\hbar V\epsilon(\omega)}\sum\frac{\vec{k}\vec{k}'}{k^2k'^2}\left(\frac{\langle\vec{k}_0|e^{-i\vec{k}'\cdot\vec{r}}|\vec{k}''\rangle\langle\vec{k}''e^{i\vec{k}\cdot\vec{r}}|\vec{k}_0\rangle}{\omega_{k'',k_0}-\omega}+\frac{\langle\vec{k}_0|e^{i\vec{k}\cdot\vec{r}}|\vec{k}''\rangle\langle\vec{k}''|e^{-i\vec{k}'\cdot\vec{r}}|\vec{k}_0\rangle}{\omega_{k''k_0}+\omega}\right). \qquad (12)$$

For a free electron, the states $|\vec{k}\rangle$ are the plane waves, and their energies are well known. It is easy to evaluate the matrix elements in Eq. (12) to give

$$\overleftrightarrow{F}(\vec{k},\vec{k}',\omega)=\frac{-4\pi e^2\vec{k}\vec{k}}{\hbar V\epsilon(\omega)k^4}\left(\frac{1}{\omega_{\vec{k}+\vec{k}_n,\vec{k}_n}-\omega}+\frac{1}{\omega_{\vec{k}_n-\vec{k},\vec{k}_n}+\omega}\right)\times\delta_{\vec{k},\vec{k}'}\,. \qquad (13)$$

We now substitute Eq. (13) into Eq. (4) to give the dispersion self-energy for a slow moving electron as

$$E_s(\vec{k}_0)=-\gamma\hbar\omega_0\left(1+\frac{1}{6}\frac{\hbar^2k_0^2}{2m}\frac{1}{\hbar\omega_0}\right)$$

with

$$\gamma=\frac{e^2}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\left(\frac{2m\omega_0}{\hbar}\right)^{1/2}, \qquad (14)$$

where the contour integration has to be performed assuming

$$\epsilon(\omega)=\epsilon(\infty)+[\epsilon(0)-\epsilon(\infty)]/[1-(\omega/\omega_T)^2]\,. \qquad (15)$$

The dispersion self-energy given in Eq. (14) is exactly the same as the familiar polaron-energy expression in the weak-coupling approximation. Thus the dispersion-energy approach provides an alternate approach to Fröhlich's electron-lattice interaction.

Although the polaron energy given by Fröhlich's theory or by the dispersion-energy formalism are identical, the two approaches are distinctly different. In the dispersion-energy approach, which is of interest in this comment, the interaction of the electron with the surrounding medium is treated in terms of the dielectric properties of the medium. If the medium has several natural frequencies or if the frequencies depend on its wave vector, such properties can be incorporated into the theory by using an appropriate form for $\epsilon(\omega_i, q_i)$ in Eq. (13).

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[1] J. Mahanty and V. V. Paranjape, Phys. Rev. B 17, 2025 (1978).

[2] J. T. Devreese, *Polarons in Ionic Crystals and Polar Semiconductors* (North-Holland, New York, 1972), p. 29.

[3] C. G. Kuper and G. D. Whitfield, *Polarons and Excitons* (Oliver and Boyd, Edinburgh, 1963) p. 1.

[4] J. Mahanty and B. W. Ninham, Dispersion Forces (Academic, London, 1976), Chap. 1.