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SOME QUESTIONS CONCERNING ADIABATIC TRANSFORMATIONS

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The old questions connected with the so-called "adiabatic theorem" ¹⁾ still play an important role in many questions of quantum field theory such as renormalization, definition of the vacuum state, etc. It may therefore be of some interest to simplify or clarify the proof of certain results, even though they are generally regarded as well known. We refer in particular to the following. A very common situation arises, when a coupling constant is switched on exponentially : $g(t) = g e^{\alpha t}$; the adiabatic limit is then obtained, of course, for $\alpha \rightarrow 0+$. For finite α , the state ψ_g attained by the system at, say, the time $t = 0$, satisfies a well known differential equation with respect to the coupling constant g . This equation was obtained by Gell-Mann and Low ²⁾ by means of a perturbation expansion in the interaction representation. We note below, Section 2, that a much simpler and more transparent derivation can be given, without resorting to a perturbation expansion. Our main topic, however, is the limit $\alpha \rightarrow 0$. As is well known, the state vector ψ_g contains a phase factor $e^{-i\theta(g,\alpha)}$ which becomes singular in the limit $\alpha \rightarrow 0$, in the sense that $\theta \sim 1/\alpha$. Physically, this infinite phase must be the integral over time, from $t = -\infty$ to $t = 0$, of $\Delta E(g)/\hbar$, where $\Delta E(g)$ is the level shift produced by the perturbation ; when α is finite, this shift operates effectively for a time of the order of $1/\alpha$, hence the above-mentioned result. Formally, the existence of the singularity can be easily checked ²⁾, if one examines the behaviour, in the limit $\alpha \rightarrow 0$, of the successive terms in the perturbation expansion ; one finds that the term of order g^n contains singular terms in α , of order $\alpha^{-1}, \alpha^{-2}, \dots, \alpha^{-n}$. It is intuitively plausible, but not obvious mathematically that these terms arise from the expansion of the exponential phase factor. If this is true, it becomes possible to eliminate the singularity at $\alpha = 0$ by renormalization of ψ_g , for example ²⁾, by the definition

$$\chi_g = \psi_g / (\phi, \psi_g) \quad (1)$$

where ϕ is the initial value (at $t = -\infty$) of the state vector. Here $(\dots, \dots)$ indicates as usual the scalar product of two vectors. It is, of course, a fundamental result that χ_g should have a finite limit for $\alpha = 0$, because it is this limit, which is then shown to be an eigenstate of the perturbed Hamiltonian, as stated by the adiabatic theorem.

Now Gell-Mann and Low content themselves with asserting that all the above statements can be verified "up to any desired order in g ", i.e., presumably as far as one's patience and willingness to be convinced allow. The direct calculations actually become quite laborious very soon. The question, however, is so fundamental and simple that it should be settled completely for an arbitrary order n . We show in the following that this is indeed possible by utilizing the differential equations in g satisfied by the state vectors ψ_g and χ_g , equations already given by the above-mentioned authors. The connection between the adiabatic solution and the Rayleigh-Schrödinger perturbation series is thus completely established.

2. - THE DIFFERENTIAL EQUATIONS

The problem to be dealt with is the following ²⁾ : the Hamiltonian of interest is of the form

$$H = H(g) \equiv H_0 + g H_1 \quad (2)$$

One asks for a solution of the time dependent Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = \{ H_0 + g e^{\alpha t} H_1 \} \psi \quad (3)$$

namely, the solution which for $t \rightarrow -\infty$ behaves asymptotically according to

$$\psi \sim \phi e^{-i\varepsilon_0 t} \quad (4)$$

where ϕ is a normalized eigenstate of the unperturbed Hamiltonian corresponding to a non-degenerate eigenvalue ε_0 :

$$(H_0 - \varepsilon_0)\phi = 0 \quad (5)$$

In Eq. (3), α is a real constant > 0 .

We now denote by ψ_g the value of this solution for $t = 0$. More explicitly, let $\psi(t, g, \alpha)$ be the unique solution of Eqs. (3) and (4), then

$$\psi_g = \psi(0, g, \alpha) \quad (6)$$

We derive a differential equation with respect to g , satisfied by ψ_g , as follows. Consider the function :

$$\psi_1(t) = e^{i\varepsilon_0 \tau} \psi(t + \tau, g, \alpha) \quad (7)$$

which, apart from a phase factor, is obtained from the solution ψ by a time-displacement τ . Clearly ψ_1 satisfies the asymptotic condition (4), and also the Schrödinger equation (3), for a different value of g : $g_1 = g e^{\alpha \tau}$. Therefore $\psi_1(t) = \psi(t, g e^{\alpha \tau}, \alpha)$ or :

$$\psi(t+\tau, g, \alpha) = e^{-i\varepsilon_0\tau} \psi(t, g e^{\alpha\tau}, \alpha) \quad (8)$$

Differentiating with respect to τ and setting $\tau = 0$, we can express the time derivative in Eq. (3) in terms of $\alpha g(\partial\psi/\partial g) - i\varepsilon_0\psi$. At $t = 0$, Eq. (3) becomes

$$i\alpha g \frac{\partial\psi}{\partial g} = \{H(g) - \varepsilon_0\}\psi \quad (9)$$

which is Gell-Mann and Low's Eq. (A5).

This derivation does not depend on a perturbation expansion and it can be easily generalized. For example, assume

$$H(g) = H_0 + gH_1 + g^2H_2 \quad (10)$$

(or even a polynomial in g of order n) and then consider the time dependent Schrödinger equation in which $H(g)$ is replaced by $H(g e^{\alpha t})$. Then everything goes through as before, and Eq. (9) is obtained. In the following, however, we shall restrict ourselves to the simple case, Eq. (2). The generalization (10) is not without interest, however, since Lagrangians and Hamiltonians with quadratic terms in the coupling constants are quite common.

Finally we notice with Gell-Mann and Low the following equations of which the second one is a differential equation for the renormalized state vector χ_g

$$i\alpha g \frac{\partial}{\partial g} (\phi, \psi_g) = (\phi, [H(g) - \varepsilon_0] \psi_g) = g (\phi, H_1 \psi_g) \quad (11)$$

$$i\alpha g \frac{\partial \chi_g}{\partial g} = \{H(g) - \varepsilon_0\} \chi_g - \chi_g i\alpha g \frac{\partial}{\partial g} \ln(\phi, \psi_g) \quad (12)$$

Both equations, of course, follow from Eq. (9). In Eq. (12), furthermore, the last term can be modified as follows

$$i\alpha g \frac{\partial}{\partial g} \ln(\phi, \psi_g) = g(\phi, H_1 \chi_g) \quad (13)$$

so that finally

$$i\alpha g \frac{\partial \chi_g}{\partial g} = \{H(g) - E(g, \alpha)\} \chi_g \quad (14)$$

$$E(g, \alpha) = \varepsilon_0 + g(\phi, H_1 \chi_g) \quad (15)$$

As we shall see, in these two last equations, one can go to the limit $\alpha = 0$ without any trouble, and $E(g, 0)$ is then the perturbed eigenvalue [of the operator $H(g)$].

3. - THE ADIABATIC LIMIT

It is customary to obtain the perturbation expansion of ψ_g

$$\psi_g = \phi + \sum_{n=1}^{\infty} g^n \frac{1}{\varepsilon_0 - H_0 + i\alpha n} H_1 \frac{1}{\varepsilon_0 - H_0 + i\alpha(n-1)} H_1 \cdots \frac{1}{\varepsilon_0 - H_0 + i\alpha} H_1 \phi \quad (16)$$

from the time-dependent equation (2). From this, in principle, one can obtain the expansion of χ_g , Eq. (1), but, as we have said, this is rather cumbersome. Notice, however, that (16) can be obtained directly from Eq. (9). It should be almost equally simple to obtain an expansion for χ_g directly from Eqs. (14) and (15). For $g = 0$, $\chi_g = \psi_g = \phi$; assume therefore

$$\chi_g = \sum_{n=0}^{\infty} g^n \phi_n(\alpha) \quad (17)$$

where $\phi_0 = \phi$. Notice also that, from (1): $(\phi, \chi_g) = 1$, so that we must have

$$(\phi, \phi_n) = \delta_{n0} \quad ; (n=0,1,2,\dots) \quad (18)$$

Substituting (17) into (15) we get

$$E(g, \alpha) = \epsilon_0 + \sum_{n=1}^{\infty} g^n \epsilon_n(\alpha) \quad (19)$$

where

$$\epsilon_n(\alpha) = (\phi, H_1 \phi_{n-1}(\alpha)) \quad (20)$$

In particular, $\epsilon_1(\alpha) = (\phi, H_1 \phi)$ is the first-order perturbation of the energy level, and is independent of α . Next substitute (17) and (19) into (14) and obtain the recurrence relation

$$\begin{aligned} (\epsilon_0 - H_0 + i\alpha n) \phi_n(\alpha) &= H_1 \phi_{n-1}(\alpha) - (\phi, H_1 \phi_{n-1}(\alpha)) \phi - \\ &- \sum_{m=1}^{n-1} \epsilon_{n-m}(\alpha) \phi_m(\alpha) \quad ; \quad (n=1,2,\dots) \end{aligned} \quad (21)$$

Thus the n -th term in the expansion of χ_g is at first sight much more complicated than the corresponding term in (16). It has, nevertheless, much simpler properties in the limit $\alpha = 0$. Notice in fact that the solution of an equation $(\epsilon_0 - H_0 + i\alpha n)\phi_n = \omega_n$ or $\phi_n = (\epsilon_0 - H_0 + i\alpha n)^{-1}\omega_n$ becomes singular as $\alpha \rightarrow 0$ only if $(\phi, \omega_n) \neq 0$. But the right-hand side of (21) may be rewritten

$$\omega_n = \Lambda H_1 \phi_{n-1} - \sum_{m=1}^{n-1} \epsilon_{n-m} \phi_m \quad (21')$$

where Λ is a projection operator (projection on the subspace orthogonal to ϕ). Together with (18) this implies that ω_n is orthogonal to ϕ , and $\phi_n = \lim_{\alpha \rightarrow 0} \phi_n(\alpha)$ exists, and may be obtained by solving the recurrence equations

$$(\epsilon_0 - H_0)\phi_n = \Lambda H_1 \phi_{n-1} - \sum_{m=1}^{n-1} \epsilon_{n-m} \phi_m \quad (22)$$

$$\epsilon_n = (\phi, H_1 \phi_{n-1}) \quad (23)$$

These are, however, precisely the equations of the Rayleigh-Schrödinger expansion of the perturbed wave function and perturbed eigenvalue

$\epsilon_0 + \Delta E(g)$. The cancellation of the singular phase factor is therefore demonstrated to arbitrary order.

4. - REMARKS AND EXTENSIONS

It is clearly possible to extend the above calculations in various directions. For example the conclusions of the last Section could be easily extended to the case of Eq. (10). Also, one could expand $\phi_n(\alpha)$ and $\epsilon_n(\alpha)$ in powers of α and examine non-adiabatic effects ; for example, terms up to order α in $\epsilon_n(\alpha)$ are

easily connected to the normalization factor in the denominator in Eq. (1), since one can prove, by means of Eq. (13), that

$$\ln(\phi, \psi_g) = -\frac{i}{\alpha} \int_0^g \Delta E(g') \frac{dg'}{g'} - i \sum_{n=1}^{\infty} \frac{g^n}{n} \varepsilon_n^{(1)} + \dots \quad (24)$$

where

$$\varepsilon_n^{(1)} = \left(d\varepsilon_n / d\alpha \right)_{\alpha=0}$$

We want to deal briefly with a different extension. The methods of perturbation theory, adiabatic switching on, and renormalization, have been applied not only to the Schrödinger equation but also directly to the field equations in the Heisenberg representation, as, for example, in the work of Källén³⁾ and of Yang and Feldman⁴⁾. The most important difference from the previous case is that the equations are non-linear. Nevertheless a method similar to that of Section 2 leads to some interesting equations. Consider as an example the scalar field equation

$$(\square + m^2)\phi(x) = -\lambda e^{\alpha t} \phi^3(x) \quad (25)$$

Here $x = (\vec{x}, t)$ and the coupling constant λ is "switched on" by the exponential factor. One seeks a solution which satisfies the boundary condition

$$\phi(x) \sim \phi_0(x) \quad \text{when } t \rightarrow -\infty \quad (26)$$

where ϕ_0 is a solution of the homogeneous equation $(\square + m^2)\phi_0 = 0$. For simplicity, we limit ourselves to the non-quantized version of the theory⁵⁾. We notice that instead of the boundary condition (26) we may consider more generally

$$\phi(x) \sim \phi_0(x+\xi) \quad \text{when } t \rightarrow -\infty \quad (26')$$

where $\xi = (\vec{0}, \tau)$ is a displacement in the time direction. In fact $\phi_0(x+\xi)$ is also a solution of the homogeneous equation [and in the quantized case, it satisfies the same commutation law as $\phi_0(x)$]. Now if we call $\Phi(x; \lambda, \xi)$ the solution of (25) and (26'), it is easy to prove by reasoning as before, that Φ satisfies the functional equation :

$$\Phi(x; \lambda, \xi) = \Phi(x+\xi; \lambda e^{-\alpha\tau}, 0) \quad (27)$$

in other words Φ depends on the three variables t, λ and τ only as a function of two variables : $t + \tau$ and $\lambda e^{-\alpha\tau}$. Hence $\Phi(n; \lambda, \xi)$ satisfies identically the differential equation

$$-\frac{\partial \Phi}{\partial t} + \alpha \lambda \frac{\partial \Phi}{\partial \lambda} + \frac{\partial \Phi}{\partial \tau} = 0 \quad (28)$$

By differentiation one derives from this

$$\frac{\partial^2 \Phi}{\partial t^2} = \frac{\partial^2 \Phi}{\partial \tau^2} + 2\alpha\lambda \frac{\partial^2 \Phi}{\partial \lambda \partial \tau} + \alpha^2 \lambda^2 \frac{\partial^2 \Phi}{\partial \lambda^2} + \alpha^2 \lambda \frac{\partial \Phi}{\partial \lambda} \quad (29)$$

We now write the differential equation (25) at time $t = 0$, replacing the second derivative with respect to time by means of (29). The boundary condition (26) is replaced by

$$\Phi = \phi_0(\vec{x}, \tau) \quad \text{when } \lambda = 0 \quad (30)$$

The equation obtained may play a similar role as Eq. (9). The solution can be expanded in powers of λ , and the coefficients of λ^n ($n = 1, 2, \dots$) obey a set of recurrent equations. We do not wish to deal with this any further here, but we shall content ourselves with the remark that the method seems to be of some interest also in the more complicated case of the quantized theory.

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