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QUANTUM ELECTRODYNAMICS BASED ON SELF-ENERGY:

SPONTANEOUS EMISSION IN CAVITIES

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QUANTUM ELECTRODYNAMICS BASED ON SELF-ENERGY: SPONTANEOUS EMISSION IN CAVITIES *

A.O. Barut ** and J.P. Dowling **

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ABSTRACT

We extend a previously developed formulation of QED based on self-energy to include the effect of perfectly conducting boundaries on spontaneous emission. The method is quite general and applicable to any quantum system and many boundary geometries. In particular, we compute the spontaneous emission rate of an atom near a conducting plate, inside a spherical cavity and between parallel plates, we give general formulas and predict both enhanced and inhibited rates, in agreement with recent experiments.

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INTRODUCTION

Recent experiments have demonstrated that there is a change in the spontaneous emission from Rydberg atoms in the vicinity of conducting walls. Both inhibited emission $^{(1)}$ and enhanced decay rates $^{(2)}$ have been observed the latter when the cavity is tuned to a transition frequency between two neighbouring Rydberg states. Inhibited decay was also seen in the case of cyclotron radiation by an electron in a Penning trap $^{(3)}$, in fluorescent decay rates $^{(4)}$, and in the suppression of black-body absorption by Rydberg atoms in a parallel-plate cavity $^{(5)}$, $^{(6)}$.

Theoretical predictions of this effect seem to go back to Purcell ⁷⁾ (see also Ref.8). There have been a number of theoretical discussions of this and related phenomena in the case of plates ^{4),9)-14)}. However all of these calculations were carried out in the context of the second quantization of the electromagnetic field and its associated vacuum fluctuations. We show in this paper that the effect can equally well be computed in the framework of the self-energy formulation of QED ^{15),16)}, where there is no field quantization and the vacuum is empty and static.

It is well known that Dirac ¹⁷⁾ in 1927 was able to derive the Einstein A coefficient of spontaneous emission from second quantization; seen as the first major success of the theory. It is perhaps less known that Fermi ¹⁸⁾ in that same year was also able to arrive at the A coefficient, simply by adding a nonlinear radiation-reaction term to the Schrödinger equation. The connection runs deeper. In 1951 Callen and Welton ¹⁹⁾, in their famous paper on the fluctuation dissipation theorem, demonstrated that there is indeed an intimate relation between zero-point fluctuations of the electromagnetic field and the phenomenon of radiation reaction. In 1973 Ackerhalt et al. ²⁰⁾, Senitzky ²¹⁾ and Milonni et al. ²²⁾ working within standard QED - were able to demonstrate that the decay of an excited state can be interpreted as being caused by the electron's perturbation by the vacuum electric field fluctuations, or by the radiation reaction of these two effects.

In view of this situation one may ask if one can reformulate QED totally in the self-energy picture, as a complement to the more conventional picture of second quantization. One approach in this direction was taken by Jaynes and his collaborators 23)-25) with their "neo-classical" theory; an elaboration of Fermi's original idea of modifying the Hamiltonian with a radiation-reaction term. More recently, a different, general theory has been advanced by Barut and Kraus 15), and Barut and van Huele 16). This formulation of QED is based entirely on self-energy without second quantization, and is developed in its full relativistic version in the first

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paper. The second paper contains a non-relativistic specialization of the theory which is used to obtain both the Einstein A coefficient and the Bethe Lamb shift for an atom in free space; all without vacuum field fluctuations.

In this account of QED the self-part of the electromagnetic four-vector potential \mathbf{A}_{μ} is eliminated from the Maxwell-Dirac equations through the use of a Green function - and so the emission from an atom depends naturally on the Green function of its environment. In the present paper we show how this idea can be used to account for the effects of nearby conducting boundaries. For simple geometries it is expedient to use the method of images, which we apply to an infinite conducting plane, a conducting spherical shell and a pair of parallel planes.

II. THE METHOD

Barut and van Huele have shown that for an isolated system in free-space the Einstein A coefficient to first order in α , is twice the imaginary part of a complex energy shift. For the n^{th} excited state (where \underline{n} stands for all the quantum numbers of the state) of the system they give $\underline{16}$ (frequency)

$$A_{n}^{o} = \frac{1}{4m_{n}^{4}} \sum_{nm} \omega_{nm} \int \frac{d\vec{k}}{\vec{k}^{2}} \sqrt{m} (\vec{k}) \sqrt{n} \sqrt{n} \left(-\vec{k} \right) \left[\vec{J}_{ij} - \hat{k}_{ij} \hat{k}_{ij} \right] \vec{J} \left(\omega_{om} - \vec{k} \right)$$
(1)

where m_0 is the electron mass, α the fine-structure constant, $\omega_{nm} = E_n - E_m$ an energy-level difference and the direction \vec{k} (summation implied over i, j). The T's are electron wave function form factors, given by 16)

$$\overrightarrow{\eta_{m}}(\vec{k}) = \int dx^{3} \, \Psi_{n}^{*}(\vec{x}) \, \overrightarrow{\nabla} \, \Psi_{m}(\vec{x}) \, e^{i \, \vec{k} \cdot \vec{x}} \tag{2}$$

with the ψ_n forming a complete set of wave functions for an atom, harmonic oscillator, electron in cyclotron motion, etc. Notice that in the dipole approximation $e^{i\vec{k}\cdot\vec{x}}\sim 1$ and $\vec{r}_m = \vec{p}_{nm}$, the matrix elements for the electron momentum.

Eq.(1) was obtained from coupled Maxwell and Dirac equations, with the Maxwell equations written as $\frac{1}{2}$

$$\Box A_{\mu}(x) + A_{\nu,\mu}(x) = -j_{\mu}(x)$$
(3)

 $\begin{array}{lll} A_{\mu}^{self} & \text{being the electron self~field, } A_{\mu} = A_{\mu}^{self} + A_{\mu}^{external} & \text{the total} \\ \text{field and} & j_{\mu} & \text{the four-vector for the electron's probability current} \\ \text{density.} & \text{Eq.(3)} & \text{is solved formally with a Green function} & D_{\mu\nu} \end{array}$

$$A_{m}^{\text{self}} = \int dy^{4} D_{m_{m}}(x-y) j^{m}(y)$$
 (4)

where in free-space with the Coulomb gauge we have, as usual

$$D_{\mu\nu}(\kappa) = -\frac{1}{(2\pi)^4} \int dk^4 \frac{e^{-ik(\pi-y)}}{|k_0^2 - |\vec{k}|^2}$$
(5)

Now in the presence of boundaries we have to use some appropriate Green's function $\widetilde{D}_{\mu\nu}$. It is well known that the electrostatic method of images 33 , in its capacity as a technique for constructing Green's functions, generalizes to the full electromagnetic field 9), 11), 26)-30). The cavity function $\widetilde{D}_{\mu\nu}$ will be then a linear combination of the freespace $D_{\mu\nu}$ and some additional image function(s). The new form factors \widetilde{T} are then computed and used in (1) to find the modified \underline{A} coefficient \overline{A}_n .

III. ATOM NEAR A CONDUCTING PLATE

An infinite, conducting plate is positioned normal to the \underline{z} axis at z = 0. If a unit test charge is placed on the \underline{z} axis at $z_0 > 0$ the plate may be replaced with a negative unit charge at $-z_0$ (see Fig.1). If in addition the real test charge has momentum $\overrightarrow{p}' \propto \overrightarrow{v}' = \{\frac{d}{dx}, \frac{d}{dy}, -\frac{d}{dx}\}$. Including both of these effects at once, Eq.(2) transforms as follows:

$$\overrightarrow{\pi}_{(\vec{k})} \rightarrow \overrightarrow{\pi}_{(\vec{k})} e^{i\vec{k}\cdot\vec{k}} - \overrightarrow{\pi}_{(\vec{k})} e^{i\vec{k}\cdot\vec{k}} = \overrightarrow{\pi}_{(\vec{k})}$$
 (6)

where $z_0 = \{0,0,z_0\}$. The form factor product in (1) becomes

$$\pi_{\widetilde{k}}(\vec{k}) = \pi_{\widetilde{k}}^{i}(-\vec{k}) \rightarrow \pi_{\widetilde{k}}^{i}(-\vec{k}) \qquad (7)$$

$$\pi_{\widetilde{k}}(\vec{k}) = \pi_{\widetilde{k}}^{i}(-\vec{k}) = \cos(2\vec{k} \cdot \vec{k}) = \pi_{\widetilde{k}}^{i}(\vec{k}) = \pi_{\widetilde{k}}^{i}(-\vec{k}) \qquad (7)$$

where factors of the form T'T' have been deleted and those of TT' multiplied by an extra $\frac{1}{2}$, due to artifacts of the imaging procedure 31). In addition

we have used symmetry in dummy sum and integration variables to combine two terms. We now make the replacement (7) in Eq.(1) and carry out the angular integration. As in the previous papers, we assume that TT and TT are functions of $|\vec{k}|^2$. (From general considerations these products are at most a linear combination of function of $|\vec{k}|^2$ and a term proportional to $\hat{\vec{a}}_{nm} \cdot \vec{k}$, where $\hat{\vec{a}}_{nm}$ is some constant vector. Then a second application of symmetry with respect to dummy variables shows that the latter always vanishes.) The exact result for the modified Einstein A coefficient near a wall is then

$$\widetilde{A}_{n} = A_{n}^{\sigma} - \frac{2\alpha}{m_{\sigma}^{2}} \sum_{m \in n} \omega_{nm} \left[n \overline{T}_{m} \right]^{2} \left[\left(1 - \overline{J}_{nm} \right) \frac{\sin \mu_{nm}}{\mu_{nm}} + \left(1 + \overline{J}_{nm} \right) \left(\frac{\cos \mu_{nm}}{\mu_{nm}^{2}} - \frac{\sin \mu_{nm}}{\mu_{nm}^{2}} \right) \right]$$
(8)

Here $\zeta_n = ||_n T_m^z||^2 / ||_n T_m||^2$ is introduced to display the asymmetry of the system with respect to the z co-ordinate, $||_n T_m||^2$ is a function of ω_{nm}^2 , and $\mu_{nm} = 2z_0 ||_{\omega_{nm}}||_{\infty}$ scales as the distance of the atom from the plate.

If the use of the dipole approximation (DA) is justified (i.e. if the atom's dimensions are small when compared to the transition wavelengths λ_{nm} contributing to the sum in (8)) then the A coefficient becomes

$$\tilde{A}_{n}^{2A} = A_{n}^{0} - 2\alpha \sum_{n \in n} \omega_{nn}^{3} |\tilde{F}_{nn}|^{\frac{1}{2}} \left[(1 - 3_{nn}) \frac{\sin \mu_{nn}}{\mu_{nn}} + (1 + 3_{nn}) \left(\frac{\cos \mu_{nn}}{\mu_{nn}} - \frac{\sin \mu_{nn}}{\mu_{nn}} \right) \right]$$
(9)

 \vec{r}_{nm} is a matrix element of the electron's co-ordinate operator, related to those of the momentum by $\vec{p}_{nm} = i \omega_{nm} m_0 \vec{r}_{nm}$. 32) Also we have the simplification $\zeta_{nm} = |z_{nm}|^2/|\vec{r}_{nm}|^2$ and thus for one-electron atoms $\vec{\xi}_{nm}$ can be computed directly 32). We shall be most interested in Rydberg transitions prepared such that $\zeta_{nm} = 0$ or 1—or an ensemble of randomly oriented atoms for which on the average ζ_{nm} can be taken to be $\frac{1}{3}$. Notice that as $z_0 \to \infty$ we recover the free-space formula, namely

$$\stackrel{\sim}{A}_{n}^{pA} \rightarrow A_{n}^{opA} = \frac{4\alpha}{3} \sum_{m \neq n} \omega_{nm}^{3} \left(\vec{r}_{nn} \right)^{2} \qquad (20)$$

III. ATOM IN A SPHERICAL CAVITY

We consider a grounded, conducting spherical shell of radius \underline{a} whose center coincides with the origin. If a unit charge is placed on the z-axis at $|z_0| |z_0| < a$, the correct Green's function is obtained by replacing the sphere with an image of charge $|z_0| = a$, which is located at $z = z_0' = A^2/z_0$. (see Fig. 2). The directions of the momenta of the two charges are related as in the single-plate case, which we again notate with $|\vec{p}|$ and $|\vec{p}|$. The form factor substitutions become

$$T_{m}^{-1}(\vec{k}) \rightarrow T_{m}^{-1}(\vec{k}) e^{-i\vec{k} \cdot \vec{k}} - i\vec{k} \cdot \vec{k}$$
 (11)

$$\pi T_{n}^{-1}(\vec{k}) \pi T_{n}^{-1}(-\vec{k}) \rightarrow \pi T_{n}^{-1}(\vec{k}) \pi T_{n}^{-1}(-\vec{k}) = e^{-\frac{1}{2}} \cos \left[\vec{k} \cdot (\vec{k} - \vec{k})\right]_{n} T_{n}^{-1}(\vec{k}) \pi T_{n}^{-1}(\vec{k}) \pi T_{n}^{-1}(\vec{k})$$
(12)

with the same conventions as used before. We can now modify Eq.(1), and straightforward manipulations yield

$$\widetilde{A}_{n} = A_{n}^{0} - 2 \frac{2\kappa}{m_{0}^{2}} \sum_{m \in n} \omega_{nm} \left| \sqrt{m_{m}} \right|^{2} \left[(1 - \tilde{J}_{nm}) \frac{\sin \nu_{nm}}{\nu_{nm}} \right]$$

$$+ \left(1 + \tilde{\zeta}_{nn}\right) \left(\frac{\cos \nu_{nm}}{\nu_{nm}^{L}} - \frac{\sin \nu_{nm}}{\nu_{nm}^{3}}\right) \tag{13}$$

with $v_{nm}=a(\eta-\frac{1}{\eta})~|\omega_{nm}|$ and ζ_{nm} as before. To obtain \widetilde{A} in the DA one simply replaces $|\overrightarrow{nT}_m|^2 \rightarrow \omega_{nm}^2~m_0^2~|\overrightarrow{\tau}_{nm}|^2$.

As a check, we notice that if we transform the sphere into a plane by letting $a \rightarrow \infty$, while keeping $a-z_0$ fixed, the single-plate result of Eq.(8) is recovered.

IV. ATOM BETWEEN PARALLEL PLATES

Two infinite, parallel conducting plates are placed normal to the z axis at $z=\pm L/2$, L being the plate separation. For a unit charge on the axis at $z=z_0$, $|z_0|< L/2$, the plates may be replaced by an <u>infinite</u> series of image charges --located on the z axis at $z_p=pL+(-1)^p z_0$, $p=\pm 1, \pm 2, \pm 3, \ldots$ and each with a charge of $(-1)^p$ (see Fig.3). The image momenta directions flip-flop, which we account for by defining

$$\frac{(i)^{p}}{\sqrt{T_{m}}(\vec{k})} := \begin{cases}
\frac{\vec{T}_{m}(\vec{k})}{\sqrt{T_{m}}(\vec{k})} & (p \text{ odd}) \\
\vec{T}_{m}(\vec{k}) & (p \text{ even})
\end{cases}$$
(14)

With this notation the form factor of (2) becomes $\begin{bmatrix} z \\ p \end{bmatrix} = (0,0,z_p)$

$$\int_{\mathbf{r}}^{\infty} (\vec{\mathbf{k}}) \rightarrow \sum_{p=-\infty}^{\infty} (-1)^p \int_{\mathbf{r}}^{\infty} (\vec{\mathbf{k}}) e^{-i \cdot \vec{\mathbf{k}} \cdot \vec{\mathbf{z}}_p} \qquad \theta \left(t_o - i \vec{\mathbf{z}}_o - \vec{\mathbf{z}}_{pl} \right) \tag{15}$$

 θ is the usual unit step function which we are using to take into account retardation. (The atom at \vec{z}_0 does not "see" the image at \vec{z}_p until time $t = \{\vec{z}_0 - \vec{z}_p\}/c.\} \quad \text{for } L << c/\tau_n = c A_n \; (\tau_n \text{ being the lifetime of the state n})$ we may set $\theta = 1.$

We need the Poisson summation formula, as used in the distribution sense 34)

$$\sum_{n=-\infty}^{\infty} e^{i \pi n \kappa} = \sum_{n=-\infty}^{\infty} J(x-n) =: \triangle(x)$$
 (16)

Using this we can now carry out the form-factor product

$$\pi_{m}^{-1}(\vec{\kappa})_{m}^{-1}(\vec{\kappa}) \rightarrow \left\{\pi_{m}^{-1}(\vec{\kappa})_{m}^{-1}(\vec{\kappa}) + \cos\left[\kappa_{k}\left(2z_{n}-L\right)\right]\pi_{m}^{-1}(\vec{\kappa})_{m}^{-1}(\vec{\kappa})\right\} \triangle\left(\frac{\kappa_{k}L}{m}\right)$$
(17)

Inserting this into expression (1), and being careful with the integration, we find

$$\widetilde{A}_{n} = \frac{1}{m_{\bullet}^{2}} \sum_{m \in n} \omega_{nm} \left[\sum_{n=1}^{k \sigma_{nm}} \left\{ \left[\left(1 + 3_{nm} \right) + \left(1 - 3 3_{nm} \right) \left(\frac{p^{2}}{\sigma_{nm}} \right)^{2} \right] - \left[\left(1 - 3 3_{nm} \right) + \left(1 + 3_{nm} \right) \left(\frac{p}{\sigma_{nm}} \right)^{2} \right] \cos \left[\pi p \left(\frac{42e}{L} - 1 \right) \right] \right\}$$
(18)

valid, as noted before, for L << cA $_n$. Here ζ_{nm} is as before. $\sigma_{nm} = L |\omega_{nm}|/\pi$ and [[k]] is the greatest integer less than k.

Milonni and Knight 12 , Philpott 26 and Barton 10 - in the framework of standard QED - have previously arrived at similar formulas. We emphasize again that what is new here is that (18) was computed, to our knowledge for the first time, from a theory which is not second-quantized

and in which there are no fluctuations in the vacuum radiation field. This is in sharp contrast to the above-mentioned derivations, all of which rely heavily on those two concepts.

V. COMPARISON TO EXPERIMENT

In their experiment Hulet, Hilfer abnd Kleppner (HHK) find both enhanced and inhibited spontaneous emission for Rydberg atoms between parallel plates $\frac{1}{2}$. Cesium atoms are prepared in a single-electron (Rydberg) circular state with principle quantum number n=22 and azimuthal quantum number n=12. The decay mode of this state is a single dipole transition, important to the experiment, since a state with several decay modes would have to have all possible transitions enhanced or suppressed in order to observe the effect on spontaneous emission. In terms of our formula (18) this means only one term will contribute to the outermost sum (n=n) and m=n'1'm'. The observed transition is $n m (22,21,21) \rightarrow n'1'm' (21,20,20)$ with wavelength $\lambda_0 \approx 0.45$ nm. Our $\alpha_0 = 0.45$ nm axis becomes a quantization axis due to an electric field directed normal to the plates; the selection rule $\alpha_0 = 0.45$ nm are in this case zero.

The plate spacing L is tuned to L $\sim \lambda_0/2$, with a variability of $\Delta L/L = 0.04$. This means that in (18), $\sigma_{nm} = \sigma \sim 1$ and $[[\sigma]] = 0.1$. For $\sigma < 1$ and $\sigma \ge 1$, respectively, and so we also have only one or zero terms in the innermost sum. The atoms sample all values of z_0 in the range $|z_0| < L/2$, and so we average formula (18) over this domain. Including all these observations, we have

$$\langle \tilde{A} \rangle_{\alpha = \frac{9}{4}} A^{\circ} \left[1 + \frac{1}{\sigma^{2}} \right] \Theta (\sigma = 1)$$
 (19)

where A^O is the free-space coefficient, $\sigma = L|\omega_0|/\pi = L/\frac{\lambda_0}{2}$ and θ a step function. As we vary L in the range $0 < L < 3\lambda_0/4$ (recall, the formula is only good for $L << cA^O$) or, equivalently, $0 < \sigma < 3/2$; we see that the spontaneous emission rate is zero unil $\sigma = 1$ ($L = \lambda_0/2$) where it jumps to $\langle \tilde{A} \rangle_{avg} = \frac{3}{2} A^O$, and then decays back towards A^O as the plate separation increases (sea Fig.4). In fact Fig.4 looks very much like the experimental plot given in HHK. In particular, their analysis indicates that a predicted enhancement to $\frac{3}{2} A^O$ at $L = \lambda_0/2$ agrees with the data to within 5%.

If one does not average (18) over z_0 , but rather localizes the atom at $z_0 = 0$ instead (cf. the Penning trap experiments), then (18), under all the same conditions as stated above, still predicts an enhancement of $\frac{3}{2}$ A^0 .

Formula (13) for an atom inside a sphere also lends itself to such an averaging procedure as used for the plates. If we average (13) over $|z_0| < a$ we get

$$\left\langle \widetilde{A}_{n}\right\rangle _{\text{avg}}^{\text{sphere}} = A_{n}^{0}$$
 (20)

i.e. the free space value -- regardless of the value of ζ_{nm} , or of the presence of a quantization axis. This difference between the parallel-plate case arises because $\widetilde{A}-A^0$ is an odd function of z_0 for the sphere formula, but even for that of the two plates. So a uniformly distributed ensemble of atoms inside a sphere should not show a change in their emission rates. Of course a localized atom will experience a change in its emission rate as per the unaveraged (13); for example, at exactly the centre of the sphere $z_0 = 0$, (13) predicts again $\widetilde{A} = A^0$. (The atom would have to be slightly off center for a non-null effect to appear.)

It is the azimuthal symmetry and the existence of a characteristic wavelength in the parallel-plate case which causes its effects to be much more pronounced than the sphere.

VI. CONCLUSIONS

In the Dirac picture of quantum electrodynamics, the spontaneous emission rate of an excited atom can be changed by a nearby boundary through their mutual coupling to the quantized vacuum field. In the present picture no such coupling occurs, as the vacuum is truly empty. Rather here the structure of the eletron's self-field depends on the presence of the boundary, and 'thus the radiation-reaction force - the cause of spontaneous emission in this view - is modified.

Our further program is to see how far we can go in understanding radiative processes from the point of view of self-energy, without second quantization. Work has been completed on Lamb shifts and the related Casimir-Polder, long-range van der Waals forces near boundaries 35). Work is in progress to include the general Casimir as well as Casimir-Polder forces, the Unruh effect and apparatus contributions

to the measured g-2 value for electrons in Penning traps. In the case of g-2, considering the recent, extremely accurate experiments $^{3),36}$, and the current theoretical controversy 27 -30) it would be advantageous to have a totally new approach to the problem.

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FIGURE CAPTIONS

- Fig.1 A unit charge (q = 1) in front of an infinite, conducting plane, and the appropriate image charge. \vec{p} and \vec{p}' are the momenta of the charges.
- Fig.2 A unit change inside a conducting spherical shell, and its associated image.
- Fig. 3 A unit charge between parallel plates, and the resultant series of image charges.
- Fig.4 The change of the spontaneous emission rate \tilde{A} , as a function of the plate spacing L averaged for an ensemble of prepared Rydberg atoms between parallel plates. A^0 is the free-space emission rate and λ_0 the wavelength of the emitted photon.

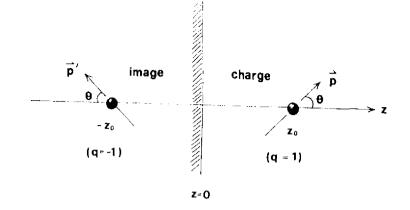


Fig.1

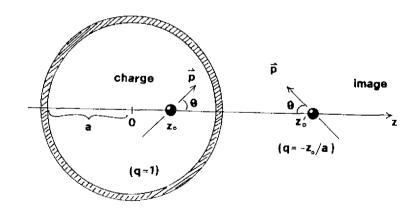


Fig.2

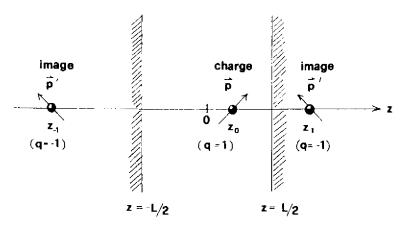


Fig.3

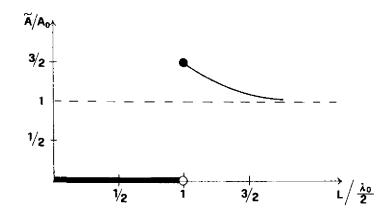


Fig.4

-15-