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On the quantum theory of dispersion at resonance

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Abstract. The perturbation expansions of the wavefunction, under the action of external monochromatic radiation are obtained, which have no secular or divergent terms, in presence of resonance (without any damping factor). Next, the expectation values of the electric dipole moment operator with respect to these characteristic states are calculated. Finally, the dispersion formulae are obtained in the neighbourhood of resonance, they are free from any divergences. The dispersion curves obtained from them have all the basic features of the usual dispersion curves in the neighbourhood of resonance.

1. Introduction

The object of this short paper is to derive expressions for the dispersion in the neighbourhood of resonance from the quantum theory. In the case of resonance, that is, when $E_j - E_k = \hbar\omega$, where E_j are the energies of the unperturbed stationary states, if one proceeds to solve the Schrödinger equation in the usual manner, one faces serious difficulty due to the vanishing of the denominators in the perturbation expansion. The conventional way of avoiding this difficulty is to introduce *ad hoc* complex energies, which is equivalent to introducing nonsteady (decaying) states (Weisskopf 1933; Heitler 1954). Alternatively, one can introduce a decaying factor in the amplitude of the incident radiation field (Weisskopf and Wigner 1930).

In this paper it is shown that, in the case of monochromatic incident radiation, such an artificial factor, which decreases exponentially with time, is redundant in obtaining the dispersion formulae which are meaningful in the neighbourhood of resonance. The case of monochromatic incident radiation is a special case of the time dependent perturbation. The solution of the Schrödinger equation without any secular or divergent term, in the general case, has been obtained by the author (Sen Gupta 1970). Following exactly the same method we first obtain a perturbation expansion which has neither any secular term nor any term with a vanishing denominator.

It may not be irrelevant to mention that some recent investigations on the stability of linear oscillatory systems with periodic perturbation or of general canonical systems of differential equations with periodic coefficients, have shown that the two cases of resonance namely: (i) $\omega_j - \omega_k = q_1\omega$ and (ii) $\omega_j + \omega_k = q_2\omega$, where ω_j the unperturbed circular frequencies and ω the fundamental frequency of the periodic perturbation (q are integers), are quite different. It is known (Gelfand and Lidskii 1955) that in the former case the system is still oscillatory while in the latter case the system is unstable. In quantum mechanics, the latter cannot appear since the Schrödinger equation is linear and the Hamiltonian is hermitian, the solutions should still be oscillatory with time. This point was noted by Schrödinger (1929) in his early papers on the time

dependent perturbation theory. It is very important for our problem. It asserts clearly that the *ad hoc* introduction of a decaying factor is redundant, and external damping is not needed as there are no divergences. This has been explicitly manifested by the solutions we have obtained in the case of resonance.

The problem of two resonating levels in the field of a monochromatic beam has been solved to a good degree of accuracy by Fleck (1966) (neglecting the nonresonating terms). Feynman *et al* (1957) have also developed a method of treating the same problem. Schwinger (1937) solved the problem of a multiresonating system of nuclear magnetic moments in the special case of a rotating magnetic field. Instead of starting with an approximate unperturbed solution of the wave equation with a two level resonating system (neglecting first and higher harmonic terms) and then obtaining the effect of the other levels as a perturbation, we have calculated directly the average electric polarization induced by the radiation field, with the help of the solution of the wave equation as obtained in the text. Wallace (1970) has investigated the solution of the time dependent Schrödinger equation by replacing it with suitable difference equations which introduces serious limitations to the problem.

Recently, Loudon (1970) has made detailed investigations of the properties of the refractive index and the propagation of electromagnetic waves at resonance (with damping) from the stand-point of classical theory. Since the classical equation of motion is inhomogeneous (though linear), one is obliged to introduce a damping term without which the solutions become aperiodic and unbounded with time at resonance. On the other hand, the Schrödinger equation is linear and homogeneous and it has solutions which are regular and bounded (in fact oscillatory) even at the resonance as noted above.

We would like to point out that the objective of the present paper is extremely modest. In all the literature, while discussing the quantum theory of dispersion in the absence of resonance, one first obtains the expectation values of the polarization from which the refractive index is calculated in a straightforward manner. But as soon as one considers the presence of resonance one introduces immediately, in an *ad hoc* manner, a damping factor (as noted in the first paragraph). The object of this paper is to show that the refractive index in the presence of resonance can also be obtained following exactly the same procedure, which is quite acceptable, as in the absence of resonance. Further, the dispersion formula thus obtained possesses all the basic characteristic features which are observed, namely, positive and negative dispersions, as well as anomalous dispersion in the neighbourhood of resonance. The physical system which corresponds to our simple model consists of a dilute gas where the mutual interaction between the molecules may be neglected. Hence, there is no need to introduce any relaxation time. We calculate directly the average electric polarization. The refractive index is obtained from the induced polarization. The introduction of the damping factor in the wavefunctions leads to serious difficulty, as the expectation values of any operator calculated from them should also be decaying with time, which is contrary to the observed facts.

In the next section, the perturbation expansion is obtained for the general case as well as that of resonance. In the case of resonance it is shown that the wave equation does not have solutions of the form usually assumed, namely to each solution of the perturbed equation there corresponds a unique unperturbed stationary state. In fact, in this case, the starting unperturbed solution does not correspond to a single stationary state, but to a suitable linear combination of all the unperturbed stationary states which are in resonance (equation (10)). Since one has to find the expectation values of the

electric polarization under the action of the radiation field, one is obliged to obtain them with respect to these characteristic perturbed states. Furthermore, only with these states is the polarization periodic, with the same period as the radiation field. In § 3 we have calculated the polarization in the simple case, when only two states are in resonance. With these two states are associated two characteristic states. The dispersion formulae obtained are regular at the resonance and are free from divergence. The dispersion with one of the characteristic states is positive while with the other it is negative. § 4 contains a short discussion of the energy density and the energy velocity. Finally, we would like to mention that the dispersion formula near resonance presented in this paper does not contain any new parameter, but is expressed in terms of the dimensionless fine structure constant.

2. The wavefunction in the presence of radiation

Let the incident radiation be described by the vector potential

$$a = ja_0 \cos \omega \left(t - \frac{n \cdot r}{c} \right) \quad j \cdot n = 0. \tag{1}$$

Since, we are interested in wavelengths large in comparison to the atomic dimensions, we can neglect the variation of phase in space and write simply

$$a = ja_0 \cos \omega t \tag{1'}$$

so that the Schrödinger equation is

$$i\hbar \frac{\partial \Psi}{\partial t} = (H_0 + H')\Psi \tag{2}$$

where H_0 is the unperturbed Hamiltonian and

$$H' = -\xi c j \cdot p \cos \omega t \quad \xi = \frac{ea_0}{mc^2}. \tag{3}$$

We have introduced the dimensionless parameter ξ , which depends on the strength of the radiation field. The eigenvalues and the normalized eigenfunctions of the unperturbed Hamiltonian are E_n and ϕ_n . We assume that the eigenfunctions form a complete set. The wave equation with respect to time is a linear homogeneous equation with periodic coefficients; hence, the solutions are of the form

$$\Psi(t) = \exp(i\lambda t)\Phi(t) \quad \Phi \left(t + \frac{2\pi}{\omega} \right) = \Phi(t) \tag{4}$$

(Halany 1966), which is a generalization of Floquet's theorem (Ince 1926). We can expand λ and $\Phi(t)$ in ascending powers of the perturbation parameter ξ . Thus, solutions of equation (2) are of the form

$$\begin{aligned} \psi(t) = \exp \left(-\frac{i}{\hbar} (E^{(0)} + \xi E^{(1)} + \xi^2 E^{(2)} + \dots) t \right) \\ \times \sum_n \phi_n (A_n^{(0)} + \xi A_n^{(1)} + \xi^2 A_n^{(2)} + \dots) \end{aligned} \tag{5}$$

where $A_k^{(N)}(t)$ are periodic, that is

$$A_k^{(N)}\left(t + \frac{2\pi}{\omega}\right) = A_k^{(N)}(t). \tag{6}$$

In the absence of resonance

$$E_\beta - E_\alpha \neq q_{\beta\alpha}\hbar\omega + O(\xi) \tag{7}$$

for any α, β . The above expression for $\psi(t)$ shows that one must start with an unperturbed wavefunction corresponding to one and only one of the unperturbed wavefunctions, that is

$$\psi_n^{(0)} = \exp\left(-\frac{i}{\hbar}E_n t\right)\phi_n \tag{8}$$

otherwise the coefficients $A_n^{(0)}(t)$ will not be periodic. However, in the case of resonance

$$E_\beta - E_\alpha = q_{\beta\alpha}\hbar\omega \tag{9}$$

the most general starting unperturbed solution satisfying equations (6) is of the form

$$\psi^{(0)}(t) = \exp\left(-\frac{i}{\hbar}E_\alpha t\right) \sum_j A_j^{(0)}(t)\phi_j \tag{10}$$

where

$$A_j^{(0)} = \exp(-iq_{j\alpha}\omega t)g_j. \tag{11}$$

The summation is only over those states satisfying equation (9), the terms g are constants and $A_j^{(0)}(t)$ are now periodic. Hence, in the case of resonance in general one should not start with only one unperturbed state but a linear combination of the states which are in resonance. It may be noted here that divergent coefficients in the conventional perturbation expansion appear only because this point is overlooked.

2.1. The perturbed wavefunction in the absence of resonance

The solutions in this case are the usual ones. They are found to be

$$\psi_n(t) = \exp\left(-\frac{i}{\hbar}E_n t\right)\left(\phi_n + \xi \sum_k F_{kn}\phi_k\right) \tag{12}$$

where

$$F_{kn} = c(\mathbf{j}, \mathbf{p})_{kn} \frac{(E_k - E_n) \cos \omega t - i\hbar\omega \sin \omega t}{(E_k - E_n)^2 - \hbar^2\omega^2} \tag{13}$$

(retaining only first order terms in ξ). ψ_n are mutually orthonormal and the transformation from ϕ_n to ψ_n is unitary.

2.2. The perturbed wavefunction in the presence of resonance

In order to avoid unnecessary complications we will take the inequality (7) to be valid for all states excluding only two which are in resonance. We designate them as ϕ_α and ϕ_β with eigenvalues E_α and E_β . Since our object is to investigate the behaviour of the system in the neighbourhood of resonance, we take

$$E_\beta - E_\alpha = \hbar(\omega + \xi\mu) \tag{14}$$

instead of a trivial equality, which corresponds to $\mu = 0$. Our aim is to study the dispersion as a function of μ , whose absolute magnitude is small ($|\xi|\mu \ll \omega$).

It can be easily checked that we can still have solutions of the form given by expression (12) for all n excluding $n = \alpha$ and $n = \beta$. To obtain the other two solutions we are obliged to start with suitable linear combinations of ϕ_α and ϕ_β as $\psi^{(0)}(t)$; from equations (10) and (11)

$$\psi^{(0)}(t) = \exp\left(-\frac{i}{\hbar}E_\alpha t\right) \{g_\alpha \phi_\alpha + \exp(-i\omega t)g_\beta \phi_\beta\}. \quad (15)$$

In order to obtain solutions as given in expressions (5) and (6), it follows that:

$$\begin{aligned} E^{(1)}g_\alpha + \frac{1}{2}c(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}g_\beta &= 0 \\ \frac{1}{2}c(\mathbf{j} \cdot \mathbf{p})_{\beta\alpha}g_\alpha + (E^{(1)} - \mu\hbar)g_\beta &= 0. \end{aligned} \quad (15')$$

So that

$$2E_\pm^{(1)} = \hbar\mu \pm \{\hbar^2\mu^2 + c^2|(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}|^2\}^{1/2} \quad (16)$$

and

$$\begin{aligned} g_\alpha^\pm &= c(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}G_\pm \exp(i\delta_\pm) & g_\beta^\pm &= -2E_\pm^{(1)}G_\pm \exp(i\delta_\pm) \\ G_\pm &= \{4E_\pm^{(1)2} + c^2|(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}|^2\}^{-1/2}. \end{aligned} \quad (16')$$

Two solutions correspond to the choice of two signs. With this choice of zeroth order solution one can find successively higher order terms, thus

$$\begin{aligned} \psi_\pm(t) &= \exp\left(-\frac{i}{\hbar}(E_\alpha + \xi E_\pm^{(1)})t\right) \\ &\times \left[\phi_\alpha \left\{ g_\alpha^\pm + \xi \left(g_\alpha^\mp l^\pm - \frac{c(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}}{4\hbar\omega} \exp(-i2\omega t)g_\beta^\pm \right) \right\} \right. \\ &+ \exp(-i\omega t)\phi_\beta \left\{ g_\beta^\pm + \xi \left(g_\beta^\mp l^\pm + \frac{c(\mathbf{j} \cdot \mathbf{p})_{\beta\alpha}}{4\hbar\omega} g_\alpha^\pm \exp(i2\omega t) \right) \right\} \\ &\left. + \xi \sum' \phi_n \{ F_{n\alpha}g_\alpha^\pm + F_{n\beta}g_\beta^\pm \exp(-i\omega t)g_\beta^\pm \} \right]. \end{aligned} \quad (17)$$

The constants l^\pm are to be determined from higher order terms, they are

$$l^\pm(E_\pm^{(1)} - E_\mp^{(1)}) + \frac{c^2}{2} \left(K_\alpha - K_\beta + \frac{|(\mathbf{j} \cdot \mathbf{p})_{\alpha\beta}|^2}{2\hbar\omega} \right) g_\alpha^\pm g_\alpha^{\mp*} = 0 \quad (18)$$

where

$$K_\gamma = \sum'_n \frac{(E_n - E_\gamma)|(\mathbf{j} \cdot \mathbf{p})_{n\gamma}|^2}{(E_n - E_\gamma)^2 - \hbar^2\omega^2} \quad (\gamma = \alpha, \beta). \quad (19)$$

The prime on the summation sign means α, β terms are to be excluded. ψ_\pm are normalized; they are mutually orthogonal and orthogonal to $\psi_n (n \neq \alpha, \beta)$. Since we are interested only in the linear response, we have retained terms up to first order in ξ . The higher order terms, on the one hand, lead to terms which oscillate with harmonics of the fundamental and on the other hand, they introduce a small correction to the terms with the fundamental frequency. The latter does not change the qualitative nature of the problem.

2.3. The completeness of the solutions and initial value problem

The solutions ψ_{\pm} , $\psi_n (n \neq \alpha, \beta)$ obtained above are linear combinations of the unperturbed solutions with coefficients depending on time. It can be easily checked that the transformation which induces the change from ϕ_n to ψ_n is unitary as the Hamiltonian is hermitian. Hence $\{\psi_n\}$ also form a complete set as they are obtained by a unitary transformation from a complete set $\{\phi_n\}$. It follows that the most general solution of equation (3) is a linear combination of ψ_{\pm} , $\psi_n (n \neq \alpha, \beta)$. So that one can easily find the solution which evolves out of any arbitrary initial state in the usual manner.

3. Dispersion

3.1. The characteristic states

The solutions obtained in the previous section are the most important ones from the point of physical significance. They correspond to the steady state solutions of time independent Hamiltonians. This is because of the fact that, for any operator \hat{Q} which does not contain time explicitly the expectation value of \hat{Q} with respect to any state as obtained above, that is, $(\psi_n \hat{Q} \psi_n)$ for all n , is periodic with the same period as the perturbation. No other solutions possess this property and expectation values with respect to any other states are not periodic but are highly oscillatory. We will call these states the characteristic states since they are characteristic of the periodic perturbation.

3.2. The dipole moment

In order to obtain the expectation values of the electric dipole moment we must calculate them with respect to these states. The expectation values of the electric dipole moment with respect to any state other than ψ_{\pm} will lead us to the usual formula for the dispersion, away from resonance. But our interest is only in the neighbourhood of resonance. Hence, we consider only

$$\mathbf{d}_{\pm} = e(\psi_{\pm} \mathbf{r} \psi_{\pm}). \quad (20)$$

Since we wish to confine ourselves only to linear response, we consider the terms which are linear in ζ and oscillate with the fundamental frequency. They are given by

$$\begin{aligned} \mathbf{d}_{\pm}^{(1)} = \zeta e \left[\mathbf{r}_{\alpha\beta} \left\{ (g_{\alpha}^{\pm} g_{\beta}^{\mp*} + g_{\alpha}^{\mp*} g_{\beta}^{\pm}) t^{\pm} \exp(-i\omega t) \right. \right. \\ \left. \left. + \frac{c(\mathbf{j} \cdot \mathbf{p})_{\beta\alpha}}{4\hbar\omega} (|g_{\alpha}^{\pm}|^2 - |g_{\beta}^{\pm}|^2) \exp(i\omega t) \right\} \right] \\ + \sum_n' (\mathbf{r}_{\alpha n} F_{n\alpha} |g_{\alpha}^{\pm}|^2 + \mathbf{r}_{\beta n} F_{n\beta} |g_{\beta}^{\pm}|^2) + \text{cc} \end{aligned} \quad (21)$$

where cc is the complex conjugate. The first term of the above expression does not contribute, as the average over the phases δ_+ and δ_- vanishes. Next, our object is to find the nature of the dispersion in the neighbourhood of resonance $E_{\beta} - E_{\alpha} = \hbar\omega_0$. Hence, we must express $\mathbf{d}_{\pm}^{(1)}$ in terms of μ . Since $\mathbf{d}_{\pm}^{(1)}$ is already linear in ζ , that is, field

intensity, we can replace ω by ω_0 as $\omega_0 - \omega = \xi\mu$. Substituting the values of g and F_{nk} from equations (16), (16') and (13), one obtains

$$\mathbf{j} \cdot \mathbf{d}_{\pm} = P_{\pm} \mathbf{j} \cdot \mathbf{E}. \quad (22)$$

P_{\pm} are given by

$$P_{\pm} = \frac{e^2}{2m\omega_0^2} \left(F_{+} \pm \frac{\mu}{(\mu^2 + \epsilon^2\omega_0^2)^{1/2}} \left(\frac{f_{\beta\alpha}}{2} + F_{-} \right) \right) \quad (23)$$

where

$$F_{\pm} = \sum_n' \left(\frac{f_{n\beta}}{\omega_{n\beta}^2 - \omega_0^2} \pm \frac{f_{n\alpha}}{\omega_{n\alpha}^2 - \omega_0^2} \right). \quad (24)$$

In the above we have used the result

$$\mathbf{p}_{kl} = im\omega_{kl}\mathbf{r}_{kl} \quad (25)$$

which is true for any spherical symmetric potential. It is important to note that there is no phase difference between \mathbf{E} (electric intensity) and \mathbf{d}_{\pm} . The oscillator strengths $f_{n\gamma}$ are (Davydov 1965)

$$f_{n\gamma} = \frac{2m}{\hbar} \omega_{n\gamma} |(\mathbf{j} \cdot \mathbf{r})_{n\gamma}|^2 \quad (26)$$

and the ratio ϵ stands for

$$\epsilon = \frac{mc}{\hbar} |(\mathbf{j} \cdot \mathbf{r})_{\alpha\beta}|^2 \quad (27)$$

that is, the modulus of the matrix element $(\mathbf{j} \cdot \mathbf{r})_{\alpha\beta}$ in units of the Compton wavelength \hbar/mc . For isotropic systems, P_{\pm} in equation (22) is the polarizability scalar and the corresponding refractive index n_{\pm} is given by

$$n_{\pm}^2 = 1 + 4\pi N P_{\pm} \quad (28)$$

where N is the number of atoms per unit volume. Hence n_{\pm} behaves smoothly in the neighbourhood of resonance $\mu = 0$. Thus, the *ad hoc* introduction of unstable decaying states is redundant. In the expression for dispersion there are no singular terms with vanishing denominator.

In the neighbourhood of resonance the nature of the dispersion is determined by the second term of expression (23). Since

$$\frac{dP_{\pm}}{d\omega} = \mp \frac{\xi\epsilon^2\omega_0^2}{(\mu^2 + \epsilon^2\omega_0^2)^{3/2}} \left(\frac{f_{\beta\alpha}}{2} + F_{-} \right) \quad (29)$$

the nature of the dispersion, that is, whether it is positive or negative, depends relatively on the sign of $f_{\beta\alpha} + 2F_{-}$ and the states ψ_{+} or ψ_{-} , considered in expression (20). If ϕ_{α} and ϕ_{β} are the ground and the adjacent excited states respectively, $f_{\beta\alpha} + 2F_{-} > 0$. So that, in this case the dispersion in the neighbourhood of resonance is negative, that is, it is anomalous for n_{+} . The dispersion curve in this case is shown in figure 1. The central full curve section is obtained from expression (23). Though the right hand side of expression (23) is meaningful for all μ , our formula is valid only in the

neighbourhood of resonance, more precisely $\xi|\mu| \ll \omega_0$. The dispersion curves on both sides away from resonance are obtained from the usual expression for the dispersion (Davydov 1965, Born and Wolf 1959). The broken sections of the curve on both sides are extrapolated. For $\omega < \omega_0$ the refractive index increases with ω but in the neighbourhood of ω_0 it decreases. Hence, it should pass through a maximum and similarly it should pass through a minimum in the region $\omega > \omega_0$. These are shown by broken lines. Their exact expressions and the position of the maximum and minimum can be obtained only with further detailed knowledge of the system. The dispersion curve thus agrees in its essential features with the usual dispersion curves obtained with damping factors (Sommerfeld 1949, Born and Wolf 1959, Davydov 1965). The dispersion which corresponds to n_- is normal at resonance and also on both sides further away from it, with two regions of anomalous dispersion between these; they should be associated with excited states.

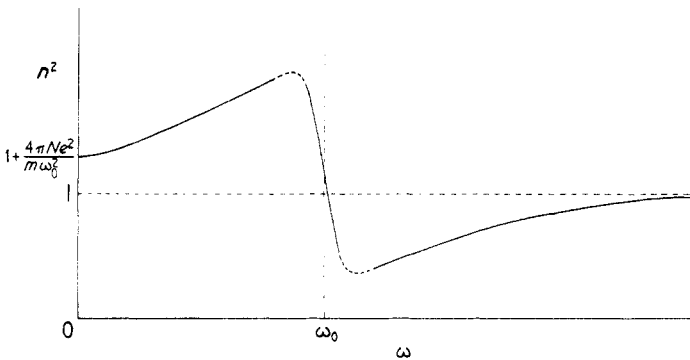


Figure 1. The dispersion curve.

With respect to the expressions (23) and (28) for the polarizability and the refractive index, the important point is to note that they are real. On the other hand, corresponding expressions obtained from complex energy states (ie decaying states) are complex (Sommerfeld 1949, Born and Wolf 1959, Davydov 1965). In our analysis, the imaginary terms which correspond to absorption do not appear as the effect of the external periodic radiation field is to produce only a periodic polarization of the system.

Next, the usual expression for the real part of the refractive index in the neighbourhood of resonance retaining the terms which depend on μ (Born and Wolf 1959, Sommerfeld 1949) is

$$n(\mu) \propto \frac{\mu}{\mu^2 + \frac{1}{4}\gamma^2} \tag{30}$$

where γ is the inverse of the halflife of the states, which is introduced *ad hoc*. While from the expression (23)

$$n(\mu) \propto \frac{\mu}{(\mu^2 + \epsilon^3 \omega_0^2)^{1/2}} \tag{31}$$

As discussed above the nature of variation for both of them for small values of μ is almost similar; both of them show anomalous behaviour near $\mu = 0$.

4. The energy density and the energy velocity

In this section we wish to examine the relation between the energy density and the energy velocity, that is, the velocity with which energy is transported through the medium. From Maxwell's equations one can write

$$\int \mathbf{S} \cdot d\boldsymbol{\sigma} + \int \left(\frac{d}{dt} \frac{1}{8\pi} (\mathbf{E} \cdot \mathbf{E} + \mathbf{H} \cdot \mathbf{H}) + \mathbf{E} \cdot \mathbf{P} \right) dv = 0 \quad (32)$$

where \mathbf{S} is Poynting's vector. Following the usual method of averaging over a cycle of variation of the field quantities (Landau and Lifschitz 1960), the integrand of the volume integral may be expressed as the time derivative of the energy density \overline{W} , averaged over a cycle of variation, so that

$$\overline{W} = \frac{\omega^2 a_0^2}{16\pi c^2} n \frac{d(n\omega)}{d\omega}. \quad (33)$$

This is obtained with the help of expressions (23) and (28) for the polarization and the refractive index. The corresponding average of the Poynting vector $\overline{\mathbf{S}} = jcn\omega a_0^2/8\pi$. So that the energy velocity is given by (Loudon 1970)

$$v_E = \frac{\overline{\mathbf{S}}}{\overline{W}} = \frac{j c}{d(n\omega)/d\omega}. \quad (34)$$

From the expressions (23) and (28) it follows that the magnitude of the energy velocity $|v_E|$ does not tend to zero at resonance ($\mu = 0$). But from the above $|v_E|$ is equal to the group velocity; hence, at resonance the magnitudes of the energy velocity and group velocity are also equal (Pelzer 1951).

5. Discussion

It is quite clear from the previous sections that one can obtain dispersion formulae which are regular at resonance without *ad hoc* introduction of the complex energy eigenvalues. We have obtained the expectation value of the dipole moment in the presence of radiation with respect to the characteristic states which correspond to steady states in the presence of radiation. The only point to be emphasized is that the zeroth orders of these states, that is $\psi_{\pm}^{(0)}$, are not pure unperturbed eigenstates when there is resonance. Further, in calculating the expectation value of r , we have followed the usual procedure in quantum mechanics that it is the diagonal elements between the states which are characteristic of the given Hamiltonian in the presence of the radiation. It should be mentioned that if one forms the expectation values of the dipole moment operator with complex energies, that is with decaying states, the dipole moment should also decay with time. As noted in the introduction this is extremely undeserving.

Finally, we do not need any new parameter to get rid of the divergence. From relations (30) and (31), it follows that the corresponding dimensionless parameter is ϵ . The term $|r_{\alpha\beta}|$ can always be expressed, in units of the Bohr radius, as

$$|r_{\alpha\beta}| = \frac{\hbar^2 R}{e^2 m} \quad (35)$$

where R is a number depending on the quantum numbers of the two states and from equation (27)

$$\epsilon = \frac{\hbar c}{e^2} R. \quad (36)$$

Thus the parameter ϵ is the inverse of the fine structure constant. It is of interest to note that from equation (23) in the trivial case when $r_{\alpha\beta} = 0$, the dispersion is regular and constant in the neighbourhood of resonance.

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