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QUANTUM MECHANICAL DISSIPATIVE SYSTEMS

by

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A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled QUANTUM MECHANICAL DISSIPATIVE SYSTEMS , submitted by Hing Hun Chan, in partial fulfillment of the requirements for the degree of Doctor of Philosophy.

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ABSTRACT

Two examples of quantum mechanical dissipative systems are studied. The first one is the multichannel Schrödinger equation with a nonlocal separable potential. This problem can be solved exactly and the partial-wave scattering amplitude can be found. A comparison is made with the well-known N/D method for one-channel and for multichannel problems. It is found that the generalization of treating N and D as matrices in the n-channel problem is not possible for this solvable example. Bound-state and resonance poles of the partial-wave amplitude are also discussed.

The second example is that of a bound electron (assumed to have two levels only) interacting with the electromagnetic field. This model is similar to the Lee model. In this model, the transition of the bound electron from the higher level to the lower level is accompanied by the emission of one photon. Results for level shift, line breadth and the probability amplitude are obtained, which correspond to the characteristics of a classical damped system, i.e. natural line breadth and the exponential decay form. Modification to this model is also considered. This modification essentially changes the eigenstates of

the photons, i.e. the bare photon becomes a coherent mixture of physical photons. Hence, the original interaction term is altered accordingly.

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Chapter 1. INTRODUCTION

In classical mechanics, when the forces acting on a particle (or particles) are known we can write down the equation of motion by virtue of Newton's Second Law of Motion. With the given initial conditions on position and velocity of the particle, the equation of motion can be integrated and thus the motion of the particle is determined completely. We note here that the force on the particle can be a function of position and velocity of the particle as well as an explicit function of time, i.e. the force may either be conservative or dissipative.

One can introduce canonical variables to form a Hamiltonian function which is the total energy of the particle (expressed in terms of canonical variables). With the Hamiltonian function, the classical equation of motion can be written concisely in Poisson brackets[1] . A natural way to quantize the classical equation of motion is to treat the canonical variables as dynamical operators (usually noncommutative) in quantum mechanics and to interpret the Poisson bracket as $1/i\hbar$ times the commutator. In this way, the classical equation of motion can be taken into quantum theory by Heisenberg's equation of motion. Another way is by the use of Schrödinger equation whose solution

corresponds to the Hamilton's principal function in the geometrical optics limit. These two methods are mathematically equivalent[2] .

When one looks at the Heisenberg picture of quantization, the imposition of the Poisson bracket on the commutator would seem an added postulate in the theory. This raises the question: "Do the equations of motion determine the quantum mechanical commutation relations?" (by Wigner)[3] . The answer is found to depend on the form of the Hamiltonian and is in the negative for a free particle and for the simple harmonic oscillator. This nonuniqueness in the commutation relation for the oscillator has been resolved by several authors[4] . Granting the Heisenberg's equations of motion for operators determine the commutation relations uniquely, there is still the question of the form of Hamiltonian.

Usually, the total energy of the system, when expressed in canonical variables, is the Hamiltonian function which can then be taken over as the Hamiltonian operator in Heisenberg picture. However, as pointed out by Havas[5] , for a given classical equation of motion many different Hamiltonians exist, one of which may be the total energy of the system. Quantization procedures using different Hamiltonian other

than the total energy will be quite different from the Heisenberg method or impossible, even though all these Hamiltonians do generate the same classical equation of motion. At this point, one would rather take the notion that equations of motion, classical or quantal, are fundamental and unique, then one would have to look for different equations for different systems. This can be done in classical mechanics, but one is lost, when dealing with quantum mechanics, in searching for the equation of motion without falling back on the Hamiltonian.

In this thesis, we are interested in dissipative system. For instance, in classical dynamics, the simple equation of motion for a damped oscillator can be solved uniquely with two given initial conditions on position and velocity of the oscillator. When we try to study this problem in quantum mechanics, we have to find the Hamiltonian that generates Heisenberg's equations of motion. However, since this Hamiltonian is not the total energy, the usual Heisenberg's quantization procedure does not apply and the correct quantization rule for this particular Hamiltonian is not known. Here, Hamilton's canonical equations are inconsistent with the usual commutation relations. Another way to consider this problem is just to "write down" the correct quantal equation of motion for the damped oscillator

avoiding the use of Hamiltonian entirely. Of course, we search in vain for this quantal equation. There seems to be a third way of trying to solve this problem by taking the total energy as the Hamiltonian (which is not explicitly time-dependent) plus the Rayleigh's dissipation function[6]. This last hope diminishes quickly, as pointed out by Brittin[7] that, for a dissipative system with a Hamiltonian not explicitly depending on time, quantization can be carried out in Heisenberg picture only if the dissipative force is a function of position and no dissipative force is possible in Schrödinger picture. Since we believe in the equivalence of these two pictures (two different methods of quantization), the above inconsistency rules out the hope to quantize a classical system with velocity-dependent dissipative force like that of the damped oscillator (classical electrodynamics is the exception). We accept the idea that a dissipative system can only be treated as a subsystem of a conservative system in quantum mechanics, in contrast to classical mechanics in which both conservative and dissipative systems can be studied separately from their respective equations of motion.

We consider some examples of dissipative systems in quantum mechanics. The multichannel problem (Chapter 3.) has been applied to inelastic nuclear reactions for some

years[8,9] . The effect of all other channels on a particular channel is to create an absorptive potential which can be considered as the quantum mechanical analogue of a damped classical system. We choose a solvable example with nonlocal separable potential to study mainly the behaviour of the S matrix and to compare the exact form of the S matrix with the well-known N/D method used in dispersion relations.

Another example (Chapter 4.) is that of a bound charged particle interacting with an electromagnetic field (non-relativistic). A bound electron (having two levels only) decays into the lower level with the emission of one photon and the reverse process. This problem, which in some ways is similar to the Lee model[10] , can be solved exactly. We obtain results for level shift and line breadth which can be compared with those obtained by time-dependent perturbation method. More important is that, in classical electrodynamics, a moving point charge emits radiation which in turn reacts on the charge's own motion. The equation of motion for the charge (Dirac's equation) is in certain ways similar to that of a damped harmonic oscillator. The emitted line by the charge is not infinitely sharp but has a certain natural breadth due to the damping force of the emitted radiation on the charge itself (Heitler's § 4.)[11] . Now our quantum mechanical dissipative system (which is a sub-

system of a conservative system) exhibits the same characteristics as a classical damped system. This convinces us that although a classical damped system cannot be quantized directly, it can always be considered as part of a conservative system which can be quantized, and then the quantum mechanical damped behaviour (quite similar to that of classical) can be found from the complete solution of the conservative system.

Modification to the above model is presented in Chapter 5, which changes the interaction term as well as the vacuum state for the photon.

Chapter 2. QUANTIZATION OF DAMPED CLASSICAL SYSTEM

A damped classical system can be specified uniquely by its equation of motion (plus initial conditions). Generally, the classical damped system cannot be quantized directly. In Section 1, we discuss some of the difficulties in quantizing a damped classical system and conclude that quantum mechanically a damped system can only be treated as a subsystem of a conservative system. We present a simple quantal system (Section 2.), similar to the Wigner-Weisskopf model, which exhibits the character of damping.

1. Quantization of Damped Classical System

It has been shown by Havas[5] that with a suitable "integrating factor" a very broad class of classical equations of motion can be derived from a variational principle and hence the Lagrangian and the Hamiltonian can also be obtained in the usual way. However, due to the multiplicity of possible integrating factors, for a given equation of motion many different Lagrangians exist. Quantization for different Lagrangian will be quite different or even impossible. In spite of this general finding, there are several papers[12] attempting to quantize the damped harmonic oscillator. The common feature in those papers is that starting from the classical

equation of motion for the damped oscillator,

$$\ddot{x} + \alpha\dot{x} + \omega^2 x = 0, \tag{2.1}$$

which is derivable from a time-dependent Hamiltonian (not the energy of the damped oscillator),

$$H = (1/2m)e^{-\alpha t}p^2 + \tfrac{1}{2}m\omega^2 e^{\alpha t}x^2, \tag{2.2}$$

where $p = me^{\alpha t}\dot{x}$. Quantization is then by the usual commutation relation

$$[x, p] = i\hbar, \tag{2.3}$$

or

$$[x, \dot{x}] = i\hbar e^{-\alpha t}/m. \tag{2.4}$$

Eq. (2.4) implies that

$$\Delta x \Delta\dot{x} \geq (\hbar/m)e^{-\alpha t} \tag{2.5}$$

violates the uncertainty principle for an oscillator,

$$\Delta x \Delta\dot{x} \geq \hbar/m, \tag{2.6}$$

which is valid even for the damped oscillator[7] .

The violation of the uncertainty principle may seem to arise from the explicit dependence of H and p on time. Some years ago Seeger[6] considered the same problem. He chose a time-independent Hamiltonian plus the Rayleigh's dissipation function (depending on velocity) and then quantized the damped oscillator by the ordinary commutation relation working entirely in the matrix form of quantum mechanics, Heisenberg representation. However, it was shown by Brittin[7] that for a dissipative system not explicitly depending on time, quantization can be carried out in the Heisenberg representation only if the dissipative force is a function of position (not velocity) and no dissipative force which is a function of position or momentum is possible in Schrödinger representation. This kind of inconsistency rules out the possibility of quantizing a dissipative system by the usual procedure. Even within the frame work of quantum mechanics, Razavy recently showed[13] that in nuclear physics an often used class of velocity-dependent Hamiltonians, which attempts to explain the strong short-range repulsion of the two-nucleon interaction at high energies, leads to unacceptable results. Though the velocity-dependent Hamiltonian satisfies the general requirements of Hermiticity and invariance properties, the Heisenberg equation of motion

for the energy operator (closely related to the Hamiltonian) cannot be satisfied.

In view of the difficulties of quantization, apparently the Hamiltonian chosen for quantization can only be the energy of the system[5] which is uniquely defined in classical mechanics. As for the quantization of a dissipative system, one should treat the dissipative system as a subsystem of a non-dissipative system. The complete system will then be solved by some approximation if needed. The behaviour of the dissipative system can then be interpreted from the solution of the complete non-dissipative system.

2. The Wigner-Weisskopf Model

A simple solvable model for inelastic processes was considered some years ago by Wigner and Weisskopf[14]. It consists of a motionless particle whose wave function is $\chi(t)$, and another moving particle of mass m with the wave function $\psi(\vec{r},t)$. These two particles act as one another's sources with a real form factor $\rho(r)$. The Schrödinger equations are

$$(i\partial/\partial t + \nabla^2/2m)\psi(\vec{r},t) = G\rho(r)\chi(t)$$

$$(id/dt - \mu)\chi(t) = G\int \rho(r)\psi(\vec{r},t)d\vec{r}. \qquad (2.7)$$

Assuming $\rho(r)$ depends on the magnitude of the radius vector, then only S-waves are coupled. Usually $\rho(r)$ is of a very short range r_o with the point interaction (local) limit as $r_o \to 0$. The solutions for (2.7) have terms in r_o^{-1}. Martin[15] studied the time development of a prepared state $|\psi=0,\chi=1\rangle$ for this model at $t = 0$. He found that such a state is not physically acceptable, since the mean energy of the system diverges at $t = 0$, which implies that the decay curve has a cusp at $t = 0$. Recently Razavy[16] remedied the above defect by a noncausal coupling in the Schrödinger equations. In the following we shall consider a similar system with nonlocal interaction, which will give results similar to Razavy's.

The Schrödinger equations for two channels coupled by a nonlocal separable potential are

$$(\nabla^2+k^2)\psi_{\vec{k}}(\vec{r}) = GV(r)\int V(r')\phi_{\vec{k}}(\vec{r}')d\vec{r}'$$

$$(\nabla^2-\kappa^2)\phi_{\vec{k}}(\vec{r}) = GV(r)\int V(r')\psi_{\vec{k}}(\vec{r}')d\vec{r}', \qquad (2.8)$$

where $\kappa^2 = \varepsilon - k^2 > 0$, ε is the internal energy of the two particles described by the wave function ϕ. Eq. (2.8) will be considered in more detail in the next chapter. Our main purpose here is to show that the phase shift in ψ is qualitatively the same as Razavy's and a state of finite mean energy can be prepared for the system at $t = 0$.

Since $V(r)$ depends on $|\vec{r}|$, Eq. (2.8) will only couple S-waves. We have assumed that $\kappa^2 > 0$, so there will be no incoming wave in ϕ as well as no spherical outgoing wave, i.e. $\phi \to e^{-\kappa r}/r$ as $r \to \infty$. With little modification, namely by putting

$$g_{11}=g_{22}=0,\ g_{12}=4\pi G,\ k_1^2=k^2,\ \text{and}\ k_2^2=-\kappa^2, \tag{2.9}$$

the results for the wave functions and the partial-wave amplitude in chapter 3, Eq. (3.11), (3.12), and (3.13), can be taken over to give

$$\tilde{\psi}_{\vec{k}}(\vec{p}) = \delta(\vec{p}-\vec{k}) + \frac{G^2\tilde{V}(k)\tilde{V}(p)}{p^2-k^2-i\varepsilon}\left[\int\frac{\tilde{V}^2(p')d\vec{p}'}{p'^2+\kappa^2}\right]\Big/\Delta$$

$$\tilde{\phi}_{\vec{k}}(\vec{p}) = -\frac{G\tilde{V}(k)\tilde{V}(p)}{p^2 + \kappa^2}\Big/\Delta \tag{2.10}$$

where

$$\Delta = 1-G^2\int\frac{\tilde{V}^2(p)d\vec{p}}{p^2-k^2-i\varepsilon}\int\frac{\tilde{V}^2(p')d\vec{p}'}{p'^2+\kappa^2} \ . \tag{2.11}$$

The tilde indicates Fourier transforms of the respective quantities. We may choose $\tilde{V}(p) \propto 1/(k^2 + b^2)$, Eq. (3.18), then from $\tilde{\psi}_{\vec{k}}(\vec{p})$, we can find $\psi_{\vec{k}}(\vec{r})$ whose asymptotic condition at $r \to \infty$ yields the scattering amplitude (S-wave),

$$a = \frac{2\pi^2G^2\tilde{V}^2(k)}{\Delta}\int\frac{\tilde{V}^2(p)d\vec{p}}{p^2+\kappa^2} = \frac{e^{i\delta}\ \sin\delta}{k} \ . \tag{2.12}$$

From this relation it follows that

$$k\cot\delta = \mathrm{Re}(a^{-1}) = [1-G^2\int\frac{\tilde{V}^2(p')d\vec{p}'}{p'^2+\kappa^2}\left(P\int\frac{\tilde{V}^2(p)d\vec{p}}{p^2-k^2}\right)]\times$$

$$[2\pi^2G^2\tilde{V}^2(k)\int\frac{\tilde{V}^2(p)d\vec{p}}{p^2+\kappa^2}]^{-1} \qquad (2.13)$$

where P stands for the principal value of the integral. Eq. (2.13) is the ratio of two polynomials in k^2 and Razavy's result is a polynomial in k^2 . Hence, our system gives qualitatively the same scattering as the one with noncausal coupling. This is to be expected. As pointed out by Gasiorowicz and Ruderman[17] that, under certain conditions, nonlocal interaction is equivalent to noncausal interaction, in the sense that they produce the same scattering amplitude.

For simplicity, we shall assume there is only one bound state ϕ_b (normalized) in ϕ when $G = 0$. Let us prepare a state $|\Psi(t = 0)\rangle = |\psi=0, \phi_b\rangle$ for our system at $t = 0$ and study its subsequent development. We can

expand $|\Psi(0)\rangle$ in terms of the eigenstates (2.10),

$$|\Psi(0)\rangle = \int d\vec{k}\lambda(\vec{k})|\psi_{\vec{k}}(\vec{r}),\phi_{\vec{k}}(\vec{r})\rangle, \tag{2.14}$$

with $\lambda(\vec{k})$ given by

$$\lambda(\vec{k}) = \langle\psi_{\vec{k}}(\vec{r}),\phi_{\vec{k}}(\vec{r})|0,\phi_b\rangle$$

$$= (2\pi)^{-3/2}\int\tilde{\phi}_{\vec{k}}(\vec{p})e^{i\vec{p}\cdot\vec{r}}d\vec{p}\phi_b(\vec{r})d\vec{r}$$

$$= (2\pi)^{-3/2}\int\tilde{\phi}_{\vec{k}}(\vec{p})e^{i\vec{p}\cdot\vec{r}}d\vec{p}(\sqrt{\kappa_b/2\pi}e^{-\kappa_b r}/r)d\vec{r}$$

$$= \sqrt{\kappa_b}/\pi\int\tilde{\phi}_{\vec{k}}(\vec{p})/(p^2 + \kappa_b^2)d\vec{p}\ . \tag{2.15}$$

At a later time, the state will be given by

$$|\Psi(t)\rangle = \int d\vec{k}\lambda(\vec{k})e^{-ik^2t}|\psi_{\vec{k}}(\vec{r}), \phi_{\vec{k}}(\vec{r})\rangle \ . \qquad (2.16)$$

The mean energy of the system at $t = 0$ is

$$\langle\Psi(0)|H|\Psi(0)\rangle = \langle\Psi(0)|i\frac{d}{dt}\Psi(t)_{t=0}\rangle = \int k^2 d\vec{k}|\lambda(\vec{k})|^2 \ , \qquad (2.17)$$

where H is the Hamiltonian (a matrix) for the two-channel Schrödinger equations (2.8). With $\lambda(\vec{k})$ given by (2.15), the mean energy above is finite. Hence, the decay curve for this model does not have a cusp at $t = 0$. The probability amplitude that the system remains in $|\Psi(0)\rangle$ after t is determined by $\langle\Psi(0)|\ \Psi(t)\rangle$ which has damped exponential behaviour for small t and ultimately goes as some inverse power of t for $t \to \infty$. More detail of a similar prepared state will be given in Chapter 4.

Chapter 3. MULTICHANNEL PROBLEM WITH NONLOCAL SEPARABLE POTENTIAL

A well-known method of treating inelastic scattering and resonance reaction is to extend the one-channel Schrödinger equation to the multichannel equation. After a brief discussion on the multichanned Schrödinger equation (Section 1.), we solve an example with a nonlocal separable potential (Section 2.). Although, for one channel, the partial-wave amplitude can be put into the often used N/D form, a straightforward generalization of N/D to multichannel is not possible for this solvable example (Section 3.). In Section 4, the analytic properties of the 2-channel partial-wave amplitude is studied with the attention to bound states and resonances.

1. The Coupled Schrödinger Equation

A general situation in nuclear scattering experiment consists of a projectile nucleon impinging on a target nucleus which can be excited into many higher levels. Such a reaction can be described by the coupled-channel Schrödinger equation[8,9]:

$$-\tfrac{1}{2}M^{-1}\nabla^2\bar{\Psi} + \bar{V}\bar{\Psi} = E\bar{\Psi} \qquad (3.1)$$

where we consider n coupled channels interacting with two-body potentials. Eq. (3.1) is written in the centre-of-mass coordinates of the two-body channels. The name "channel" has the following meaning: the incoming nucleon plus the target nucleus in its ground state is designated the incident channel which is capable of going into n exit channels having an out-going nucleon plus the target nucleus in one of its excited states or its ground state. We confine ourselves to two-body interactions by $\bar{V}$ so that particles in each channel are grouped into two bodies, e.g. projectile plus target, out-going particle plus excited nucleus. The diagonal matrix M has elements μ_α, the reduced mass of the two bodies in a certain channel α. The matrix ξ has elements $\xi_{\alpha\beta} = (E - \varepsilon_\alpha)\delta_{\alpha\beta}$, where E is the total energy of the whole system or the kinetic energy of the incident nucleon (taking ground state energy of the target as zero), and ε_α is the internal energy of the two bodies in channel α or the excitation energy of the target nucleus. We shall call ε_α the "threshold" of channel α because it is the minimum kinetic energy that the incident nucleon must possess in order to make the interaction energetically possible in channel α. The potential matrix $\bar{V}$ is symmetric due to time-reversal invariance[18]. $\bar{\Psi}$ is the wave-function matrix describing the interaction between n channels. Each column of $\bar{\Psi}$ and the whole matrix $\bar{\Psi}$ are solutions of

(3.1).

Eq. (3.1) can be reduced to a simpler form by defining

$$\Psi \equiv M^{-\frac{1}{2}}\overline{\Psi}$$

$$V \equiv 2M^{\frac{1}{2}}\,\overline{V}\,M^{\frac{1}{2}} \qquad (3.2)$$

where $M^{\pm 1/2}$ is the diagonal matrix with elements $\mu_\alpha^{\pm 1/2}$. Substitution of (3.2) into (3.1) yields

$$-\nabla^2\Psi + V\Psi = K^2\Psi \qquad (3.3)$$

where K is the diagonal matrix of the channel wave numbers, $k_\alpha = \sqrt{2\mu_\alpha(E - \varepsilon_\alpha)}$. We may, therefore, consider all channels having the same reduced mass $1/2$, and take (3.3) as our coupled-channel equation. At a given total energy E it may be possible to excite the target nucleus into some levels and still have some (positive) kinetic energy left over for the out-going particle; other higher levels may not be so accessible. The channels corresponding to the former are said to be open, i.e. $E > \varepsilon_\alpha$, and those corresponding to the latter are said to be closed, $E < \varepsilon_\alpha$. The energy

at which a channel opens up is its threshold.

2. A Solvable Example of Nonlocal Separable Potential

It is well known that effects of many-body forces[19], exchange forces (Majorana[20], particle-exchange[21]), velocity-dependent forces, and the usual relativistic correction to the energy, all give rise to nonlocal potentials in the Schrödinger equation. In the coupled equation (3.3) with local (real) interaction, we can single out a particular channel, e.g. the incident channel 1, by eliminating all other channels. The resulting Schrödinger equation for channel 1 contains a generalized "optical" potential[9] whose imaginary part is negative definite. This means that the effect of other channels on 1 is to produce an absorptive potential since the incident nucleon may be "absorbed" (not literally but with kinetic energy changed) in different ways through n exit channels. This generalized "optical" potential is nonlocal though not separable *. This is the quantum mechanical analogue of the damped classical system.

In our discussion we shall take a real nonlocal separable potential matrix, which will be specified later,

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* A general type of nonlocal potentials, with separable and local as two extreme cases, can be expressed as a sum of separable potentials.[22]

and shall ignore spin variables in the coupled Schrödinger equation (3.3). Let us make the usual partial-wave decomposition for the wave function and the nonlocal potential,

$$\Psi_{\alpha\beta}(\vec{r}) = \sum_{\ell} u_{\alpha\beta}^{(\ell)}(r)/r \; P_{\ell}(\cos\theta)$$

$$V_{\alpha\gamma}(\vec{r},\vec{r}') = \sum_{\ell}(2\ell+1)V_{\alpha\gamma}^{(\ell)}(r,r')/(4\pi rr') \; P_{\ell}(\hat{r}\cdot\hat{r}') \; , \qquad (3.4)$$

where we have assumed the nonlocal potential to be "central", i.e. depending only on the magnitude of the distance $\vec{r}-\vec{r}'$ ($\hat{r}$ and $\hat{r}'$ are the unit vectors in the directions of $\vec{r}$ and $\vec{r}'$ respectively). The nonlocal potential is not only symmetric in α and γ, as mentioned in the last section, but also symmetric in $\vec{r}$ and $\vec{r}'$ due to the requirement of Hermiticity.[23] Then Eq. (3.3) becomes

$$[d^2/dr^2 + k_{\alpha}^2 - \ell(\ell+1)/r^2]u_{\alpha\beta}^{(\ell)}(r)$$

$$- \sum_{\gamma=1}^{n} \int_0^{\infty} V_{\alpha\gamma}^{(\ell)}(r,r')u_{\gamma\beta}^{(\ell)}(r')dr' = 0 \qquad (3.5)$$

which shows that only partial waves of the same order are coupled. For our real nonlocal separable potential, we choose the simple form,

$$V^{(\ell)}_{\alpha\gamma}(r,r') = g^{(\ell)}_{\alpha\gamma} v^{(\ell)}(r) v^{(\ell)}(r'), \qquad (3.6)$$

where $g^{(\ell)}_{\alpha\gamma} = g^{(\ell)}_{\gamma\alpha}$ are the real coupling constants. The S matrix for the ℓ-th partial wave is determined by the boundary condition at $r \to \infty$[24] :

$$u^{(\ell)}_{\alpha\beta}(r) \underset{\sim}{r\to\infty} e^{i\frac{1}{2}\pi(\ell+1)}(k_\alpha k_\beta)^{-\frac{1}{2}}(\delta_{\alpha\beta} e^{-ik_\alpha r} - e^{ik_\beta r} e^{-i\pi\ell} S^{(\ell)}_{\alpha\beta}). \qquad (3.7)$$

In the following discussion we shall suppress the ℓ indices in $\bar{u}^{(\ell)}_{\alpha\beta}$, $g^{(\ell)}_{\alpha\gamma}$, $v^{(\ell)}$, and $S^{(\ell)}_{\alpha\beta}$.

Eq. (3.5), with the potential given by (3.6), can be written in momentum space by the following transform:

$$u_{\alpha\beta}(r)/r = \sqrt{2/\pi} \int_0^\infty \tilde{u}_{\alpha\beta}(p) j_\ell(pr) p^2 dp$$

$$v(r)/r = \sqrt{2/\pi} \int_0^\infty \tilde{v}(p) j_\ell(pr) p^2 dp$$

$$\tilde{u}_{\alpha\beta}(p) = \sqrt{2/\pi} \int_o^\infty u_{\alpha\beta}(r)/r \; j_\ell(pr) r^2 dr$$

$$\tilde{v}(p) = \sqrt{2/\pi} \int_o^\infty v(r)/r \; j_\ell(pr) r^2 dr \; . \qquad (3.8)$$

From (3.6) and (3.8), we obtain for (3.5)

$$(k_\alpha^2 - p^2)\tilde{u}_{\alpha\beta}(p) - \sum g_{\alpha\gamma} \tilde{v}(p) \int_o^\infty \tilde{v}(p')\tilde{u}_{\gamma\beta}(p') p'^2 dp' = 0 \qquad (3.9)$$

with the general solution:

$$\tilde{u}_{\alpha\beta}(p) = \delta_{\alpha\beta} \frac{\delta(k_\alpha - p)}{k_\alpha^2} - \frac{\tilde{v}(p)}{p^2 - k_\alpha^2 - i\varepsilon} \sum g_{\alpha\gamma} \int_o^\infty \tilde{v}(p')\tilde{u}_{\gamma\beta}(p') p'^2 dp' \; . \qquad (3.10)$$

The integration constants $\int_o^\infty \tilde{v}(p)\tilde{u}_{\gamma\beta}(p) p^2 dp$ can be evaluated from a set of simultaneous equations obtained by substitutions of (3.10) into the constants themselves. We get finally

$$\tilde{u}_{\alpha\beta}(p) = \delta_{\alpha\beta} \frac{\delta(k_\alpha - p)}{k_\alpha^2} - \frac{\tilde{v}(p)}{p^2 - k_\alpha^2 - i\varepsilon} \sum g_{\alpha\gamma} (A^{-1})_{\gamma\beta} \tilde{v}(k_\alpha), \qquad (3.11)$$

where the matrix A is given by

$$A_{\alpha\beta} = \delta_{\alpha\beta} + g_{\alpha\beta} \int_0^\infty \frac{\tilde{v}^2(p) p^2 dp}{p^2 - k_\alpha^2 - i\varepsilon} \quad . \tag{3.12}$$

The S matrix can be obtained by writing $\tilde{u}_{\alpha\beta}(p)$ in configuration space, Eq. (3.8), and from the asymptotic condition (3.7),

$$S_{\alpha\beta} = \delta_{\alpha\beta} - i\pi\sqrt{k_\alpha k_\beta}\,\tilde{v}(k_\alpha)\tilde{v}(k_\beta)\sum g_{\alpha\gamma}(A^{-1})_{\gamma\beta}$$

$$= \delta_{\alpha\beta} + 2i\sqrt{k_\alpha k_\beta}\; a_{\alpha\beta} \,, \tag{3.13}$$

where $a_{\alpha\beta}$ is the ℓ- th partial-wave amplitude. As implied by time-reversal invariance, the S matrix is symmetric, which can also be shown explicitly from (3.13) and (3.12). We note that, from (3.12), $A_{\alpha\beta}$ can be considered as a function of the total energy $E = k_\alpha^2 + \varepsilon_\alpha$, which may also be analytically continued for a complex E in a certain region if we choose $\tilde{v}^2(p)$ analytic in that region (and of course vanishing fast enough for large p to make the integral in (3.12) convergent). As a function of the complex variable E,

$A_{\alpha\beta}$ will have a cut on the positive real axis starting from the threshold ε_α to infinity (the ground state energy ε_1 can be taken as zero). Since we have taken $\tilde{v}^2(p)$ to vanish for large p, $A_{\alpha\beta} \to \delta_{\alpha\beta}$ as $E \to \infty$, i.e. $A_{\alpha\beta}$ is analytic and normalized for $E = \infty$. In the following sections, we shall study the analytic properties of the S matrix in more detail.

3. The N/D Form for the Partial-Wave Amplitude

It has been shown by many authors[25] that, for a one-channel problem, the partial-wave amplitude a(s) is a function of s, the total centre-of-mass energy squared. It has a right-hand cut (kinematical cut) in the complex s plane coming from the unitarity of the S matrix and a left-hand cut (dynamical cut) due to the interaction between the two particles in the channel. For nonrelativistic potential scattering[26] that we are interested in, $s = k^2$ the centre-of-mass momentum squared if we take the internal energy of the two particles as zero, i.e. the threshold for this interaction is at $k^2 = 0$. The general analytic behaviour mentioned above enables one to write

$$a = N/D \ , \qquad (3.14)$$

where D has the same right-hand cut as a but no left-hand cut, while N has the same left-hand cut as a with no right-hand cut. D is normalized at $k^2 = \infty$ and its zeros with $\mathrm{Im}(k) > 0$ ($\mathrm{Re}\ k = 0$) correspond to the bound states. N and D can then be expressed as some kind of dispersion relations. These two dispersion relations, two coupled integral equations, may be solved by successive approximations. This is a roundabout way to solve a scattering problem, though we do not need it to solve potential scattering since it is easier to solve the Schrödinger equation. However, at high energies, where the governing equations are not solvable or simply are nonexistent, the N/D method furnishes an approximation that can be handled without knowing the exact dynamical structure of the system. Usually when the projectile gets more and more energetic it is capable of producing different kinds of reactions, elastic, inelastic, rearrangements. In these cases, a single-channel formulation will not be sufficient. One must take account of the channels that are most relevant to the problem concerned.

There have been many attempts to generalize the single-channel N/D method to multichannel processes[27,28,29]. An obvious way to generalize (3.14) is to treat N and D as matrices[27] because the partial-wave amplitude becomes an $n \times n$ matrix $a_{\alpha\beta}$ for n coupled channels:

$$a_{\alpha\beta} = \sum N_{\alpha\gamma}(D^{-1})_{\gamma\beta} \tag{3.15}$$

with the usual respective analytic properties assigned to the N and D matrices, namely that:

(a) dynamical cut only in N;

(b) physical cut (unitarity cut) only in D; and

(c) bound-state poles are produced by zeros of D (the determinant of matrix D).

Another way to account for the effect of other channels on a particular channel is to introduce an "absorptive parameter" into the single-channel scattering amplitude[29] and thus keep the simple form of single-channel N/D. However, it has been shown that results obtained from "absorptive parameter" N/D are not equivalent to those from multichannel N/D[30]. Though D still has only the right-hand cut, N will have both the left and the right-hand cut. Moreover, condition (c) is not fulfilled[31].

For our solvable example, it is easy to check if the N/D form (single or multichannel) is acceptable with the above three conditions imposed. For one channel, from (3.13) and (3.12), we obtain the partial-wave amplitude,

$$a(k^2) = N(k^2)/D(k^2)$$

$$= -\tfrac{1}{2}\pi g\tilde{v}^2(k) \Big/ \left(1+g\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k^2-i\varepsilon}\right) , \qquad (3.16)$$

which fulfills conditions (a), (b), and (c), provided that[32]

$$v(r)/r \sim O(r^{-5/2}) \quad \text{for} \quad r \to 0,$$

and

$$v(r)/r \sim \text{const.}\ \exp(-br) \quad \text{for} \quad r \to \infty . \qquad (3.17)$$

We may then assume that our potential (3.8) is of the form

$$\tilde{v}(k) \propto 1/(k^2+b^2), \qquad (3.18)$$

where $1/b$ can be considered as the range of the potential. With Eq. (3.18), the left-hand cut of N becomes an isolated double pole.

For multichannel, we have already noticed, at the end of last section, that matrix $A_{\alpha\beta}$ of (3.12) (with (3.17)) is equivalent to the D matrix in (3.15). If we make the assumption that all channels have the same threshold, say 0, we can write an exact N/D form for our partial-wave amplitude, i.e.

$$a_{\alpha\beta} = \sum N_{\alpha\gamma}(D^{-1})_{\gamma\beta}$$

with

$$N_{\alpha\beta}(k) = -\tfrac{1}{2}\pi\tilde{v}^2(k)g_{\alpha\beta}$$

$$D_{\alpha\beta}(k) = A_{\alpha\beta}(k) = \delta_{\alpha\beta} - \frac{2}{\pi}\int_0^\infty \frac{N_{\alpha\beta}(p)p^2dp}{p^2-k^2-i\varepsilon} , \qquad (3.19)$$

from Eqs. (3.12) and (3.13). In general, however, different channels will have different thresholds, as the target nucleus would have excited states other than the ground state. From (3.13), the partial-wave amplitude (matrix) can be written in matrix form

$$a = -\tfrac{1}{2}\pi\tilde{v}gA^{-1}\tilde{v} , \qquad (3.20)$$

where $\tilde{v}$ is the diagonal matrix with elements $\tilde{v}(k_\alpha)$, (containing the left-hand cut), g the symmetric matrix of the coupling constants $g_{\alpha\beta}$, and matrix A is given by (3.12). Eq. (3.20) is no longer in the exact N/D form. If one still insists upon writing $a_{\alpha\beta} = \sum N_{\alpha\gamma}(D^{-1})_{\gamma\beta}$ with $D_{\gamma\beta}$ given by (3.12) a different N matrix will be found. From the matrix equation (3.20) (a, N, and D are now matrices)

$$a = ND^{-1} = -\tfrac{1}{2}\pi\tilde{v}gD^{-1}\tilde{v}$$

$$\therefore \quad N = -\tfrac{1}{2}\pi\tilde{v}gD^{-1}\tilde{v}D \ , \qquad (3.21)$$

which shows that N will have the right-hand cut (from D) in addition to the usual left-hand cut (from $\tilde{v}$). This may be compared with the situation in the "absorptive parameter" N/D[29,31] , except that the zeros of det (D) in (3.21) do produce bound states.

In conclusion, a straightforward generalization of the N/D form for the partial-wave amplitude from one-channel to multichannel, Eq. (3.15) plus the three restrictions, is not applicable to our simple solvable example, and we doubt its validity in the much more complicated problems though it has already been used in the treatment of strong interactions.

4. Analytic Properties of the Partial-Wave Amplitude (2 - channel)

We shall study the analytic properties of the partial-wave amplitude in the simple case of two coupled

channels. The general behaviour of the n-channel amplitude is similar to that of the two-channel amplitude. The matrix elements $a_{\alpha\beta}$ of the partial-wave amplitude can be found from Eqs. (3.13) and (3.12).

$$a_{11} = n_{11}/\Delta = \frac{-\pi\tilde{v}^2(k_1)}{2\Delta}[g_{11}+(g_{11}g_{22}-g_{12}^2)\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_2^2-i\varepsilon}]$$

$$a_{22} = n_{22}/\Delta = \frac{-\pi\tilde{v}^2(k_2)}{2\Delta}[g_{22}+(g_{11}g_{22}-g_{12}^2)\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_1^2-i\varepsilon}]$$

$$a_{12} = a_{21} = n_{12}/\Delta = -\pi\tilde{v}(k_1)\tilde{v}(k_2)g_{12}/2\Delta \qquad (3.22)$$

where Δ is the determinant of the matrix A, Eq. (3.12),

$$\Delta = [1+g_{11}\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_1^2-i\varepsilon}]\times[1+g_{22}\int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2-k_2^2-i\varepsilon}] -$$

$$-g_{12}^2 \int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_1^2-i\varepsilon} \int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2-k_2^2-i\varepsilon} \ . \tag{3.23}$$

Let us suppose that channel 2 has a higher threshold than channel 1, i.e. $\varepsilon_2 > \varepsilon_1 (= 0$, the ground state energy). The channel momenta , k_1 and k_2 are not independent (their signs are independent) but are related to the total energy E of the system (the kinetic energy of the incident particle) by

$$k_1^2 = E \ , \quad k_2^2 = E - \varepsilon_2 \ , \tag{3.24}$$

where we have taken the channel reduced mass as 1/2. When $a_{\alpha\beta}$ are considered as functions of the complex variable E, they have (kinematical) cuts (from the integrals) on the positive real axis, starting from the thresholds at $E = 0$ and $E = \varepsilon_2$ to infinity, and (dynamical) cuts (from the potential) below the thresholds along the real axis to $-\infty$. We also note that $a_{\alpha\beta} \to 0$, and $\Delta \to 1$, for $|E| \to \infty$. In the following discussion, we shall follow a paper by Peierls[33] .

The characteristics of the 2-channel processes depend on the incident energy E (real and positive). If E

is less than ε_2 the only possible real process is elastic scattering in channel 1. If E is above the threshold for channel 2, inelastic scattering is also possible. The zeros of Δ, with certain restrictions on k_1 and k_2, corresponds to the bound-state and resonant poles of $a_{\alpha\beta}$. Their positions are determined from the (complex) roots of (3.23).

Let us look at the bound-state poles first. There are two kinds of bound states, one has the bound-state energy below all the thresholds (the ordinary kind) and the other has the bound-state energy between the two thresholds. The latter kind is called the bound state embedded in the continuum[34] because it looks like an ordinary bound state in channel 2 but with an energy in the continuum of channel 1, so it is not a bound state in channel 1. Bound states of the first kind are given by the roots of (3.23) with both k_1 and k_2 positive imaginary, i.e.

$$[1+g_{11}\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2+\kappa_1^2}]\times[1+g_{22}\int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2+\kappa_2^2}]$$

$$- g_{12}^2\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2+\kappa_1^2}\int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2+\kappa_2^2} = 0 \ , \qquad (3.25)$$

where $k_1 = iK_1 = +i\sqrt{E_b}$, $k_2 = iK_2 = +i\sqrt{E_b - \varepsilon_2}$, and E_b is the negative bound-state energy. It is seen that no matter what the diagonal elements of the potential matrix are (attractive or repulsive), if the off-diagonal elements are large enough in magnitude, there will be a bound state, because only the square of g_{12} enters in Δ. This corroborates the fact that the coupling term, e.g. V_{12}, of the Hamiltonian always is effectively attractive[9]. However, there is no way of identifying the channel in which the bound state occurs, it belongs to both channels. For a bound state embedded in the continuum with bound-state energy E'_b, $0 < E'_b < \varepsilon_2$, we must look for a root of (3.23) at a positive real value of $k_1 (= +\sqrt{E'_b})$ and at a positive imaginary value of $k_2 (= iK_2 = +i\sqrt{E'_b - \varepsilon_2})$,

$$\left[1+g_{11}\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_1^2-i\varepsilon}\right]\times\left[1+g_{22}\int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2+\kappa_2^2}\right]$$

$$- g_{12}^2\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2-k_1^2-i\varepsilon}\int_0^\infty \frac{\tilde{v}^2(p')p'^2dp'}{p'^2+\kappa_2^2} = 0 \ . \qquad (3.26)$$

The real and imaginary parts of this equation must vanish, i.e.

$$1 + g_{22}\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2+\kappa_2^2} = 0$$

$$g_{11}[1+g_{22}\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2+\kappa_2^2}] = g_{12}^2\int_0^\infty \frac{\tilde{v}^2(p)p^2dp}{p^2+\kappa_2^2} . \qquad (3.27)$$

The first equation determines E_b', so g_{22} should be negative (attractive), while the second equation will require $g_{12} = 0$ and g_{11} may be positive or negative. This means that channels 1 and 2 are not coupled, then, of course, channel 2 can have bound state above the threshold of channel 1. However, this is a special situation, we expect that, for more than two channels, some zeros of Δ would give rise to bound states embedded in the continuum without too severe a restriction on the off-diagonal elements of the potential matrix.

Resonant poles, in the one-channel problem, occur in

the fourth quadrant close to the positive real axis in the complex momentum plane. In the two-channel case, there are two fourth quadrants, one for each channel momentum. Poles, in either one or both of the two fourth quadrants and close to the real axis, will correspond to resonances. When the resonances are sharp, i.e. the width of the resonances is small compared to their spacing, a more convenient way of determining the resonance energy E_r is to require the real part of Δ to vanish at E_r .[28] In this way, we are working with the real energy E instead of complex E. On writing (3.23) into real and imaginary parts, $\Delta(E) = \Delta_R(E) + i\Delta_I(E)$, E_r is then determined by $\Delta_R(E_r) = 0$ and the resonance width Γ is proportional to $\Delta_I(E_r)$. For E near E_r, we can expand

$$\Delta(E) \approx (E-E_r)\Delta_R'(E_r) + i\Delta_I(E_r) , \qquad (3.28)$$

where $\Delta_R'(E)$ is the derivative of $\Delta_R(E)$ with respect to E. Thus, near resonance, the partial-wave amplitude $a_{\alpha\beta}$ has the denominator (3.28) which can be put into the usual form of resonance denominator,

$$(E-E_r) + i\Delta_I(E_r)/\Delta_R'(E_r) = (E-E_r) + i\Gamma/2 , \qquad (3.29)$$

where Γ is the width of the resonance. The channel in which the resonance occurs is determined by the conditions of $E_r>0$ or ε_2 . If $E_r<0$, then $\Delta_I=0$ (since Δ is real for $E<0$) so that $\Gamma=0$. Hence, there is no resonance below the lowest threshold $E=0$. We can rewrite $a_{\alpha\beta}$ (3.22) with the common resonance denominator (3.29) for $E\approx E_r$,

$$a_{\alpha\beta}(E)\approx r_{\alpha\beta}/[(E-E_r)+i\Gamma/2], \tag{3.30}$$

where

$$r_{\alpha\beta} = n_{\alpha\beta}(E_r)/\Delta'_R(E_r) . \tag{3.31}$$

which may be taken to be real, i.e. principal values of the integrals in $n_{\alpha\beta}$ are taken, since the width Γ is assumed to be small. If $0<E_r<\varepsilon_2$, then, from (3.23), the integrals involving k_1^2 $(=E_r)$ will be complex, while those involving k_2^2 $(=E_r-\varepsilon_2)$ will be real. We can find Γ from Eqs. (3.29), (3.23), (3.22), and (3.31),

$$\Gamma/2 = \Delta_I(E_r)/\Delta'_R(E_r) = -r_{11}\sqrt{E_r} , \tag{3.32}$$

which is the partial width for channel 1. If $E_r > \varepsilon_2 > 0$, then all integrals in (3.23) will be complex, and we find similarly

$$\Gamma/2 = \Delta_I(E_r)/\Delta'_R(E_r) = -r_{11}\sqrt{E_r} - r_{22}\sqrt{E_r - \varepsilon_2} \quad , \quad (3.33)$$

which shows that if both channels are open ($E > \varepsilon_2$), then the total width is the sum of the partial widths for each channel.

Chapter 4. A SOLVABLE MODEL IN NONRELATIVISTIC ELECTRODYNAMICS

In this chapter we shall discuss the interaction of a nonrelativistic charged particle with an electromagnetic field. The charged particle is assumed to be spinless and bound in a nuclear or atomic potential, i.e. it satisfies the ordinary Schrodinger equation. An example is furnished by the electron of a hydrogen atom interacting with an electromegnetic field. We shall limit ourselves to processes involving a single charged particle with the emission or absorption of one photon.

After a description of the model (Section 1.), which is similar to the well-known Lee model, and the discussion of the processes of the interaction, we arrive at the Hamiltonian that will be used throughout this chapter. Our main interest is in the decay behaviour of a prepared state (Section 2.) which leads to the level shift and the line breadth of the emitted photon (Section 3.). We show that the prepared state is physically acceptable (Section 4.). In Section 5, we obtain a complete set of states and give an alternative form for the Hamiltonian, since the results of previous sections are also obtainable by expanding the

prepared state in such a complete set. We conclude this chapter by considering a simple form of spin-dependent interaction in the Hamiltonian.

1. The Hamiltonian

The complete Hamiltonian for a nonrelativistic bound charged particle of zero spin interacting with an electromagnetic field is,[35] ($\hbar = c = 1$)

$$H_{com} = \int[(1/2m)\nabla\psi^*(\vec{r},t)\cdot\nabla\psi(\vec{r},t)+V(\vec{r})\psi^*(\vec{r},t)\psi(\vec{r},t)]d\vec{r}$$

$$+ (1/8\pi)\int[\vec{E}^2(\vec{r},t)+(\nabla\times\vec{A}(\vec{r},t))^2]d\vec{r}$$

$$+ (ie/2m)\int\vec{A}(\vec{r},t)\cdot[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t)-\nabla\psi^*(\vec{r},t)\psi(\vec{r},t)]d\vec{r}$$

$$+ (e^2/2m)\int\vec{A}^2(\vec{r},t)\psi^*(\vec{r},t)\psi(\vec{r},t)d\vec{r} \quad +$$

$$+ (e^2/2)\iint \frac{\psi^*(\vec{r},t)\psi^*(\vec{r}',t)\psi(\vec{r}',t)\psi(\vec{r},t)}{|\vec{r} - \vec{r}'|} \, d\vec{r}d\vec{r}' \, . \tag{4.1}$$

The first term describes the charged particle with mass m bound in a nuclear potential V. The nucleus can be considered fixed (infinitely massive). The second term, where we have used Gaussian units, is the radiation energy of the electromagnetic field. Both $\vec{E}$ and $\vec{A}$ are transverse fields. The third and fourth terms give rise to the interaction between the charged particle and the electromagnetic field. However, the fourth term is much smaller than the third and can produce two-photon processes. The last term is the electrostatic interaction between charges which does not contribute in one-electron processes. Hence, we shall omit the last two terms in the Hamiltonian for our discussion.[36] We shall come back to consider the fourth term in the next chapter.

Let us expand ψ and ψ^* in a complete orthonormal set of eigenfunctions for a single electron in a nuclear potential. The vector field $\vec{A}$ can also be expanded in plane waves with periodic boundary conditions in a box of unit normalization volume. We then have

$$\psi(\vec{r},t) = \sum_n b_n(t)u_n(\vec{r})$$

$$\psi^*(\vec{r},t) = \sum_n b_n^\dagger(t)u_n^*(\vec{r})$$

$$\vec{A}(\vec{r},t) = \sum_\lambda \hat{e}_\lambda\sqrt{2\pi/k_\lambda}(a_\lambda(t)e^{i\vec{k}_\lambda\cdot\vec{r}} + a_\lambda^\dagger(t)e^{-i\vec{k}_\lambda\cdot\vec{r}})$$

$$\vec{E}(\vec{r},t) = -\partial\vec{A}/\partial t = \sum_\lambda i\hat{e}_\lambda\sqrt{2\pi k_\lambda}(a_\lambda(t)e^{i\vec{k}_\lambda\cdot\vec{r}} - a_\lambda^\dagger(t)e^{-i\vec{k}_\lambda\cdot\vec{r}}) \ , \qquad (4.2)$$

where $u_n(r)$ form a complete orthonormal set of eigenfunctions which satisfy the Schrödinger equation

$$(-\nabla^2/2m + V(\vec{r}))u_n(\vec{r}) = E_n u_n(\vec{r}) \quad . \tag{4.3}$$

The photon energy is $k_\lambda = |\vec{k}_\lambda|$ and $\hat{e}_\lambda$ is the unit polarization vector orthogonal to $\vec{k}_\lambda$. The sum over λ includes momentum eigenstates and polarization, different direction of polarization is denoted by different λ . The expansion coefficient $b_n^\dagger$ (b_n) is the creation (annihilation) operator for an electron in the electron eigenstate n. Similarly, $a_\lambda^\dagger$ (a_λ) creates (annihilates) a photon of momentum $\vec{k}_\lambda$, polarization $\hat{e}_\lambda$. The b's and a's satisfy the usual commutation relations,

$$[b_n(t), b_{n'}^\dagger(t)]_+ = b_n(t)b_{n'}^\dagger(t)+b_{n'}^\dagger(t)b_n(t) = \delta_{nn'}$$

$$[a_\lambda(t), a_{\lambda'}^\dagger(t)] = a_\lambda(t)a_{\lambda'}^\dagger(t)-a_{\lambda'}^\dagger(t)a_\lambda(t) = \delta_{\lambda\lambda'}$$

$$[b_n(t), b_{n'}(t)]_+ = [b_n^\dagger(t), b_{n'}^\dagger(t)]_+ = 0$$

$$[a_\lambda(t),a_{\lambda'}(t)] = [a_\lambda^\dagger(t),a_{\lambda'}^\dagger(t)] = 0$$

$$[a_\lambda(t),b_n(t)] = [a_\lambda(t),b_n^\dagger(t)] = [a_\lambda^\dagger(t),b_n(t)] = [a_\lambda^\dagger(t),b_n^\dagger(t)] = 0.$$

(4.4)

We further assume that there are only two energy levels in (4.3), or only two eigenstates contribute significantly to the interaction, the higher level E_2 and the lower level E_1, e.g. we can take two bound states in the hydrogen atom. If we are restricted to processes of the following type:

One electron in level 2↔one electron in level 1 + one photon

(4.5)

as indicated at the beginning of this chapter, we will obtain a simple Hamiltonian by substituting (4.2) into (4.1), (ignoring last two terms in (4.1))

$$H = H_0 + H_1$$

where

$$H_0 = E_2 b_2^\dagger(t) b_2(t) + E_1 b_1^\dagger(t) b_1(t) + \sum_\lambda k_\lambda a_\lambda^\dagger(t) a_\lambda(t)$$

and

$$H_1 = e\sum_\lambda (1/\sqrt{2k_\lambda})(\beta_\lambda b_2^\dagger(t) b_1(t) a_\lambda(t) + \beta_\lambda^* b_1^\dagger(t) a_\lambda^\dagger(t) b_2(t)) \ . \qquad (4.6)$$

The infinite zero-point energy of the radiation field, $\sum k_\lambda /2$, has been subtracted. The quantities β_λ are given by

$$\beta_\lambda = (i\sqrt{4\pi/m}) \int u_2^*(\vec{r}) e^{i\vec{k}_\lambda \cdot \vec{r}} \hat{e}_\lambda \cdot \nabla u_1(\vec{r}) d\vec{r} \ , \qquad (4.7)$$

which are essentially the one-photon interaction matrix elements (p.143, Heitler)[11].

The Hamiltonian, as given in (4.6), is in Heisenberg representation since the a's and b's are time-dependent operators. We can transform (4.6) into Schrödinger representation which coincides with Heisenberg representation at a particular time $t = 0$. The transformation of operators is achieved by

$$O(t) = e^{iHt}\, O(t=0)\, e^{-iHt} \quad . \tag{4.8}$$

Hence, the Hamiltonian in Schrödinger representation has the same form as (4.6) but with the a's and b's specified at $t = 0$ which we shall simple rewrite omitting the time parameter. In the following sections the Hamiltonian in Schrodinger representation will be used, since we shall try to solve the time-dependent Schrödinger equation for a prepared state of our physical system. The Hamiltonian (4.6) is very similar to that of the Lee model[10,37-41], except that we do not have to introduce a "cutoff" for the interaction energy, since β_λ, as defined in Eq. (4.7) will provide a natural cutoff for all integrals involved.

So far we have not really specified the two levels of the bound electron (4.3). If those two levels are two discrete states of an electron in an atom, then Hamiltonian (4.6) describes radiative transitions between two discrete states by emission or absorption of one photon. Generalization to transitions of an atom, or nucleus, from any state of higher to one of lower energy can be easily carried out. We can choose the appropriate wave functions

for those two states, either or both of which may be in the discrete or in the continuous energy spectrum. Hence, for atoms, the photoeffect, the radiative capture, (discrete $\leftrightarrow$ continuous transitions) and Bremsstrahlung (continuous $\leftrightarrow$ continuous transitions) can be studied along the same lines. Similarly for nuclear photoeffect and γ-decay of nuclear levels, but the wave functions for the charged particle in a nuclear field (not necessarily Coulomb potential) will be very complicated or simply unobtainable since the behaviour of nuclear forces for very short ranges is not known.

2. The Development of a Prepared State

We will be using Hamiltonian (4.6) in Schrödinger representation. Let us first define a vacuum state $|0\rangle$ for our system, i.e. a state with no electron and photon present,

$$b_2|0\rangle = b_1|0\rangle = a_\lambda|0\rangle = 0 \ , \tag{4.9}$$

which is also an eigenstate of (4.6) with eigenvalue zero. This vacuum state is, therefore, time-independent and we can build up the states we want for our system by applying

a's and b's to it.

Suppose that we prepare our system at $t = 0$ to be at the higher level 2 with no photon, i.e. in the initial state

$$\Psi(0) = b_2^\dagger |0\rangle \ , \tag{4.10}$$

and we shall study its subsequent development due to the Hamiltonian (4.6). At a later time $t > 0$, our system will be in the state $\Psi(t)$ which is governed by the time-dependent Schrödinger equation,

$$i\partial\Psi(t)/\partial t = H\Psi(t) \ , \tag{4.11}$$

where H is the Hamiltonian operator (4.6). The formal solution of the time-dependent wave function $\Psi(t)$ has the explicit form

$$\Psi(t) = e^{-iHt}\Psi(0) \ , \tag{4.12}$$

which satisfies the specified boundary condition (4.10) at $t = 0$. For $t > 0$, we can rewrite (4.12) as[42]

$$\Psi(t) = (-1/2\pi i)\int_{-\infty}^{+\infty} \frac{dE e^{-iEt}}{E+i\varepsilon-H}\,\Psi(0), \tag{4.13}$$

where $\varepsilon \to 0(+)$ and E is a real variable.

Our main problem now is to find the quantity

$$\frac{1}{E+i\varepsilon-H}\,\Psi(0) = \frac{1}{E+i\varepsilon-H}\,b_2^{\dagger}|0\rangle\ . \tag{4.14}$$

Using the identity, valid for operators as well as c-numbers,

$$\frac{1}{a+b} = \frac{1}{a} - \frac{1}{a+b}b\frac{1}{a}\ , \tag{4.15}$$

and putting $a = E + i\varepsilon - H_0$, $b = -H_1$, we can write (4.14) as

$$\frac{1}{E+i\varepsilon-H} b_2^\dagger|0\rangle = \frac{1}{E+i\varepsilon-E_2} (b_2^\dagger|0\rangle + e\sum_\lambda \frac{\beta_\lambda^*}{(2k_\lambda)^{1/2}} \frac{1}{E+i\varepsilon-H} b_1^\dagger a_\lambda^\dagger|0\rangle) .$$

(4.16)

Using a formula in Schweber p. 359 [43],

$$\frac{1}{E+i\varepsilon-H} a_\lambda^\dagger = a_\lambda^\dagger \frac{1}{E+i\varepsilon-H-k_\lambda} + \frac{1}{E+i\varepsilon-H} [H_1, a_\lambda^\dagger] \frac{1}{E+i\varepsilon-H-k_\lambda} ,$$

(4.17)

we obtain

$$\frac{1}{E+i\varepsilon-H} b_1^\dagger a_\lambda^\dagger|0\rangle = \frac{1}{E+i\varepsilon-E_1-k_\lambda} (b_1^\dagger a_\lambda^\dagger|0\rangle + \frac{e\beta_\lambda}{\sqrt{2k_\lambda}} \frac{1}{E+i\varepsilon-H} b_2^\dagger|0\rangle) .$$

(4.18)

Substituting (4.18) into (4.16), we finally get

$$\frac{1}{E+i\varepsilon-H}\, b_2^\dagger|0\rangle = (E+i\varepsilon-E_2+e^2 \sum_\lambda \frac{|\beta_\lambda|^2}{2k_\lambda} \frac{1}{k_\lambda+E_1-E-i\varepsilon})^{-1} \times$$

$$(b_2^\dagger|0\rangle - e\sum_{\lambda'} \frac{\beta^*_{\lambda'}}{\sqrt{2k_{\lambda'}}} \frac{1}{k_{\lambda'}+E_1-E-i\varepsilon}\, b_1^\dagger a_{\lambda'}^\dagger|0\rangle) \,. \tag{4.19}$$

Eq. (4.13) together with the above expression determines the complete behaviour of our system which was prepared in the state $\Psi(0)$ at $t = 0$.

We are mostly interested in the probability of finding the system in its initial state after time t. The probability amplitude for the system remaining in $\Psi(0)$ at a later time t is given by

$$\langle\Psi(0)|\Psi(t)\rangle = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} \frac{dE\ e^{-iEt}}{E+i\varepsilon-E_2+e^2\sum_{\lambda}\frac{|\bar{\beta}_{\lambda}|^2}{2k_{\lambda}}\frac{1}{k_{\lambda}+E_1-E-i\varepsilon}} \quad .$$

(4.20)

In the denominator, the sum over λ (including sum over two directions of polarization) can be written as an integral when the normalization volume tends to infinity.

$$f(E-E_1+i\varepsilon) = \frac{e^2}{2\pi^2}\int_0^{\infty}\frac{|\beta(k)|^2kdk}{k+E_1-E-i\varepsilon}$$

$$= \frac{e^2}{2\pi^2}\,P\int_0^{\infty}\frac{|\beta(k)|^2kdk}{k+E_1-E} + i\frac{e^2}{2\pi}\,|\beta(E-E_1)|^2(E-E_1)\ ,$$

(4.21)

which is defined for real E. We have assumed that β_λ does not depend on the direction of the momentum vector $\vec{k}_\lambda$ but only on its magnitude $|\vec{k}_\lambda|$. The symbol P stands for the principal value of the integral. Let us write down the denominator in (4.20) as

$$h(E-E_1-i\varepsilon) = E+i\varepsilon-E_2+f(E-E_1+i\varepsilon) \ , \tag{4.22}$$

which is also defined for real E, and can be analytically continued for a general complex E provided that the same can be done for $|\beta(k)|^2$.[39]

Let us define a complex variable

$$z = E - E_1 = x + iy \ , \tag{4.23}$$

where E is now complex, and E_1 is real, the lower energy level. On the first Riemann sheet, for $0 < \arg(z) < 2\pi$.

$$h^I(z) = z + E_1 - E_2 + f(z) \ , \tag{4.24}$$

which has a cut along the positive real axis as can be easily seen from (4.21) and (4.22). Integral (4.20) may be obtained by the following contour integration on the first Riemann sheet:

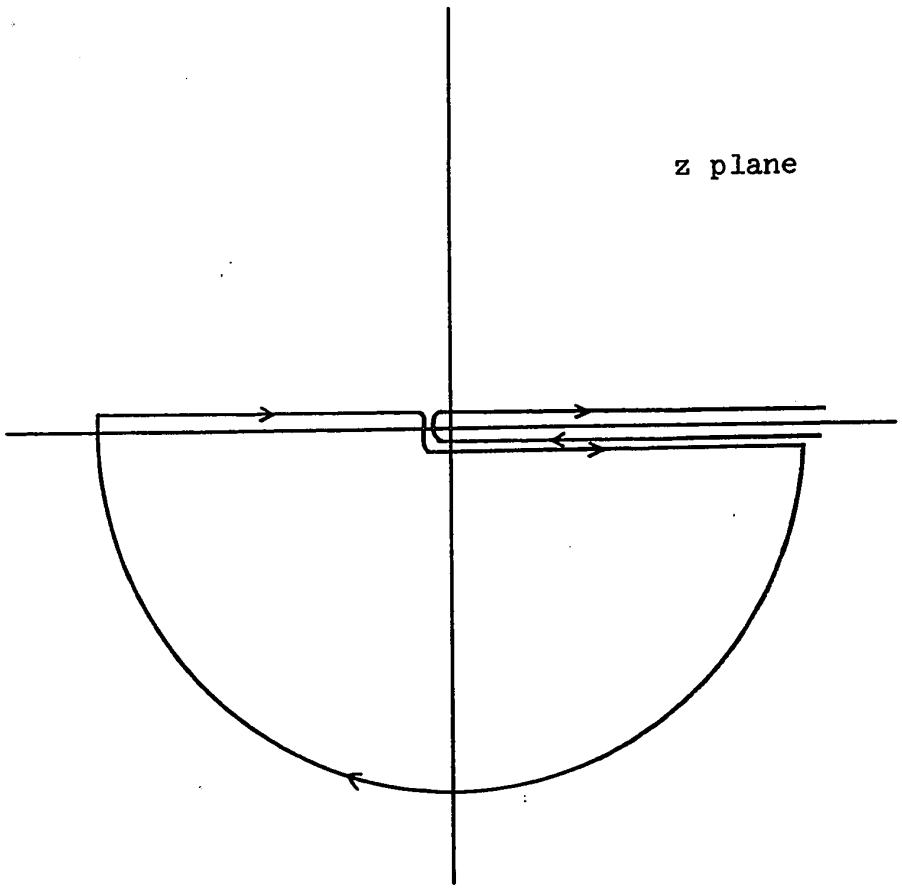

Fig. 1. Contour for Integral (4.20) Closed on the First Sheet.

We, therefore, must find the roots of $h^I(z)$ in the lower half plane, excluding the cut. A simple substitution of $z = x + iy$ into $h^I(z) = 0$ will require

$$y = 0$$

and

$$x = E_2 - E_1 - (e^2/2\pi^2)\int_0^\infty |\beta(k)|^2 k dk/(k-x) \tag{4.25}$$

for $x < 0$. Eq. (4.25) has no solution below $x = 0$, if

$$E_2 - E_1 > (e^2/2\pi^2)\int_0^\infty |\beta(k)|^2 dk \ , \tag{4.26}$$

which we shall assume E_2 and E_1 satisfy. We expect that the behaviour of (4.20) is some kind of damped exponential which arises from a complex root of the denominator with negative imaginary part. Hence, we search further onto the second Riemann sheet.

Analytic continuation onto the second Riemann sheet, for $0 > \arg(z) > -2\pi$, is effected by defining for real $z\ (= x)$,

$$h^{II}(x - i\varepsilon) = h^I(x + i\varepsilon) \ . \tag{4.27}$$

Then, for $z = x + iy$, we have[39]

$$h^{II}(z) = h^{I}(z) + i(e^2/\pi)|\beta(z)|^2 z \ . \qquad (4.28)$$

Now we can evaluate integral (4.20) by closing the contour on the second Riemann sheet as shown in Fig. 2.[39]

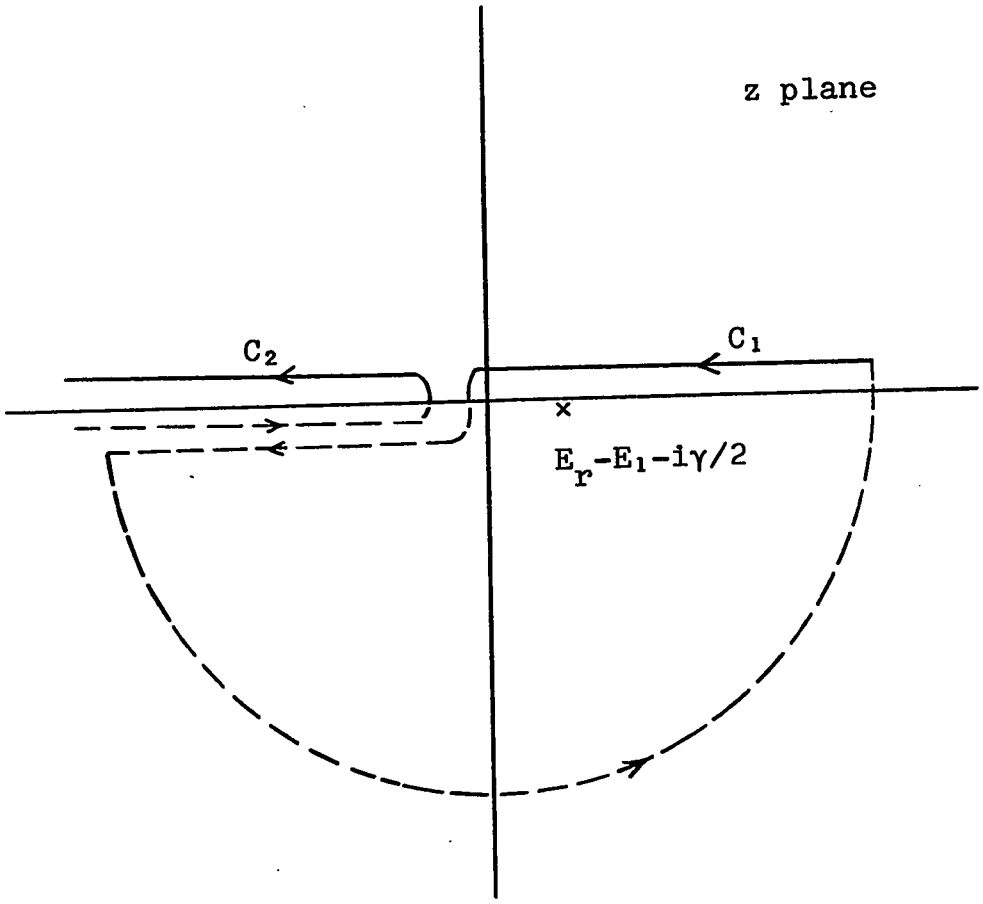

Fig. 2. Contour for Integral (4.20) Closed on the Second Sheet.

The solid portion of the contour is on the first Riemann sheet while the dotted portion is on the second. The integral of the closed contour C_1 can be obtained from Cauchy's integral formula, so we must find the zeros in $h^{II}(z)$. Assuming for simplicity that $h^{II}(z)$ has only one solution, i.e. the integrand in (4.20) has a simple pole, at $z = (E_r - E_1) - i\,\gamma/2$, then from (4.28), (4.24), and (4.21) we obtain the determining equations for E_r and γ,[38]

$$E_r - E_2 + \frac{e^2}{2\pi^2}\int_0^\infty \frac{|\beta(k)|^2 k\,dk}{(k+E_1-E_r)^2+\gamma^2/4}(k+E_1-E_r) - \frac{e^2}{\pi}\eta = 0$$

$$\frac{\gamma}{2}\left(1+\frac{e^2}{2\pi^2}\int_0^\infty \frac{|\beta(k)|^2 k\,dk}{(k+E_1-E_r)^2+\gamma^2/4}\right) - \frac{e^2}{\pi}\zeta = 0\,, \qquad (4.29)$$

where

$$\zeta + i\eta \equiv |\beta(E_r - E_1 - i\gamma/2)|^2 (E_r - E_1 - i\gamma/2) \ . \qquad (4.30)$$

Integral (4.20) can be written as contour integrals

$$\langle \Psi(0) | \Psi(t) \rangle = \frac{e^{-iE_1 t}}{2\pi i} \left(\int_{C_1} + \int_{C_2} \right) \frac{dz e^{-izt}}{h(z)} \ , \qquad (4.31)$$

where C_1 and C_2 are shown in Fig. 2. The denominator $h(z)$ will be either $h^{I}(z)$ or $h^{II}(z)$ depending on whether the contour is on the first or on the second Riemann sheet. The integrals over C_1 and C_2 are then,

$$\frac{e^{-iE_1 t}}{2\pi i} \int_{C_1} \frac{dz e^{-izt}}{h^{II}(z)} = \frac{e^{-iE_r t - \gamma t/2}}{(dh^{II}(z)/dz)_{z=E_r - E_1 - i\gamma/2}}$$

and

$$\frac{e^{-iE_1t}}{2\pi i}\int_{C_2}\frac{dz\ e^{-izt}}{h(z)} = \frac{e^{-iE_1t}}{2\pi i}\left(\int_{-\infty}^{0}\frac{dx\ e^{-ixt}}{h^{II}(x)} + \int_{0}^{-\infty}\frac{dx\ e^{-ixt}}{h^{I}(x)}\right)$$

$$= \frac{-e^2}{2\pi^2}\int_{-\infty}^{0} dx e^{-ixt}\left[\frac{|\beta(x)|^2}{h^{I}(x)h^{II}(x)}\right] xe^{-iE_1t}\ ,$$

(4.32)

where we have used (4.28) with $z = x$ (real) for the integral over C_2. On comparing the above two integrals, we see that for weak coupling and not too large t the first one dominates while the second one will only become appreciable after a sufficiently long time. However, by this time (4.31) may have already become extremely small indeed. As t tends to infinity the behaviour of the second integral in (4.32) is determined by the "critical

point" at $x = 0$ [44], which means that most contribution comes from the end point $x = 0$. We can obtain the asymptotic expansion for the second integral by expanding the square bracket about $x = 0$,

$$\left[\frac{|\beta(x)|^2}{h^{I}(x)h^{II}(x)}\right] \approx [\cdots\cdots]_{x=0} + x\frac{d}{dx}[\cdots\cdot]_{x=0} + \cdots\cdot , \tag{4.33}$$

and by inserting the above expansion into the integral which can then be evaluated at $x = 0$ to yield

$$\int_{C_2} \underset{t\to\infty}{\sim} \frac{-e^2}{2\pi^2} \frac{|\beta(0)|^2}{h^{I}(0)h^{II}(0)} \frac{e^{-iE_1 t}}{t^2} + O(t^{-3}) . \tag{4.34}$$

The manner in which (4.34) is obtained tells us that the asymptotic behaviour of the probalility amplitude depends on the dynamic structure of the system and on how one prepares the initial state[40]. For example, if we start with the system in the initial state

$$\Psi(0) = \sum_{\lambda} \phi_{\lambda} b_1^{\dagger} a_{\lambda}^{\dagger} |0\rangle \ , \tag{4.35}$$

which describes an electron in level 1 plus a packet of photons of arbitrary shape ϕ_{λ}. A similar calculation will give the exponential form for small t, and for large t an integral over C_2, which is dominated by the contribution from $x = 0$,

$$\frac{1}{2\pi i}\int_{C_2} dz e^{-izt} \left|\sum_{\lambda} \frac{e}{\sqrt{2k_{\lambda}}} \frac{\phi_{\lambda}\beta_{\lambda}}{k_{\lambda}-z}\right|^2 \frac{e^{-iE_1 t}}{h(z)}$$

$$= \frac{-e^2}{2\pi^2}\int_{-\infty}^{0} dx e^{-ixt} \left[\left|\sum_{\lambda} \frac{e}{\sqrt{2k_{\lambda}}} \frac{\phi_{\lambda}\beta_{\lambda}}{k_{\lambda}-x}\right|^2 \frac{|\beta(x)|^2}{h^{I}(x)h^{II}(x)}\right] x e^{-iE_1 t} \ . \tag{4.36}$$

Again, we expand the square bracket about $x = 0$, like (4.33)

$$[\,|\sum_{\lambda}\frac{e}{\sqrt{2k_\lambda}}\,\frac{\phi_\lambda\beta_\lambda}{k_\lambda - x}|^2\,\frac{|\beta(x)|^2}{h^{I}(x)h^{II}(x)}] \approx [\cdots]_{x=0} + x\frac{d}{dx}[\cdots]_{x=0} + \cdots \quad , \tag{4.37}$$

where ϕ_λ is the arbitrary shape of the wave packet that we prepare our system at $t = 0$. This means that we can pick the leading term in t for the asymptotic expansion of (4.36) by choosing suitable ϕ_λ ; e.g. if the first term in (4.37) vanishes for a particular choice of ϕ_λ , then

$$\text{Eq. (4.36)} \overset{t\to\infty}{\sim} \text{constant}(e^{-iE_1 t}t^{-3}) + O(t^{-4}) \quad , \tag{4.38}$$

which has a leading term t^{-3} instead of t^{-2} as was in (4.34).

Let us come back to the time evolution of our system. The probability of finding the system in the initial state at time t is represented by $|\langle\Psi(0)|\Psi(t)\rangle|^2$. We can, therefore, conclude from (4.31). (4.32). and (4.34) that this probability decreases exponentially with lifetime $1/\gamma$ for small t ($\approx 1/\gamma$), and ultimately decays as t^{-4}. However, one must note that the preparation of the initial state affects greatly the asymptotic behaviour of the above mentioned probability.

3. Level Shift and Line Breadth

The complex root $z = E_r - E_1 - i\gamma/2$ for $h^{II}(z)$ as determined by (4.29) has simple physical interpretation. Let us first look at the weak coupling limit in which e^2 is very small, $E_r \approx E_2$, and $E_r - E_1 >> \gamma/2 \approx O(e^2)$. In this limit we can solve for E_r and γ without knowing the exact form of $\beta(k)$. From (4.29) and (4.30) then,

$$\zeta \approx |\beta(E_2-E_1)|^2(E_2-E_1)$$

$$\eta \approx 0 \ ,$$

and therefore,

$$E_r - E_2 \equiv \Delta E \approx \frac{-e^2}{2\pi^2} P \int_0^\infty \frac{|\beta(k)|^2 k dk}{k+E_1-E_2}$$

$$\gamma \approx (e^2/\pi)|\beta(E_2-E_1)|^2(E_2-E_1) \ . \qquad (4.39)$$

The results for ΔE and γ agree with that by first order time-dependent perturbation calculation for the level shift and the line breadth respectively.[11(§18)] When the electron at level 2 decays spontaneously to level 1 with the emission of a photon, the spectral line of the emitted photon will have a maximum at frequency = $E_r - E_1$ with a half width γ, instead of a perfectly sharp line with frequency = $E_2 - E_1$. Or one may say that when the electron at level 2 interacts with an electromagnetic field according to (4.6), its original level E_2 will shift to E_r with a breadth γ, i.e. it has lifetime of $1/\gamma$ due to the radiative transition to the lower level 1. Eq. (4.39) also

gives the correct behaviour of our system when there is no interaction ($e^2 = 0$), such that $\Delta E = \gamma = 0$. In this case the electron will remain at level 2 indefinitely, since it is an eigenstate of the Hamiltonian when $e^2 = 0$.

Suppose we can increase the coupling strength e^2 between the bound electron and the electromagnetic field without affecting the other part of our system, i.e. E_2 , E_1 , and $\beta(k)$ will not change if e^2 changes. A look at the second equation of (4.29) will show us that there is another solution for $\gamma = 0$ with $e^2 \neq 0$. If such a solution exists for a certain $e^2 = e_s^2$, then we would have an emitted photon with a perfectly sharp spectral line. This solution will require $\zeta = 0$ which implies $E_r = E_1$. When this condition is applied to the first equation of (4.29), we find that E_1 and E_2 must satisfy

$$E_1 - E_2 = (-e_s^2/2\pi^2) \int_0^\infty |\beta(k)|^2 dk \ , \qquad (4.40)$$

which is the equation that determines e_s^2 . However, in order to obtain (4.29) such that the electron at level 2 can decay spontaneously, we had already assumed that E_1 and E_2 must fulfil the inequality (4.26) which holds for all values of e^2 . Eq. (4.40) is, therefore, invalid, and there is no emitted photon with perfectly sharp line. Let us suppose for the moment that $e^2 \rightarrow e_s^2$ without the above contradiction, can e^2 be increased further still? If E_r and γ are both continuous functions of e^2 , when e^2 increases from 0 to e_s^2 , E_r decreases from E_2 to E_1 and γ from 0 back to 0. So if $e^2 > e_s^2$, $E_r = E_1 - \delta E$ where δE is a small positive energy. Substitution of $E_r = E_1 - \delta E$ into the second equation of (4.29) will yield a negative γ which means $\langle \Psi(0) | \Psi(t) \rangle$ grows indefinitely, and hence not acceptable.

We conclude this section by remarking that we cannot increase the coupling parameter e^2 infinitely even if it does not affect the other structure of the system. The exact form of $\beta(k)$ must be specified if we want to find the exact solutions for E_r and γ .

4. The Mean Energy and the Rate of Energy Dissipation for the Initial State

We have prepared our system at $t = 0$ in the initial state (4.10) which evolves according to the time-dependent Schrödinger equation (4.11). We have also studied the decay behaviour of the system in Section 2. In this section, we want to show that the initial state (4.10) for our system is physically acceptable.

The mean energy and the rate of energy dissipation for an acceptable state should be expected to be finite. Otherwise we cannot simply prepare at $t = 0$ such a state of infinite energy or a state of finite energy but with infinite time derivative. In the latter case the initial state jumps discontinuously into another state and thus $\Psi(t)$ is no longer a continuous function of t as described by (4.11). The mean energy of the initial state $\Psi(0)$ is determined by $\langle \Psi(0)|H|\Psi(0)\rangle$ where $\Psi(0)$ and H are given by (4.10) and (4.6) respectively. A simple calculation will yield the result

$$\langle \Psi(0)|H|\Psi(0)\rangle = E_2 \ , \tag{4.41}$$

which is just the bound state energy of the electron at level 2 and has a finite value. The rate of energy dissipation for $\Psi(0)$ at $t = 0$ is proportional to the expectation value of H^2 in the initial state,

$$\langle\Psi(0)|H^2|\Psi(0)\rangle = (E_2)^2 + e^2\sum_{\lambda}|\beta_\lambda|^2/(2k_\lambda) \ , \qquad (4.42)$$

by a similar calculation as (4.41). The first term in (4.42) is again finite. The second term is also finite with β_λ given by (4.7) which will provide the necessary converging factor in the sum. We have demonstrated that $\Psi(0)$ for our system is physically acceptable and its subsequent decay is exponential for small t, and for large t asymptotically in inverse powers of t.

We should mention here that all results obtained so far, (4.20) in particular, can also be derived by expanding the initial state in terms of a certain complete set of eigenstates of the Hamiltonian (4.6), providing E_1 and E_2 satisfy condition (4.26). In the next section we shall obtain this complete set of eigenstates.

5. A Complete Orthonormal Set of Eigenstates of the Hamiltonian and An Alternative Form for the Hamiltonian

We construct here a certain complete orthonormal set of eigenstates of the Hamiltonian (4.6) in the subspace spanned by $b_2^\dagger|0\rangle$ and $b_1^\dagger a_\lambda^\dagger|0\rangle$.[37] These eigenstates are solutions of the Schrödinger equation

$$H|1,\lambda\rangle = (E_1+k_\lambda)|1,\lambda\rangle \ , \tag{4.43}$$

where $|1,\lambda\rangle$ are the eigenstates which are states describing the scattering of a photon by the electron in level 1. we can write $|1,\lambda\rangle$ as the electron wave function in level 1 plus an incoming plane wave of a photon, $b_1^\dagger a_\lambda^\dagger|0\rangle$, and an outgoing scattered wave $|\chi\rangle$, then

$$|1,\lambda\rangle = b_1^\dagger a_\lambda^\dagger|0\rangle + |\chi\rangle \ . \tag{4.44}$$

Substitution of (4.6) and (4.44) into (4.43) yields the solution for the outgoing scattered wave

$$|\chi\rangle = \frac{e\beta_\lambda}{\sqrt{2k_\lambda}} \frac{1}{E_1+k_\lambda-H+i\varepsilon} b_2^\dagger|0\rangle \ . \tag{4.45}$$

The operation of $(E_1 + k_\lambda - H + i\varepsilon)^{-1}$ on $b_2^\dagger|0\rangle$ is given by (4.19), so we obtain finally,

$$|1,\lambda\rangle = b_1^\dagger a_\lambda^\dagger|0\rangle + \frac{e\beta_\lambda}{\sqrt{2k_\lambda}}\left(E_1+k_\lambda+i\varepsilon-E_2+e^2\sum_{\lambda'}\frac{|\beta_{\lambda'}|^2}{2k_{\lambda'}}\frac{1}{k_{\lambda'}-k_\lambda-i\varepsilon}\right)^{-1}\times$$

$$\left(b_2^\dagger|0\rangle - e\sum_{\lambda''}\frac{\beta^*_{\lambda''}}{\sqrt{2k_{\lambda''}}}\frac{b_1^\dagger a_{\lambda''}^\dagger|0\rangle}{k_{\lambda''}-k_\lambda-i\varepsilon}\right) . \qquad (4.46)$$

The proof that $|1,\lambda\rangle$ form a complete orthonormal set in the subspace mentioned at the beginning, namely

$$\sum_\lambda |1,\lambda\rangle\langle\lambda,1| = \sum_\lambda b_1^\dagger a_\lambda^\dagger|0\rangle\langle 0|a_\lambda b_1 + b_2^\dagger|0\rangle\langle 0|b_2$$

$$\langle\lambda,1|1,\lambda'\rangle = \delta_{\lambda\lambda'} \quad , \qquad (4.47)$$

is the same as given by Glaser and Källén[37], where we have the occasion to evoke the inequality (4.26).

Next we shall write an alternative form for the Hamiltonian which is quadratic in oprators and is very similar to Henley's[45]. We note in the subspace that we have considered the Hamiltonian will be operating on $b_2^\dagger|0\rangle$ and $b_1^\dagger|0\rangle$ (plus a packet of photon). From the type of allowed transitions (4.5), we would like to have operators that change $b_2^\dagger|0\rangle$ to $b_1^\dagger|0\rangle$ and vice versa. Let us define new operators T_+ and $T_- = T_+^\dagger$ that possess the desired property,

$$T_+ = b_1^\dagger b_2 \ , \text{ and } \ T_- = b_2^\dagger b_1 \ , \tag{4.48}$$

such that

$$T_+(b_2^\dagger|0\rangle) = b_1^\dagger|0\rangle \ , \quad T_+(b_1^\dagger|0\rangle) = 0 \ ,$$

$$T_-(b_2^\dagger|0\rangle) = 0 \ , \quad T_-(b_1^\dagger|0\rangle) = b_2^\dagger|0\rangle \ . \tag{4.49}$$

The commutator of T_+ and T_- is defined as

$$T_3 = [T_+, T_-] = b_1^\dagger b_1 - b_2^\dagger b_2 \ , \qquad (4.50)$$

which has the following property

$$T_3(b_2^\dagger|0\rangle) = -b_2^\dagger|0\rangle \ , \quad T_3(b_1^\dagger|0\rangle) = b_1^\dagger|0\rangle \ . \qquad (4.51)$$

In our particular subspace spanned by $b_2^\dagger|0\rangle$ and $b_1^\dagger a_\lambda^\dagger|0\rangle$, the operator $(b_1^\dagger b_1 + b_2^\dagger b_2)$ has eigenvalue 1, so we can write

$$b_2^\dagger b_2 = (1-T_3)/2 \ , \quad b_1^\dagger b_1 = (1+T_3)/2 \ . \qquad (4.52)$$

Substitution of (4.48) and (4.52) into (4.6) yields the result for the Hamiltonian

$$H = (E_2+E_1)/2 - (E_2-E_1)T_3/2 + \sum_\lambda k_\lambda a_\lambda^\dagger a_\lambda$$

$$+ e\sum_\lambda (2k_\lambda)^{-\frac{1}{2}} (\beta_\lambda a_\lambda T_- + \beta_\lambda^* a_\lambda^\dagger T_+) \ , \qquad (4.53)$$

which is meaningful only in the special subspace concerned.

6. Spin-Dependent Interaction

The interaction between electron spin and the radiation field will modify the Hamiltonian (4.1), and an additional term,

$$H_{sp} = (-e/2m)\int \psi^*(\vec{r},t)\vec{\sigma}\cdot\vec{H}(\vec{r},t)\psi(\vec{r},t)d\vec{r}$$

$$= (-e/2m)\int \psi^*(\vec{r},t)\vec{\sigma}\cdot(\nabla\times\vec{A}(\vec{r},t))\psi(\vec{r},t)d\vec{r} \quad , \qquad (4.54)$$

should be added to (4.1). In this equation $\vec{\sigma}$ is the usual Pauli spin matrix. The spin-orbit interaction is neglected in the nonrelativistic limit. However, the contribution from H_{sp} is still extremely small in causing transitions when compared with the third term in (4.1), unless the third term is highly forbidden for a certain kind of transition. We are interested in H_{sp} mainly because it is linear in $\vec{A}$ and thus involves processes of one photon which may be combined with the third term.

A similar expansion for the first three terms in

(4.1) and H_{Sp} can be carried out as before but with ψ now being a two-component field,

$$\psi(\vec{r},t) = \sum_n \begin{pmatrix} b_{n+}(t) \\ b_{n-}(t) \end{pmatrix} u_n(\vec{r}) \ , \tag{4.55}$$

where $u_n(r)$ are eigenfunctions of (4.3). Operators b_{n+} and b_{n-} are annihilation operators for an electron in state n with spin up and spin down respectively. For simplicity, the magnetic field $\vec{H}$ is assumed to be polarized in the z direction, i.e. the electromagnetic vector potential $\vec{A}$ is propagated in the x direction and polarized in the y direction, so we obtain

$$\vec{H}(\vec{r},t) = \nabla\times\vec{A}(\vec{r},t) = \sum_\lambda i\sqrt{2\pi k_\lambda}\hat{z}(a_\lambda(t)e^{i\vec{k}_\lambda\cdot\vec{r}} - a_\lambda^\dagger(t)e^{-i\vec{k}_\lambda\cdot\vec{r}}) \ , \tag{4.56}$$

where $\hat{z}$ is a unit vector in the z direction. Note that sum over λ here, and what follows in this section, sums over momentum eigenstates only, since there is only one direction of polarization, the y direction. Then

$$\vec{\sigma}\cdot(\nabla\times\vec{A}) = \sum_{\lambda} i\sqrt{2\pi k_\lambda}\,\left(a_\lambda(t)e^{i\vec{k}_\lambda\cdot\vec{r}} - a_\lambda^\dagger(t)e^{-i\vec{k}_\lambda\cdot\vec{r}}\right)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{4.57}$$

If we again consider a two-level system with allowed transitions of the type (4.5), a similar Hamiltonian as (4.6) can be obtained in Schrödinger representation,

$$\begin{aligned} H = {} & E_2(b_{2_+}^\dagger b_{2_+} + b_{2_-}^\dagger b_{2_-}) + E_1(b_{1_+}^\dagger b_{1_+} + b_{1_-}^\dagger b_{1_-}) + \sum_\lambda k_\lambda a_\lambda^\dagger a_\lambda \\ & + e\sum_\lambda (1/\sqrt{2k_\lambda})(\beta_\lambda(b_{2_+}^\dagger b_{1_+} + b_{2_-}^\dagger b_{1_-})a_\lambda + \beta_\lambda^*(b_{1_+}^\dagger b_{2_+} + b_{1_-}^\dagger b_{2_-})a_\lambda^\dagger) \\ & + e\sum_\lambda (1/\sqrt{2k_\lambda})(\alpha_\lambda(b_{2_+}^\dagger b_{1_+} - b_{2_-}^\dagger b_{1_-})a_\lambda + \alpha_\lambda^*(b_{1_+}^\dagger b_{2_+} - b_{1_-}^\dagger b_{2_-})a_\lambda^\dagger)\,, \end{aligned} \tag{4.58}$$

where β_λ are given by (4.7), and

$$\alpha_\lambda = (-i\sqrt{\pi}k_\lambda/m)\int u_2^*(\vec{r})e^{i\vec{k}_\lambda\cdot\vec{r}}u_1(\vec{r})d\vec{r} \ . \qquad (4.59)$$

Operators a_λ and $b_{n\pm}$ obey the commutation relations (4.4) with the addition that operators of different spin commute. The development of a prepared state like (4.10), $\Psi(0) = b_{2+}^\dagger|0\rangle$, can be analysed following the same procedures as before and similar results obtained. For example, the probability amplitude at time t of finding the system in the initial state $b_{2+}^\dagger|0\rangle$ is given by

$$\langle\Psi(0)|\Psi(t)\rangle = \frac{-1}{2\pi i}\int_{-\infty}^{\infty}\frac{dEe^{-iEt}}{E+i\varepsilon-E_2+e^2\sum_\lambda\frac{|\beta_\lambda+\alpha_\lambda|^2}{2k_\lambda}\frac{1}{k_\lambda+E_1-E-i\varepsilon}} \ , \qquad (4.60)$$

which can be compared with (4.20) and discussed in the same way.

Chapter 5. APPROXIMATION FOR THE $\vec{A}^2$ TERM IN THE HAMILTONIAN

It was mentioned in Section 1 of last chapter that we shall return to study the $\vec{A}^2$ term in the Hamiltonian (4.1). We can see from expansion (4.2) for $\vec{A}^2$ that this term will connect states, initial, final, or intermediate, that differ by two or no photons. In Section 1, we make the approximation, valid for small t, which is equivalent to fixing the number of electrons at $t = 0$ in our system. This approximate H_2 is then treated together with H_{rad}, Eq. (5.7), classically by canonical transformations to yield a diagonalized form which, in turn, is quantized (Appendix). The quantized expression (A.13) contains a new zero-point energy which is different from the original zero-point energy of the radiation field. Only when the coupling strength e^2 vanishes identically, are these two zero-point energies equal, since H_2 will also vanish identically. The old creation or annihilation operator for the photon will be transformed into an infinite sum of new creation and annihilation operators. This implies that a "free" photon corresponds to a superposition of "transformed" photons (Section 2). Section 3 deals with the "physical" and the "bare" vacua for the photon and the possibility of preparing our system at $t = 0$ in terms of the bare vacuum. If one can switch

off H_2 initially, one is led strongly to the idea that an initial state can be built up from the bare vacuum. Under very special assumptions, that both (5.15) and (5.19) are finite, this idea is indeed possible. However, we would rather take the usual notion in quantum field theory that one should not and cannot separate out a bare particle from the physical particles. So a physically acceptable state can only be prepared from the physical vacuum.

1. The Approximation

The $\vec{A}^2$ term in (4.1) is given by

$$(e^2/2m)\int \vec{A}^2(\vec{r},t)\psi^*(\vec{r},t)\psi(\vec{r},t)d\vec{r} \ , \tag{5.1}$$

where $\vec{A}$ is the electromagnetic field and ψ the field for the bound electron. Our approximation is to replace

$$|\psi(\vec{r},t)|^2 \approx |\psi(\vec{r},0)|^2 \ , \tag{5.2}$$

which is no longer the dynamical operator but a real form factor, e.g. the charge distribution for the bound electron at $t = 0$. This approximation is valid for small t and we shall be mainly interested in studying the behaviour of our system at small t. The charge distribution may be normalized,

i.e.

$$\int |\psi(\vec{r},0)|^2 d\vec{r} = 1 \ , \tag{5.3}$$

if we assume that at $t = 0$ there is one electron in our system, at level 2 or 1.

For the time being, we shall treat $\vec{A}$ as a classical field and make the following plane-wave expansion:

$$\vec{A}(\vec{r},t) = 2\sqrt{\pi}\sum_{\lambda}\hat{e}_{\lambda}(q_{\lambda}(t)\cos(\vec{k}_{\lambda}\cdot\vec{r}) - (1/k_{\lambda})p_{\lambda}(t)\sin(\vec{k}_{\lambda}\cdot\vec{r})) \ . \tag{5.4}$$

The amplitudes q_{λ} and p_{λ} are pairs of canonical variables which are real. Quantization of field $\vec{A}$ can be accomplished by interpreting p_{λ} and q_{λ} as operators in Heisenberg representation satisfying the usual commutation relation,

$$[q_{\lambda}(t), p_{\lambda'}(t)] = i\delta_{\lambda\lambda'} \ . \tag{5.5}$$

Further, a system of creation and annihilation operators, $a_{\lambda}^{\dagger}$ and a_{λ}, can be introduced (second quantization),

$$q_{\lambda} = \sqrt{1/2k_{\lambda}}\ (a_{\lambda} + a_{\lambda}^{\dagger}) \ , \quad p_{\lambda} = i\sqrt{k_{\lambda}/2}\ (a_{\lambda}^{\dagger} - a_{\lambda}) \ . \tag{5.6}$$

The above quantization procedures have already been carried out in the previous plane-wave expansion for $\vec{A}$ in (4.2). We use expansion (5.4) here because we want to treat

$$H_{rad} + H_2 = (1/8\pi)\int(\vec{E}^2(\vec{r},t)+(\nabla\times\vec{A}(\vec{r},t))^2)d\vec{r}$$

$$+ (e^2/2m)\int\vec{A}^2(\vec{r},t)|\psi(\vec{r},0)|^2d\vec{r} \qquad (5.7)$$

as a classical Hamiltonian expressed in canonical variables p_λ and q_λ. After $H_{rad} + H_2$ has been diagonalized by canonical transformations, which will then be quantized as indicated in (5.5) and (5.6), introducing a new set of creation and annihilation operators. The diagonalization of (5.7) is shown in the appendix.

2. The Transformed Hamiltonian

In this "transformed" Hamiltonian, we must put the previously subtracted infinite zero-point energy of the radiation field, $\sum k_\lambda/2$, back to (4.6), since it is included in H_{rad}, and of course H_2 will also be present. The Hamiltonian becomes

$$H_T = (H+\sum_\lambda k_\lambda/2) + H_2$$

$$= (E_2 b_2^\dagger b_2 + E_1 b_1^\dagger b_1 + H_{rad} + H_1) + H_2 \ ,$$

(5.8)

where H is given by (4.6). Using Eqs. (5.6), (A.3), and (A.8), the old annihilation (or creation) operator a_λ is transformed into,

$$a_\lambda = \sqrt{k\lambda/2} \sum_\nu \sqrt{1/2K_\nu}(a'_\nu(\mathcal{F}_{\nu\lambda} - \mathcal{G}_{\nu\lambda}) + a'^\dagger_\nu(\mathcal{F}_{\nu\lambda} + \mathcal{G}_{\nu\lambda})) \ ,$$

(5.9)

where

$$\mathcal{F}_{\nu\lambda} = \sum_{\lambda'}(\mathcal{D}_{\lambda\lambda'} + (i/k_\lambda)\mathcal{B}_{\lambda\lambda'})(T^{-1})_{\nu\lambda'}$$

and

$$\mathcal{G}_{\nu\lambda} = \sum_{\lambda'} iK_\nu(\mathcal{C}_{\lambda\lambda'} + (i/k_\lambda)\mathcal{A}_{\lambda\lambda'})T_{\lambda'\nu} \ . \qquad (5.10)$$

The new set of annihilation and creation operators, a'_ν and $a'^\dagger_\nu$, are defined by relations similar to (5.6). With (5.9) we can write

$$H'_T = H_T - \sum_\nu K_\nu/2 = E_2 b_2^\dagger b_2 + E_1 b_1^\dagger b_1 + \sum_\nu K_\nu a_\nu'^\dagger a'_\nu$$

$$+ e\{b_2^\dagger b_1 \sum \sqrt{1/2K_\nu}(a'_\nu(F_\nu - G_\nu) + a_\nu'^\dagger(F_\nu + G_\nu))$$

$$+ b_1^\dagger b_2 \sum \sqrt{1/2K_\nu}(a'_\nu(F_\nu^* + G_\nu^*) + a_\nu'^\dagger(F_\nu^* - G_\nu^*))\} \quad , \tag{5.11}$$

where

$$F_\nu = \sum_\lambda \beta_\lambda \mathcal{F}_{\nu\lambda}/2 \quad ,$$

and

$$G_\nu = \sum_\lambda \beta_\lambda \mathcal{G}_{\nu\lambda}/2 \quad . \tag{5.12}$$

In Eq. (5.11) the summation is over the "transformed" eigenstates of the photon. The new infinite zero-point energy may be subtracted from H_T. We notice that the first three terms in H'_T are very similar to H_o of (4.6) but H_1 of (4.6) has a different dependence on the creation and annihilation operators. The form of H'_T implies that the electron in level 1 or 2 can absorb or emit an arbitrary number of "transformed" photons of eigenstates ν. With the Hamiltonian (4.6), the bound electron could only emit or absorb one "free" photon of eigenstate λ. This means that a "free" photon corresponds to a *superposition of* "transformed" photons, which was actually implied by (5.9). We should mention that if we treat (5.1) in another way, i.e. replacing $\vec{A}^2(\vec{r},t)\approx\vec{A}^2(\vec{r},0)$, which would have no direct physical meaning like that of (5.2). The H_2 term will modify the energy levels of the bound electron and the electron operators, $b_{1,2}$ and $b^{\dagger}_{1,2}$. We can say, similarly, that a "free" electron, bound in a nuclear field but free from H_2, corresponds to a cloud of "transformed" electrons.

3. Physical and Bare Vacua for the Photon

We shall call the "transformed" photons physical and the "free" photons bare. The new zero-point energy $\Sigma K_\nu/2$, will be subtracted from the Hamiltonian H_T, instead of subtracting $\Sigma k_\lambda/2$ as was done in (4.6). Let us define

the physical vacuum state $|\Phi_o'\rangle$ as that state with no physical photon but one electron at level 1 or 2. The presence of one electron in $|\Phi_o'\rangle$ is to satisfy the condition given by (5.3), so that H_2 in (5.7) will not vanish identically, otherwise we would have the same Hamiltonian as (4.6). For definiteness we shall put this electron at level 2. Then the physical vacuum state for the photon is defined by

$$a_\nu' |\Phi_\delta'\rangle = 0 \quad , \tag{5.13}$$

for all ν. Similarly, we can also define a bare vacuum state $|\Phi_o\rangle$ for the photon as

$$a_\lambda |\Phi_0\rangle = 0 \quad , \tag{5.14}$$

which is a state with no photon but one electron at level 2.

Let us assume that initially there is no perturbation H_2 in our system so we can make up our initial state by applying a_λ to $|\Phi_o\rangle$. Recall, from Section 4 of last chapter, that the mean energy and the rate of energy dissipation should be finite for a physically acceptable state. It is, therefore, sufficient to test that if $\langle\Phi_o|H_T'|\Phi_o\rangle$ and $\langle\Phi_o|H_T'^2|\Phi_o\rangle$ are finite, our initial state will be physically acceptable. Rewriting H_T' from (5.11) and (5.8), and then

expanding $\vec{A}$ by (4.2) in terms of operators $a_\lambda^\dagger$ and a_λ, a straightforward calculation yields

$$\langle\Phi_0|H_T'|\Phi_0\rangle = E_2+\sum k_\lambda/2-\sum K_\nu/2+(e^2\pi/m)\sum 1/k_\lambda \ . \qquad (5.15)$$

The three sums are separately divergent at high frequencies, the first two quartically, the last quadratically. We cannot say offhand that the divergences completely compensate each other at high frequencies[46], since K_ν cannot be solved simply. However, there is still hope that (5.15) may be finite due to the difference in signs for the three sums. For the case of a point charge distribution, $|\psi(\vec{r})|^2 = \delta(\vec{r})$, we have

$$H_2 = (e^2 2\pi/m)\sum_{\lambda\lambda'} \hat{e}_\lambda\cdot\hat{e}_{\lambda'} q_\lambda q_{\lambda'} \ , \qquad (5.16)$$

which can be diagonalized with H_{rad} by Van Kampen's method[47]. Instead of (A.11), we have a simple equation for the eigenvalues K_ν^2,

$$(e^2 4\pi/m) \sum_\lambda 1/(K^2-k_\lambda^2) = 1 \ . \qquad (5.17)$$

Since we want to examine the high-frequency behaviour of K_ν, we can take $(e^2 4\pi/m) << k_\lambda^2$ for large λ's. At high frequencies (5.17) will be dominated by the term $K \approx k_\lambda + \delta$ where δ is a small positive frequency. With the above approximations, we obtain

$$K_\nu \approx k_\lambda + e^2 2\pi/(mk_\lambda) \tag{5.18}$$

at high frequencies. We can see from (5.18) and (5.15) that the divergences in (5.15) exactly compensate each other at high frequencies. Hence, the mean energy for the bare vacuum is finite if $\sum K_\nu/2$ is subtracted from the Hamiltonian, instead of subtracting $\sum k_\lambda/2$ as is done usually. Let us proceed to evaluate

$$\langle \Phi_0 | H_T'^2 | \Phi_0 \rangle = (\langle \Phi_0 | H_T' | \Phi_0 \rangle)^2 + e^2 \sum |\beta_\lambda|^2/(2k_\lambda) +$$

$$+ (e^4 2\pi^2/m^2) \sum_{\lambda\lambda'} (\hat{e}_\lambda \cdot \hat{e}_{\lambda'})^2/(k_\lambda k_{\lambda'}) \left| \int e^{i(\vec{k}_\lambda + \vec{k}_{\lambda'})\cdot\vec{r}} |\psi(\vec{r})|^2 d\vec{r} \right|^2 . \tag{5.19}$$

The last term diverges for point charge distribution, while the second term converges due to $|\beta_\lambda|^2$. We can say that states built up from the bare vacuum is not physically acceptable at least for the point charge distribution. If we assume a spread-out charge distribution concentrated in a region of radius $1/k_c$ about the origin, then $|\int\cdots\cdot|^2$ in (5.19) will provide a cutoff for frequencies $> k_c$ to make the last term finite. However, there is no guarantee that (5.15) will remain finite for a spread-out charge distribution. The arguments above lead us to conclude that the concept of the bare vacuum is not physically acceptable. This is connected to the well known situation in quantum field theory that one cannot separate out a bare particle from the physical particles, since a physical particle always associates with a cloud of bare particles. On the other hand, we can show that, at $t = 0$,

$$\langle\Phi_0'|H_T'|\Phi_0'\rangle = E_2$$

and

$$\langle\Phi_0'|H_T'^2|\Phi_0'\rangle = (E_2)^2 + e^2\sum|F_\nu-G_\nu|^2/(2K_\nu) \quad ,$$

(5.20)

which are both finite. Hence, we should prepare our initial states from the physical vacuum.

Chapter 6. SUMMARY AND CONCLUSION

We have studied two examples of quantum mechanical dissipative systems. They are subsystems of conservative systems. In the first example, the conservative system consists of two interacting particles which can make transitions to n different final states (real or virtual). A single channel in this case will be the (dissipative) subsystem. Here, assuming a nonlocal separable potential, we can obtain exact result for the partial-wave amplitude which contains the usual kinematical cuts from the unitarity condition and dynamical cuts from the interaction. However, there is no simple way to generalize the one-channel N/D method to the multichannel problem. Of course, in our solvable example, there is a matrix A which has all the properties of the desirable D matrix, but the complete expression for the partial-wave amplitude cannot be written as a quotient of two matrices, ND^{-1}. Bound states and resonances are given by zeros of det(A) as expected.

The second example concerns a solvable model in nonrelativistic electrodynamics. Results of level shift and line breadth, corresponding to a damped classical point charge, are obtained. The decay behaviour of a state has the usual exponential form for small time ($\approx$ half life

of the state). This damped exponential and the line breadth can be considered typical characteristics of a quantum mechanical dissipative system.

In the last chapter, we have considered modification of the second example, which changes a bare photon to a superposition of physical photons as implied by (5.9). We have also argued that, for physically acceptable states, the transformed zero-point energy $\sum K_\nu/2$ should be subtracted rather than the radiation field (free) zero-point energy $\sum k_\lambda/2$. One notices that $\sum K_\nu/2$ arises from the Heisenberg's equations of motion for a'_ν, i.e.

$$\dot{a}'_\nu(t) = i[H_T, a'_\nu(t)] \quad , \tag{6.1}$$

by the usual commutation relation

$$[a'_\nu(t), a'^{\dagger}_{\nu'}(t)] = \delta_{\nu\nu'} \quad . \tag{6.2}$$

On the other hand, the equations of motion for the bare photon operators,

$$\dot{a}_\lambda(t) = i[H_T, a_\lambda(t)] \quad , \tag{6.3}$$

is obtained by assuming

$$[a_\lambda(t),\ a^\dagger_{\lambda'}(t)] = \delta_{\lambda\lambda'} \ . \tag{6.4}$$

An entirely different zero-point energy $\sum k_\lambda/2$ arises. If we demand that (6.3) should also give the physically acceptable result, namely the zero-point energy $\sum K_\nu/2$, then the commutation relation (6.4) will no longer hold and it should be modified. This leads us back to Wigner's result that from Heisenberg's equations of motion (6.3), the zero-point energy $\sum K_\nu/2$ can be obtained if one assumes a different commutation relation.

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APPENDIX DIAGONALIZATION OF $H_{rad} + H_2$

In this appendix we shall deal with the diagonalization of $H_{rad} + H_2$ in some detail. Substitution of (5.4) into (5.7) yields

$$H_{rad} + H_2 = (1/2)\sum_{\lambda}(p_\lambda^2+k_\lambda^2 q_\lambda^2) + (e^2/2)\sum_{\lambda\lambda'}(g_{\lambda\lambda'}p_\lambda p_{\lambda'}+f_{\lambda\lambda'}q_\lambda q_{\lambda'} + h_{\lambda'\lambda}p_\lambda q_{\lambda'}+h_{\lambda\lambda'}q_\lambda p_{\lambda'}) , \tag{A.1}$$

where

$$g_{\lambda\lambda'} = (4\pi/mk_\lambda k_{\lambda'})\hat{e}_\lambda\cdot\hat{e}_{\lambda'}\int\sin(\vec{k}_\lambda\cdot\vec{r})\sin(\vec{k}_{\lambda'}\cdot\vec{r})|\psi|^2 d\vec{r} = g_{\lambda'\lambda} ,$$

$$f_{\lambda\lambda'} = (4\pi/m)\hat{e}_\lambda\cdot\hat{e}_{\lambda'}\int\cos(\vec{k}_\lambda\cdot\vec{r})\cos(\vec{k}_{\lambda'}\cdot\vec{r})|\psi|^2 d\vec{r} = f_{\lambda'\lambda} ,$$

$$h_{\lambda\lambda'} = (-4\pi/mk_{\lambda'})\hat{e}_\lambda\cdot\hat{e}_{\lambda'}\int\cos(\vec{k}_\lambda\cdot\vec{r})\sin(\vec{k}_{\lambda'}\cdot\vec{r})|\psi|^2 d\vec{r} . \tag{A.2}$$

We shall consider (A.1) as a classical Hamiltonian of finite degrees of freedom, i.e. $\lambda = 1, 2, \ldots N$. Assume that the final result can be carried through for $N \to \infty$ if all sums remain finite.

First let us eliminate the cross terms in p_λ and q_λ by the following transformation:

$$p_\lambda = \sum_{\lambda'} (\mathcal{A}_{\lambda\lambda'} p'_{\lambda'} + \mathcal{B}_{\lambda\lambda'} q'_{\lambda'})$$

$$q_\lambda = \sum_{\lambda'} (\mathcal{C}_{\lambda\lambda'} p'_{\lambda'} + \mathcal{D}_{\lambda\lambda'} q'_{\lambda'}) \,. \qquad \text{(A.3)}$$

The transformation matrices, $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, and $\mathcal{D}$, are determined by the two requirements:

(a) transformation (A.3) is canonical, viz. the fundamental Poisson bracket relations are invariant under canonical transformations; [1] and

(b) cross terms in (A.1) vanish after the transformation.

Condition (a) leads to

$$\sum_{\lambda''} (\mathcal{D}_{\lambda\lambda''} \mathcal{A}_{\lambda'\lambda''} - \mathcal{C}_{\lambda\lambda''} \mathcal{B}_{\lambda'\lambda''}) = \delta_{\lambda\lambda'}$$

$$\sum_{\lambda''} (\mathcal{A}_{\lambda\lambda''} \mathcal{B}_{\lambda'\lambda''} - \mathcal{B}_{\lambda\lambda''} \mathcal{A}_{\lambda'\lambda''}) = 0$$

$$\Sigma_{\lambda''}(\mathcal{C}_{\lambda\lambda''}\mathcal{D}_{\lambda'\lambda''} - \mathcal{D}_{\lambda\lambda''}\mathcal{C}_{\lambda'\lambda''}) = 0, \qquad (A.4)$$

while the second condition demands

$$\Sigma_{\lambda}(\mathcal{A}_{\lambda\lambda_1}\mathcal{B}_{\lambda\lambda_2} + k_{\lambda}^2\mathcal{C}_{\lambda\lambda_1}\mathcal{D}_{\lambda\lambda_2}) + e^2\Sigma_{\lambda\lambda'}(g_{\lambda\lambda'}\mathcal{A}_{\lambda\lambda_1}\mathcal{B}_{\lambda'\lambda_2} +$$

$$+ f_{\lambda\lambda'}\mathcal{C}_{\lambda\lambda_1}\mathcal{D}_{\lambda'\lambda_2} + h_{\lambda'\lambda}\mathcal{A}_{\lambda\lambda_1}\mathcal{D}_{\lambda'\lambda_2} + h_{\lambda\lambda'}\mathcal{C}_{\lambda\lambda_1}\mathcal{B}_{\lambda'\lambda_2}) = 0 \quad . \qquad (A.5)$$

Equations (A.4) and (A.5), in principle, can be solved and thus determine transformation (A.3). Then (A.1) becomes

$$H_{rad} + H_2 = \tfrac{1}{2}\Sigma_{\lambda_1\lambda_2}(\mathcal{L}_{\lambda_1\lambda_2}p'_{\lambda_1}p'_{\lambda_2} + \mathcal{M}_{\lambda_1\lambda_2}q'_{\lambda_1}q'_{\lambda_2}) \quad , \qquad (A.6)$$

where

$$\mathcal{L}_{\lambda_1\lambda_2} = \Sigma_{\lambda}(\mathcal{A}_{\lambda\lambda_1}\mathcal{A}_{\lambda\lambda_2} + k_{\lambda}^2\mathcal{C}_{\lambda\lambda_1}\mathcal{C}_{\lambda\lambda_2}) + e^2\Sigma_{\lambda\lambda'}(g_{\lambda\lambda'}\mathcal{A}_{\lambda\lambda_1}\mathcal{A}_{\lambda'\lambda_2} +$$

$$+ f_{\lambda\lambda'}\mathcal{C}_{\lambda\lambda_1}\mathcal{C}_{\lambda'\lambda_2} + h_{\lambda'\lambda}\mathcal{A}_{\lambda\lambda_1}\mathcal{C}_{\lambda'\lambda_2} + h_{\lambda\lambda'}\mathcal{C}_{\lambda\lambda_1}\mathcal{A}_{\lambda'\lambda_2}) = \mathcal{L}_{\lambda_2\lambda_1}$$

and

$$\mathcal{M}_{\lambda_1\lambda_2} = \sum_\lambda (\mathcal{B}_{\lambda\lambda_1}\mathcal{B}_{\lambda\lambda_2} + k_\lambda^2 \mathcal{D}_{\lambda\lambda_1}\mathcal{D}_{\lambda\lambda_2}) + e^2 \sum_{\lambda\lambda'} (g_{\lambda\lambda'}\mathcal{B}_{\lambda\lambda_1}\mathcal{B}_{\lambda'\lambda_2} +$$

$$+ f_{\lambda\lambda'}\mathcal{D}_{\lambda\lambda_1}\mathcal{D}_{\lambda'\lambda_2} + h_{\lambda'\lambda}\mathcal{B}_{\lambda\lambda_1}\mathcal{D}_{\lambda'\lambda_2} + h_{\lambda\lambda'}\mathcal{D}_{\lambda\lambda_1}\mathcal{B}_{\lambda'\lambda_2}) = \mathcal{M}_{\lambda_2\lambda_1} \cdot$$

(A.7)

The sum of $H_{rad} + H_2$ is positive-definite and real, as should be expected from the radiation energy plus a perturbation energy ((5.7) and (A.1)). Then (A.6) consists of two real positive-definite quadratic forms which can be diagonalized simultaneously.[48] The canonical transformation is

$$p'_\lambda = \sum_\nu T_{\lambda\nu} P_\nu \quad , \quad q'_\lambda = \sum_\nu (T^{-1})_{\nu\lambda} Q_\nu \quad , \qquad (A.8)$$

which satisfies condition (a). In order that (A.8) reduces (A.6) to a form like H_{rad} , the first sum in (A.1), we require

$$\sum_{\lambda\lambda'} (T_{\lambda\nu}\mathcal{L}_{\lambda\lambda'}T_{\lambda'\nu'}) = \delta_{\nu\nu'} \quad ,$$

and

$$\Sigma_{\lambda\lambda'}(T^{-1})_{\nu\lambda}\mathcal{M}_{\lambda\lambda'}(T^{-1})_{\nu'\lambda'} = K_\nu^2\delta_{\nu\nu'} \quad , \qquad (A.9)$$

where K_ν^2 are the eigenvalues to be determined. From (A.9), we find

$$\Sigma_{\lambda'}(\mathcal{M}_{\lambda\lambda'} - K_\nu^2(\mathcal{L}^{-1})_{\lambda\lambda'})(T^{-1})_{\nu\lambda'} = 0 \quad , \qquad (A.10)$$

which may be considered as a set of N homogeneous algebraic equations for the transformation matrix elements $(T^{-1})_{\nu\lambda'}$, where ν is fixed. The necessary and sufficient condition that these equations have a solution is that the determinant of their coefficients vanishes, i.e. the eigenvalues K_ν^2 are the roots of the secular equation

$$\det \begin{vmatrix} \mathcal{M}_{11}-K^2(\mathcal{L}^{-1})_{11}, & \mathcal{M}_{12}-K^2(\mathcal{L}^{-1})_{12}, \cdots & \mathcal{M}_{1N}-K^2(\mathcal{L}^{-1})_{1N} \\ \mathcal{M}_{21}-K^2(\mathcal{L}^{-1})_{21}, & \mathcal{M}_{22}-K^2(\mathcal{L}^{-1})_{22}, \cdots & \mathcal{M}_{2N}-K^2(\mathcal{L}^{-1})_{2N} \\ \vdots & \vdots & \vdots \\ \mathcal{M}_{N1}-K^2(\mathcal{L}^{-1})_{N1}, & \mathcal{M}_{N2}-K^2(\mathcal{L}^{-1})_{N2}, \cdots & \mathcal{M}_{NN}-K^2(\mathcal{L}^{-1})_{NN} \end{vmatrix} = 0 \, .$$

(A.11)

As $N\to\infty$, we have a secular determinant of infinite dimension in (A.11). To obtain such a determinant, mathematical induction is employed to determine a general solution for arbitrary dimension N and then N is allowed to approach infinity.[49] Another method to diagonalize (A.6) is given by Van Kampen[47] for the special case that $\mathcal{L}_{\lambda\lambda'}=\delta_{\lambda\lambda'}$ and $\mathcal{M}_{\lambda\lambda'} = M_\lambda\delta_{\lambda\lambda'}+m_\lambda m_{\lambda'}$. We obtain finally, from (A.6), (A.8), and (A.9),

$$H_{rad} + H_2 = \tfrac{1}{2}\sum_{\nu=1}^{N}(P_\nu^2 + K_\nu^2 Q_\nu^2) \ , \qquad (A.12)$$

where K_ν^2, as determined from (A.11), are positive and real since we have assumed that $H_{rad}+H_2$ is positive and real. For simplicity, we shall also assume that K_ν^2 are all distinct. In (A.12) we can let $N\to\infty$ as the diagonalized form of $H_{rad}+H_2$. Quantization can be carried out to yield

$$H_{rad} + H_2 = \sum_\nu K_\nu(a_\nu'^\dagger a_\nu' + \tfrac{1}{2}) \ , \qquad (A.13)$$

where $a_\nu'^\dagger$ and a_ν' are the new set of creation and annihilation operators defined similar to (5.6). A new infinite zero-point energy, $\sum K_\nu/2$, appears. One should note that

$$K_\nu^2 = k_\lambda^2 \quad \text{for} \quad e^2 \equiv 0 \ , \qquad (A.14)$$

as one compares (A.12) with (A.1).