POSSIBLE DETERMINATION OF THE DIELECTRIC CONSTANT FROM DATA ON POSITRONIUM SCATTERING IN A POLAR MEDIUM

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The complex dielectric constant of a condensed polar medium is currently studied by the method of dielectric relaxtion [1] by which method one can determine the frequency dependence of this constant in the longwave limit $\lim_{k\to 0} \varepsilon(k, \omega)$. We show below that spatial–temporal dispersion $\varepsilon_{\alpha\beta}(\mathbf{k}, \omega)$ can be determined from data on positronium scattering in a polar medium. For this purpose we take up the problem of the scattering of nonrelativistic positronium in a homogeneous and isotropic nonmagnetic medium. Assuming the positronium wavelength to be much greater than the average separation d of particles in the medium, we can adopt a continuum model for this medium.

We write the differential cross section for the scattering of positronium per unit volume in the Born approximation as

$$d\Sigma^{i'i}_{\mathbf{p'p}} = \frac{2m}{p}\frac{2\pi}{\hbar}\sum_{\nu\nu'}\exp\left\{\frac{1}{T}(F-\mathscr{E}_\nu)\right\}\left|V^{\nu'\nu}_{\substack{i'i\\ \mathbf{p'p}}}\right|^2\delta(\hbar\omega+\hbar\omega_{i'i}+\mathscr{E}_{\nu'}-\mathscr{E}_\nu)\frac{d\mathbf{p}'}{(2\pi\hbar)^3}, \tag{1}$$

where $\mathscr{E}_\nu$ and $\mathscr{E}_{\nu'}$ are the initial and final energies of the medium, F is the free energy of the medium, m is the mass of an electron, $\mathbf{p}$ and $\mathbf{p}'$ are the momenta of the center of mass of the positronium before and after the scattering, $\hbar\omega_{i'i}=\varepsilon_{i'}-\varepsilon_i$ is the change in the internal-state energy, $\hbar\omega=\frac{1}{4m}(p'^2-p^2)$ is the change in the kinetic energy of the positronium, and $V^{\nu'\nu}_{\substack{i'i\\ \mathbf{p'p}}}$ is the matrix element of the operator representing the positronium–medium interaction. Using the integral representation for the δ-function, we convert Eq. (1) to

$$\frac{d^2\Sigma}{d\omega d\Omega}=\frac{4m^2}{\hbar(2\pi\hbar)^3}\frac{p'}{p}K^{\mathbf{p}}_{i'i}(\mathbf{q},\omega+\omega_{i'i}) \tag{2}$$

where Ω is the solid angle for direction $\mathbf{p}'$,

$$K^{\mathbf{p}}_{i'i}(\mathbf{q},\omega)=\int_{-\infty}^{\infty}d\tau e^{i\omega\tau}\mathrm{Sp}\left\{\exp\left\{\frac{1}{T}(F-\hat{\mathscr{H}}_m)\right\}[\hat{V}^+_{\mathbf{p}}(\mathbf{q},0)]_{ii'}[\hat{V}_{\mathbf{p}}(\mathbf{q},\tau)]_{i'i}\right\}, \tag{3}$$

where the spur (Sp) or trace is taken over the index ν; $\hat{\mathscr{H}}_m$ is the Hamiltonian of the medium, $\hbar\mathbf{q}=\mathbf{p}'-\mathbf{p}$; and

$$\hat{V}_{\mathbf{p}}(\mathbf{q},\tau)=\frac{1}{\sqrt{v}}\int d\mathbf{r}\exp\left\{\frac{i}{\hbar}(\hat{\mathscr{H}}_m\tau-\mathbf{p}'\mathbf{r})\right\}V(\mathbf{r})\exp\left\{-\frac{i}{\hbar}(\hat{\mathscr{H}}_m\tau-\mathbf{p}\mathbf{r})\right\} \tag{4}$$

($\mathbf{r}$ is the coordinate of the center of mass of the positronium).

To determine the operator representing the positronium–medium interaction, we use the expression for the Hamiltonian of a free electron in an external electromagnetic field [2]. In our nonrelativistic approximation, this Hamiltonian is, within terms $\sim 1/c^2$,

$$\mathscr{H}=\frac{\hat{p}^2}{2m}\left(1-\frac{\hat{p}^2}{4m^2c^2}\right)+e\hat{\Phi}+\frac{e}{2mc}(\hat{\mathbf{p}}\hat{\mathbf{A}}+\hat{\mathbf{A}}\hat{\mathbf{p}})-\hat{\boldsymbol{\mu}}\hat{\mathbf{H}}-\frac{1}{2mc}\hat{\boldsymbol{\mu}}[\hat{\mathbf{E}}^{\parallel},\hat{\mathbf{p}}]-\frac{\mu_0\hbar}{4mc}\mathrm{div}\,\hat{\mathbf{E}}, \tag{5}$$

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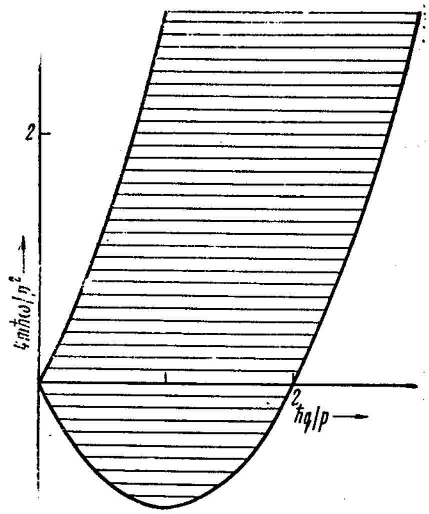

Fig. 1. The hatched region shows the region of possible values of ω and q (in dimensionless coordinates) in experiments in the scattering of particles having a mass of 2m.

where $\hat{\Phi}$ and $\hat{\mathbf{A}}$ are the scaler and vector potentials of the fluctuating electromagnetic field $\hat{\mathbf{E}}$, $\hat{\mathbf{H}}$ of the medium (here and below, $\parallel$ and $\perp$ represent the longitudinal and transverse components of the vectors), μ_0 is the Bohr magneton, and $\boldsymbol{\mu} = \mu_0\sigma$. [In Eq. (5) we have taken account of the fact that we have $H \sim A \sim (1/c)E$ in a nonmagnetic medium.] Introducing the relative-motion coordinate and momentum **R** and **P**, and using $\boldsymbol{\mu}_{\pm} = \mu_0(\sigma_{\pm} + 1)$ for the bound state of an electron and a positron, we find the following operator for the positronium–medium interaction:

$$\begin{aligned} V(\mathbf{r}) = {} & |e|\left\{\hat{\Phi}\left(\mathbf{r} + \frac{1}{2}\mathbf{R}\right) - \hat{\Phi}\left(\mathbf{r} - \frac{1}{2}\mathbf{R}\right)\right\} - \frac{|e|}{2mc}\left\{\left(\hat{\mathbf{p}} + \hat{\mathbf{P}}\right)\hat{\mathbf{A}}\left(\mathbf{r} + \frac{1}{2}\mathbf{R}\right)\right. \\ & - (\hat{\mathbf{p}} - \hat{\mathbf{P}})\hat{\mathbf{A}}\left(\mathbf{r} - \frac{1}{2}\mathbf{R}\right) + \hat{\mathbf{A}}\left(\mathbf{r} + \frac{1}{2}\mathbf{R}\right)(\hat{\mathbf{p}} + \hat{\mathbf{P}}) - \left.\hat{\mathbf{A}}\left(\mathbf{r} - \frac{1}{2}\mathbf{R}\right)(\hat{\mathbf{p}} - \hat{\mathbf{P}})\right\} \\ & - \frac{|\mu_0|\hbar}{4mc}\{\operatorname{div}\hat{\mathbf{E}}|_{\mathbf{r}+1/2\mathbf{R}} - \operatorname{div}\hat{\mathbf{E}}|_{\mathbf{r}-1/2\mathbf{R}}\} + \frac{|\mu_0|}{2mc}\left\{(\hat{\sigma}_+ + \hat{1})\left[\hat{\mathbf{E}}^{\parallel}\left(\mathbf{r} + \frac{1}{2}\mathbf{R}\right), \hat{\mathbf{p}}\right.\right. \\ & \left. + \hat{\mathbf{P}}\right] - (\hat{\sigma}_- + \hat{1})\left.\left[\hat{\mathbf{E}}^{\parallel}\left(\mathbf{r} - \frac{1}{2}\mathbf{R}\right), \hat{\mathbf{p}} - \hat{\mathbf{P}}\right]\right\} + |\mu_0|\left\{(\hat{\sigma}_+ + \hat{1})\hat{\mathbf{H}}\left(\mathbf{r} + \frac{1}{2}\mathbf{R}\right)\right. \\ & \left. - (\hat{\sigma}_- + \hat{1})\hat{\mathbf{H}}\left(\mathbf{r} - \frac{1}{2}\mathbf{R}\right)\right\}. \end{aligned} \tag{6}$$

Omitting the lengthy computation, we list the nonvanishing matrix elements for the scattering involving a change in the spin rate of the positronium for $n = n' = 1$:

$$[\hat{V}_{\mathbf{p}}(\mathbf{q}, \tau)]\begin{matrix} n' = n = 1 \\ s' = 1, s = 0 \\ s'_z = s_z = 0 \end{matrix} = [V_{\mathbf{p}}(\mathbf{q}, \tau)]\begin{matrix} n' = n = 1 \\ s' = 0, s = 1 \\ s'_z = s_z = 0 \end{matrix} = -2\mu_0\left\{(\xi\hat{\mathbf{e}}_{\mathbf{q}})\hat{H}(\mathbf{q}, \tau) + (\xi\mathbf{v})\frac{p'p\sin\theta}{2\hbar mcq}\hat{E}^{\parallel}(\mathbf{q}, \tau)\right\}, \tag{7}$$

where ξ is the polarization vector for the magnetic moment of the positronium, $\boldsymbol{\nu} = ([\mathbf{p}'\,\mathbf{p}]/p'\,p)(1/\sin\theta)$; θ is the scattering angle, $\mathbf{e}_{\mathbf{q}} \perp \mathbf{q}$, $|\mathbf{e}|_{\mathbf{q}}^2 = 1$. (In calculating the nonvanishing matrix elements we used the condition $qr_B < gd \ll 1$, where r_B is the first Bohr radius.) Then for this case of the scattering of an unpolarized beam, the double differential cross sections are

$$\begin{aligned} \frac{d^2\Sigma^{s\to t}_{n'=n=1}}{d\omega d\Omega} & \equiv \frac{d^2\Sigma}{d\omega d\Omega}\left|\begin{matrix} n' = n = 1 \\ s' = 1, s = 0 \\ s'_z = s_z = 0 \end{matrix}\right. \\ & = \frac{8}{3}\frac{\alpha}{\pi^2}\frac{1}{c}\frac{p'}{p}\frac{(\omega + \Delta\omega)^2}{q^2c^2}\left[\exp\left\{\frac{\hbar}{T}(\omega + \Delta\omega)\right\} - 1\right]^{-1} \\ & \times\left\{\frac{\operatorname{Im}\varepsilon^{\perp}(q, \omega + \Delta\omega)}{|\varepsilon^{\perp}(q, \omega + \Delta\omega)|^2} + \frac{p'^2 p\sin^2\theta}{4\hbar^2 m^2(\omega + \Delta\omega)^2}\frac{\operatorname{Im}\varepsilon^{\parallel}(q, \omega + \Delta\omega)}{|\varepsilon^{\parallel}(q, \omega + \Delta\omega)|^2}\right\}, \\ \frac{d^2\Sigma^{t\to s}_{n'=n=1}}{d\omega d\Omega} & \equiv \frac{d^2\Sigma}{d\omega d\Omega}\left|\begin{matrix} n' = n = 1 \\ s' = 0, s = 1 \\ s'_z = s_z \end{matrix}\right. \\ & = \frac{8}{3}\frac{\alpha}{\pi^2}\frac{1}{c}\frac{p'}{p}\frac{(\omega - \Delta\omega)^2}{q^2c^2}\left[\exp\left\{\frac{\hbar}{T}(\omega - \Delta\omega)\right\} - 1\right]^{-1} \\ & \times\left\{\frac{\operatorname{Im}\varepsilon^{\perp}(q, \omega - \Delta\omega)}{|\varepsilon^{\perp}(q, \omega - \Delta\omega)|^2} + \frac{p'^2 p^2\sin^2\theta}{4\hbar^2 m^2(\omega - \Delta\omega)^2}\frac{\operatorname{Im}\varepsilon^{\parallel}(q, \omega - \Delta\omega)}{|\varepsilon^{\parallel}(q, \omega - \Delta\omega)|^2}\right\}, \end{aligned} \tag{8}$$

where $\Delta\omega = \omega n' = 1$, $s' = 1$, $s_z' = 0$; $n=1$, $s=0$, $s_z = 0 = (^7/_{12})\alpha^2 m(e^4/\hbar) = 1.4\cdot 10^{12}$ sec^{-1}. In deriving these relations we took account of the fact that, according to linear theory, the longitudinal and transverse field components in a homogeneous and anisotropic medium are not correlated; we carried out an averaging over the directions of the vectors

$$\hat{e}_q\left(\overline{e_q^\alpha e_q^\beta} = \frac{1}{2}\left(\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2}\right)\right) \text{and } \xi\left(\xi_\alpha\xi_\beta = \frac{1}{3}\delta_{\alpha\beta}\right);$$

and, in accordance with the fluctuation-dissipation theorem [3], we expressed the field correlators in terms of the dielectric constant with an account of $\omega \lessgtr pq/m \ll cq$.

We turn now to a discussion of the possible use of Eqs. (8) to determine the complex dielectric constant from data on positronium scattering in a polar medium. Since in practice it is difficult to distinguish between scattered atoms having $n' = 1$ and $n' > 1$, we will analyze the contribution of $n=1$, $n' > 1$ transitions to the scattering cross section. A straightforward direct calculation shows that the scattering cross section has a dependence on the quantum number n such that this cross section is proportional to $\operatorname{Im}\varepsilon(q, \omega \pm \Delta\omega + \omega_{n'n})$, where $\hbar\omega_{n'n} = \varepsilon_{n'} - \varepsilon_n$. In particular, for $n=1$ and $n'=2$, we find $\omega_{21} = 3.3\cdot 10^{15}$ sec^{-1}. On the other hand, the frequency range of interest here has an upper limit imposed by the relation $\omega \lessgtr pq/m \sim \hbar^2 q/m \ll 10^{15}$ sec^{-1}; i.e., we have $\omega \ll \omega_{21}$. Since low-frequency absorption is usually much greater than high-frequency absorption in polar media, i.e., since $\operatorname{Im}\varepsilon(\omega) \gg \operatorname{Im}\varepsilon(\omega_{21})$, we see that the contribution to the scattering cross section from transitions to excited levels having $n' > 1$ is negligible. In addition, account should be taken of the fact that the quantity $\operatorname{Im}\varepsilon(\omega_{21})$ can be nonvanishing essentially only if there is a random resonance between the transition frequencies ω_{21} in the positronium atom and some electronic levels of the molecules of the medium. These remarks naturally hold both for scattering involving a change in spin state and for scattering not involving such a change. In the latter case, however, the decrease in $\operatorname{Im}\varepsilon$ in a transition to $n' > 1$ levels may be offset by the fact that the matrix elements due to the first term in (6), which vanish identically for transitions involving a change in spin state, give a large nonvanishing contribution to the cross section (physically, these matrix elements correspond to the dipole moment of the positronium for the case $n' > 1$ with a polar medium). Accordingly, using

$$\frac{d^2\Sigma^{s\to t}}{d\omega\, d\Omega} \simeq \frac{d^2\Sigma^{s\to t}_{n'=n=1}}{d\omega\, d\Omega}, \quad \frac{d^2\Sigma^{t\to s}}{d\omega\, d\Omega} \simeq \frac{d^2\Sigma^{t\to s}_{n'=n=1}}{d\omega\Omega},$$

we will derive an expression for the dielectric constant in terms of the cross section for scattering involving a change in spin state. Solving system (8) and introducing

$$F^{\parallel}(q,\omega) \equiv \frac{c}{\sin^2\theta}\frac{m^2(\hbar\omega)^2}{p_-'^2 p_-^2 - p_+'^2 p_+^2}\left\{\frac{p_-}{p_-'}\frac{d^2\Sigma^{s\to t}}{d\omega\, d\Omega}(q,\theta,\omega-\Delta\omega) - \frac{p_+}{p_+'}\frac{d^2\Sigma^{t\to s}}{d\omega\, d\Omega}(q,\theta,\omega+\Delta\omega)\right\};$$

$$F^{\perp}(q,\omega) \equiv \frac{c}{4}\frac{1}{p_-'^2 p_-^2 - p_+'^2 p_+^2}\left\{\frac{p_+'^2 p_+^2 p_-}{p_-'}\frac{d^2\Sigma^{s\to t}}{d\omega\, d\Omega}(q,\theta,\omega-\Delta\omega) - \frac{p_-'^2 p_-^2 p_+}{p_+'}\frac{d^2\Sigma^{t\to s}}{d\omega\, d\Omega}(q,\theta,\omega+\Delta\omega)\right\}, \tag{9}$$

where p_+, p_+', and p_-' are found from

$$(p_\pm')^2 - (p_\pm)^2 = 4m(\omega \pm \Delta\omega), \quad (p_\pm')^2 - (p_\pm)^2 - 2p_\pm' p_\pm\cos\theta = \hbar^2 q^2, \tag{10}$$

we find

$$\frac{\operatorname{Im}\varepsilon^{\parallel,\perp}(q,\omega)}{|\varepsilon^{\parallel,\perp}(q,\omega)|^2} = \frac{3}{2}\frac{\pi^2}{\alpha}(e^{\hbar\omega/T} - 1)\frac{q^2c^2}{\omega^2}F^{\parallel,\perp}(q,\omega). \tag{11}$$

By experimentally varying p and θ, we can use Eqs. (11) and (9) to measure $\dfrac{\operatorname{Im}\varepsilon^{\parallel}(q,\omega)}{|\varepsilon^{\parallel}(q,\omega)|^2}$ and $\dfrac{\operatorname{Im}\varepsilon^{\perp}(q,\omega)}{|\varepsilon^{\perp}(q,\omega)|^2}$ over a wide range of ω and q values. From

$$\frac{\hbar(q - p/\hbar)^2}{4m} - \frac{p^2}{4m\hbar} \leqslant \omega \leqslant \frac{\hbar(q + p/\hbar)}{4m} - \frac{p^2}{4m\hbar},$$

which limit the ω range for scattering involving a change in the momentum $\hbar q$ for a given p. In addition, the condition $q \ll 1/d$ must be used for valid use of the continuum approximation. Accordingly, we can study $\operatorname{Im}\varepsilon_{\alpha\beta}^{-1}(q,\omega)$ at frequencies $\omega \sim 10^{14}$ sec^{-1} for $q \sim p/\hbar \sim 10^7$ cm^{-1}. Accordingly, we can construct $\varepsilon_{\alpha\beta}(q,\omega)$ (in this frequency range) from the $\operatorname{Im}\varepsilon_{\alpha\beta}^{-1}(q,\omega)$ data on the basis of the Kramers-Kronig relations if frequencies $\omega > 10^{14}$ sec^{-1} correspond to the transparency band for the case $q \gtrless 10^7$ cm^{-1}. Obviously, these results will be those of the greatest interest, since with $q \lessgtr 10^6$ cm^{-1} the function $\varepsilon(q, \omega)$ lies beyond the longwave limit.

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