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Adiabatic Process and the Stationary State

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The transformation function has singularity when the interaction has been switched off adiabatically. A procedure to remove this singularity is presented. As a result of this procedure we can find the displacement of energy spectrum of total Hamiltonian from that of free Hamiltonian.

§ 1. Introduction

General theories of scattering have been proposed by many authors. These authors attempted to investigate the properties of stationary states of total Hamiltonian $H$ and to obtain the expressions of cross section of various processes. But in these theories, the displacement of energy spectrum of the total Hamiltonian from that of the free Hamiltonian has not been, or has been only incompletely, taken into consideration. Here we call this displacement of spectrum briefly the energy displacement.

For example, Möller and Goldberger presented their theories of scattering assuming that there is no energy displacement. Lippmann and Schwinger have assumed that the collision process of two wave packets, which are completely separated from each other at infinite past, can be described by their integral equation which has the factor of switching off interactions. This assumption necessitates to neglect the energy displacement. On the other hand Gell-Mann and Goldberger took the energy displacement into consideration. But in their method, the energy displacements are determined by the limiting process in which normalizing volume tends to infinity. It is doubtful whether the operator giving the energy displacement is completely determined, namely whether we can have the closed expression of the energy displacement.

As is well known, we can always find the energy displacement for the co-existent systems of various fields as well as for some cases where the interaction between two particles does not vanish even at an infinite distance. Therefore, it is necessary to take account of the energy displacement in these cases. On the other hand there always appears the ultraviolet divergence in Tamm-Dancoff's formalism for quantized fields. This divergence constitutes one of the difficulties with Tamm-Dancoff's formalism. In order to avoid this difficulty, it seems necessary to analyse the energy displacement and find the wave matrix which explicitly includes the effect of the energy displacement in its structure.

In this paper, it will be shown how to construct the stationary states of $H$, taking account of the energy displacement. For this purpose, the adiabatic switching off process for the interaction is used. In this case there are some difficulties. The difficulties lie in
the singularity which appears gradually as the adiabatic factor approaches to unity. Hereafter, we call this singularity adiabatic singularity for the sake of convenience. In this paper, the difficulty accompanying this adiabatic singularity is avoided by factorizing the transformations function into two factors corresponding to the amplitude and the phase factor, and by pushing completely the adiabatic singularity into the latter factor.* To show the possibility of such a factorization is an essential point of this paper. The above amplitude, free from adiabatic singularities, tends to non-singular matrix as the adiabatic factor approaches to unity. This limiting matrix satisfies the generalized equation for Møller's wave matrix, in which the energy displacement appears in a closed form.

§ 2. Factorization of \( U(t, -\infty; \varepsilon) \)

In this chapter, it is shown that the transformation function \( U(t, -\infty; \varepsilon) \) which satisfies the Schrödinger equation in the interaction representation**

\[
i\partial U(t, -\infty; \varepsilon)/\partial t = g e^{itH_1(t)} U(t, -\infty; \varepsilon)
\]

and the boundary condition

\[ U(-\infty, -\infty; \varepsilon) = 1, \]

can be factorized in the following way, using Dyson's chronological operator \( P \),

\[
U(t, -\infty; \varepsilon) = V(t) P e^{-i\int_{-\infty}^{t} e^{-it'H_1(t')V(t')} dt'}
\]

This \( V(t) \) is given by the equation,

\[
i\partial V(t)/\partial t = g e^{it}[H_1(t)V(t) - V(t)'H_1(t)V(t)']
\]

and the initial condition,

\[ V(-\infty) = 1 \]

Generally, the elements of matrix depend upon the system of basic vectors of representation. In this paper, we use the eigenstates of \( H_0 \) as the system of basic vectors. For this representation, the symbol \( \langle A \rangle \) means a diagonal matrix derived from \( A \), whose elements are the diagonal ones of \( A \). In the same manner, we use the symbol \( A \) which means matrix \( A - \langle A \rangle \). Namely \( A \) is non-diagonal matrix, whose elements are the non-diagonal ones of \( A \).

To show the above results, we separate \( U(t, -\infty; \varepsilon) \) in the following way,

\[
U(t, -\infty; \varepsilon) = U(t, -\infty; \varepsilon) + \langle U(t, -\infty; \varepsilon) \rangle.
\]

Now we put***

\[
V(t) = 1 + U(t, -\infty; \varepsilon) \langle U(t, -\infty; \varepsilon) \rangle^{-1},
\]

* Dr. S. Tani attempted to remove this singularity. (Private communication)

** We used \( e^{it} \) as the switching-off factor in the interaction term. But, generally, \( g(t) = \int_{0}^{t} dG(t) e^{iv} \)

may be used as such a factor, too.

*** It is assumed in this paper that \( U(t, -\infty; \varepsilon) \) can be expanded in a power series when \( g \leq g_r \).

From this assumption, we can assert that the inverse of \( \langle U(t, -\infty; \varepsilon) \rangle \) always exists and its power series in \( g \) converges when \( g \leq g_r \).
then
\[ U(t, -\infty ; \varepsilon) = V(t) \langle U(t, -\infty ; \varepsilon) \rangle. \] (8)

\( V(t) \) has a structure: 1 + nondiagonal matrix.

We insert (8) into (1)
\[ i \frac{\partial V(t)}{\partial t} \langle U(t, -\infty ; \varepsilon) \rangle + V(t) i \frac{\partial}{\partial t} \langle U(t, -\infty ; \varepsilon) \rangle = g e^{itH} V(t) \langle U(t, -\infty ; \varepsilon) \rangle. \] (9)

On account of the structure of \( V(t) \),
\[ \langle \frac{\partial V(t)}{\partial t} \rangle = 0, \quad \langle V(t) \rangle = 1. \]

Therefore, we put \( \langle \quad \rangle \) in the both sides of (9),
\[ i \frac{\partial}{\partial t} \langle U(t, -\infty ; \varepsilon) \rangle = g e^{it} \langle H(t) V(t) \rangle \langle U(t, -\infty ; \varepsilon) \rangle. \] (10)

From this,
\[ \langle U(t, -\infty ; \varepsilon) \rangle = P e^{-i \int t \frac{\partial}{\partial t} \langle V(t) \rangle \langle U(t, -\infty ; \varepsilon) \rangle}. \] (11)

By inserting (10) into (9)
\[ i \frac{\partial}{\partial t} \langle U(t, -\infty ; \varepsilon) \rangle = g e^{it} \langle H(t) V(t) \rangle \langle U(t, -\infty ; \varepsilon) \rangle - \langle V(t) \rangle \langle H(t) V(t) \rangle \langle U(t, -\infty ; \varepsilon) \rangle, \] (12)

then
\[ i \frac{\partial}{\partial t} H(t) V(t) = g e^{it} (H(t) V(t) - V(t) \langle H(t) V(t) \rangle). \]

(8) and \( \langle U(-\infty, -\infty ; \varepsilon) \rangle = U(-\infty, -\infty ; \varepsilon) = 1 \) give
\[ V(-\infty) = 1. \]

Thus we have proved that the factorization of (3) is possible.

\[ \text{§ 3. The adiabatic singularity} \]

Rewriting (4) in a form of integral equation,
\[ V(t) = 1 - i g \int_{-\infty}^{t} dt' e^{it'\epsilon}[H(t') V(t') - V(t') \langle H(t') V(t') \rangle]. \] (13)

Developing \( V(t) \) into a power series of \( g \) and putting \( 1 = V(0)(t) \),
\[ V(t) = \sum_{n=0}^{\infty} (-i g)^n V^{(n)}(t). \] (14)

Inserting (14) into (13)
\[ V^{(n+1)}(t) = \int_{0}^{t} dt' e^{it'\epsilon} [H(t') V^{(n)}(t') - \sum_{k=0}^{n} V^{(k)}(t') V^{(n-k)}(t')] \] (15).

Putting \( n = 0 \),
\[ V^{(1)}(t) = \int_{-\infty}^{t} dt' e^{it'\epsilon} H(t'). \]
Let $\Phi_0$ be an arbitrary eigen-function of $H_0$ and $E_0$ the corresponding eigen-value, then we have

$$V^{(1)}(t) \Phi_0 = \int dt' \frac{e^{i(H_0 - E_0) t'}}{i(H_0 - E_0) + \epsilon} H_0(0) \Phi_0 = e^{i(H_0 - E_0)t + \epsilon H_1(0) \Phi_0} = e^{i(H_0 - E_0)t + \epsilon} V^{(1)}(0) \Phi_0.$$  

(16)

It is clear that the right hand side of (16) has no adiabatic singularity when eigen-values of $H_0$ are discrete at $E_0$.

Even if the eigenvalues of $H_0$ are continuous in the neighbourhood of $E_0$, it may be shown in the following way that the situation is not changed.

For this purpose, we make the scalar products between the right hand side of (16) and the arbitrary state which does not involve $\epsilon$. If this scalar products are not singular for the limiting process $\epsilon \rightarrow 0$, it may be natural to say that the right hand side of (17) is not singular.

For the arbitrary state $\Psi_0$ which does not involve $\epsilon$, we put

$$\Psi_0 = \int \Phi_0(E') \Phi_E dE'.$$

Then

$$\langle \Psi_0, e^{i(H_0 - E_0)t + \epsilon} V^{(1)}(0) \Phi_0 \rangle = e^{i(E' - E_0)t + \epsilon} \int \Phi_0(E') \frac{1}{i(E' - E_0) + \epsilon} e^{\epsilon H_1(E')} \langle E'|H_1(0)|E_0\rangle dE'. $$

(17)

As we have no interest in the dynamical system, in which the interaction Hamiltonian may change suddenly everywhere, namely, $\langle E^0 - 0|H_1(0)|E_0\rangle = \langle E^0 + 0|H_1(0)|E^0\rangle$ at the set of points $E_0$ having finite Lebesgue measure, we can evaluate (17) in the following way:

$$[\int dE' + \int dE'] \left[ \Phi_0^{*}(E') / i(E' - E_0) + \epsilon \cdot e^{\epsilon H_1(E')} \langle E'|H_1(0)|E_0\rangle \right]$$

$$= [\int dE' + \int dE'] \left[ \Phi_0^{*}(E') / i(E' - E_0) + \epsilon \cdot e^{\epsilon H_1(E')} \langle E'|H_1(0)|E_0\rangle \right]$$

$$- i \epsilon H_1 \Phi_0^{*}(E_0) M \ln \frac{\epsilon - i\delta}{-\epsilon - i\delta}.$$  

(18)

$M$ is defined as follows:

$$M = \langle E_0 - 0|H_1(0)|E_0\rangle = \langle E_0 + 0|H_1(0)|E_0\rangle.$$

Clearly the right hand side of (18) has no singularity for $\epsilon \rightarrow 0$. In abbreviation, the right hand side of (18) has the singularity only when $\langle E'|H_1(0)|E_0\rangle$ is strongly singular at $E' = E_0$. On the other hand, $\langle E_0|H_1(0)|E_0\rangle = 0$ according to the non-diagonal character of $H_1(0)$. Of course, even if $\langle E_0|H_1(0)|E_0\rangle = 0$, adiabatic singularity appears when $\langle E'|H_1(0)|E_0\rangle \approx (E' - E_0)^{-\delta}$ for $\delta \geq 1$ or $\langle E_0 - 0|H_1(0)|E_0\rangle = \langle E_0 + 0|H_1(0)|E_0\rangle$. We do not discuss this case in the present paper.
Furthermore, we can show by the method of mathematical induction that $V^{(n)}(t)$ also has no adiabatic singularity. For this purpose, we assume that for $l \leq n$,

(i) $V^{(l)}(t) \Phi_0 = e^{i(H_0-E_0)t+il\delta t} V^{(l)}(0) \Phi_0$,

(ii) $\langle E_0 - 0 | V^{(l)}(0) | E_0 \rangle = \langle E_0 + 0 | V^{(l)}(0) | E_0 \rangle$,

(iii) $V^{(l)}(t) \Phi_0$ has no adiabatic singularity.

If we can show that the assertions (i) (ii) (iii) for $l = n + 1$ follow from the ones $l \leq n$, it may be concluded that above (i) (ii) (iii) are right for all $l$'s, since the case for $l = 1$ was already discussed. As $\Phi_0$ is an eigen-state of $H_0$, $\langle H_1(t') V^{(n)}(t') \rangle \Phi_0$ is also one, because

$H_0 \langle H_1(t') V^{(n)}(t') \rangle \Phi_0 = \langle H_1(t') V^{(n)}(t') \rangle H_0 \Phi_0 = E_0 \langle H_1(t') V^{(n)}(t') \rangle \Phi_0$.

Therefore, when the right hand side of (15) operates on $\Phi_0$, we can use the form (i) for $V^{(l)}(t')$ in (15) as well as for $V^{(n)}(t')$ or $V^{(n-1)}(t')$. Then

$V^{(n+1)}(t) \Phi_0 = e^{i(H_0-E_0)t+(n+1)\delta t} \frac{1}{i(H_0-E_0)} + (n+1) \delta t \times [H_1(0) V^{(n)}(0) - \sum_{s=1}^{n} V^{(s)}(0) \langle H_1 V^{(n-s)}(0) \rangle] \Phi_0$

$= e^{i(H_0-E_0)t+(n+1)\delta t} V^{(n+1)}(0) \Phi_0$.

Certainly (i) is right for $l = n + 1$. It is easy to show (ii) for $l = n + 1$. By the same reduction as for $n = 1$, we can conclude (iii) is also right for $l = n + 1$. This is what was to be proved.

We put

$\lim_{\epsilon \to 0} V^{(n)}(t) = \mathfrak{R}^{(n)}(t)$.

Convergence of

$V(t) = \sum_{n=0}^{\infty} (-ig)^n \mathfrak{R}^{(n)}(t)$

does not always give convergence of

$\sum_{n=0}^{\infty} (-ig)^n \mathfrak{R}^{(n)}(t)$.

Then we assume uniform convergence of the right hand side over $0 \leq \epsilon \leq \epsilon_0$. This assumption may be followed by the results:

$\lim_{\epsilon \to 0} V(t) = \sum_{n=0}^{\infty} (-ig)^n \mathfrak{R}^{(n)}(t)$.

§ 4. General wave matrix

Using (i) in the preceding chapter,

$V(t) \Phi_0 = \sum_{n=0}^{\infty} (-ig)^n e^{i(H_0-E_0)t+n\epsilon \delta t} V^{(n)}(0) \Phi_0$.

Differentiating the both sides with respect to $t$,

$i \frac{\partial}{\partial t} V(t) \Phi_0 = -[H_0, V(t)] \Phi_0 + i\epsilon \sum_{n=0}^{\infty} (-ig)^n n \times V^{(n)}(t) \Phi_0$. 


Therefore
\[ i \frac{\partial}{\partial t} V(t) = -[H_0, V(t)] + i\varepsilon \sum_{n=0}^{\infty} (-i\gamma)^n \times n \times V^{(n)}(t). \] (22)

From (13) and (22)
\[ g e^{it[H_1(t) V(t) - V(t) \langle H_1(t) V(t) \rangle]} = -[H_0, V(t)] + i\varepsilon \tilde{\chi}(t), \]
here
\[ \sum_{n=0}^{\infty} (-i\gamma)^n \times n \times V^{(n)}(t) = \chi(t). \]

Having transformed several terms, we have
\[ [H_0 + g e^{it H_1(t)}] V(t) = V(t) [H_0 + g e^{it} \langle H_1(t) V(t) \rangle] + i\varepsilon \tilde{\chi}(t). \] (23)

If the power series of \[ g, \sum_{n=0}^{\infty} (-i\gamma)^n \times n \times V^{(n)}(t) \] uniformly converges when \[ g \leq g_c \] over \[ 0 \leq \varepsilon \leq \varepsilon_0 \],
\[ \sum_{n=0}^{\infty} (-i\gamma)^n \times n \times V^{(n)}(t) \]
does uniformly converge when \[ g < g_c \] over \[ 0 \leq \varepsilon \leq \varepsilon_0 \]. Then generally we can assert
\[ \lim_{\varepsilon \to 0} \chi(t) = \sum_{n=0}^{\infty} (-i\gamma)^n \times n \times V^{(n)}(t), \]
namely
\[ \lim_{\varepsilon \to 0} \chi(t) \]
is not singular for the limiting process \( \varepsilon \rightarrow 0 \). Thus we reached final results:
\[ H(t) \Psi(t) = \Psi(t) [H_0 + g \langle H_1(t) \Psi(t) \rangle] = \Psi(t) \langle H(t) \Psi(t) \rangle. \] (24)

Especially for \( t = 0 \),
\[ H \Psi = \Psi[H_0 + g \langle H_1 \Psi \rangle] = \Psi \langle H \Psi \rangle, \] (25)
here
\[ \Psi = \Psi(0). \]

This is the generalized formula of Möller's wave matrix. 4

It is also possible to acquire the similar results as (23) for \( U(t, -\infty ; \varepsilon) \). But, in this case, the term corresponding to the last one of the right hand side of (23) may essentially be singular for \( \varepsilon \rightarrow 0 \).

Matrix \( \langle gH_1, \Psi \rangle \) is not always completely diagonal for the arbitrary sets of eigenfunction of \( H_1 \). Let \( \{ \Phi_\lambda \} \) be the set of eigenfunctions for which \( \langle gH_1, \Psi \rangle \) is completely diagonal. Then \( \Psi \Phi_\lambda \) is the eigenstate of \( H \). The eigenvalue is \( E_\lambda \pm \Delta E_{\lambda\alpha} \) where \( \Delta E_{\lambda\alpha} \) is one of the diagonal elements of \( \langle gH_1, \Psi \rangle \) for \( \{ \Phi_\lambda \} \).

When the eigenfunction \( \Phi_0 \) is not degenerate for the particular eigenvalue,
\[ U(t, -\infty ; \varepsilon) \Phi_0 = V(t) \Phi_0 \Phi_0 e^{-\frac{i}{\hbar} \int_{t_0}^{t} \langle H_1, \Phi_0 \rangle \Phi_0 \rangle}, \]
and
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\[
(\Phi_0^*, V(t) \Phi_0) = 1.
\]

Then
\[
\lim_{\varepsilon \to 0} U(t, -\infty; \varepsilon) \Phi_0 / (\Phi_0^*, U(t, -\infty; \varepsilon) \Phi_0) = \lim_{\varepsilon \to 0} V(t) \Phi_0 = \mathbb{B}(t) \Phi_0. 
\tag{26}
\]

Even in the field theory, the eigenfunction for the lowest eigenvalue of \( H_0 \) or the so-called particle vacuum may not be degenerate. Therefore \( \mathbb{B} \Phi_0 \) is the true vacuum state when \( \Phi_0 \) is the particle vacuum state.\(^5\)

\[\text{§ 5. Discussions}\]

From the result of § 3
\[
\langle H_j(t) V(t) \rangle \Phi_0 = \sum_{n=0}^{\infty} (-i\gamma)^n e^{int} \langle H_j V^{(n)}(0) \rangle \Phi_0.
\]
Then we can presume that \( \langle H_j(t) V(t) \rangle \) is independent of \( t \) in the limiting case \( \varepsilon \to 0 \). Thus \( P \)-symbol in (3) may be neglected in this case. Consequently
\[
U(t, -\infty; \varepsilon) \approx \mathbb{B}(t) \exp \left[ -i\gamma (1/\varepsilon)^{\infty} \sum_{n=0}^{\infty} (-i\gamma)^n (1/n+1)e^{int} \langle H_j \mathbb{B}^{(n)} \rangle \right]
\]
\[
= \mathbb{B}(t) \exp \left[ -i\gamma (1/\varepsilon) \langle H_j \mathbb{B} \rangle -igt \langle H_j \mathbb{B} \rangle + \text{higher order term of } \varepsilon \right].
\]
From this form of \( U(t, -\infty; \varepsilon) \) a few assertions can be derived.

\( U(t, -\infty; \varepsilon) \) has certainly adiabatic singularity and the character of singularity is essential.

\( V(t) \) describes the change of amplitude of the state function which has been under interaction from infinite past time.

Both \(-i\gamma (1/\varepsilon) \langle H_j \mathbb{B} \rangle\) and \(-ig \langle H_j \mathbb{B} \rangle t\) are the phase of system. The term \(-i\gamma (1/\varepsilon) \langle H_j \mathbb{B} \rangle\) is infinite for \( \varepsilon \to 0 \), namely, this term may be interpreted as the infinite part of the phase of the dynamical system. Our dynamical system starts movement at the infinite past time. This situation produces the infinite part of the phase of the state function. On the contrary, \(-ig \langle H_j \mathbb{B} \rangle t\) is finite. This finite phase corresponds to energy deviation of systems, that is to say, \( g \langle H_j \mathbb{B} \rangle \).

If \( D \) is an arbitrary operator which commutes with \( H_0 \), \( D^{-1} g \langle H_j \mathbb{B} \rangle D \) has the same eigenvalues as \( g \langle H_j \mathbb{B} \rangle \). Putting
\[
W = \mathbb{B} D,
\tag{27}
\]
\( W \) is the general wave matrix, too. Because of (25), we can easily gain
\[
HW = W[H_0 + \mathcal{A}],
\tag{28}
\]
where
\[
\mathcal{A} = gD^{-1}\langle H_j \mathbb{B} \rangle D.
\tag{29}
\]
\( \mathbb{B} \) has a special property, that is to say,
\[
\langle \mathbb{B} \rangle = 1,
\]
but \( W \) has no such special property.

Certainly \( U(t, -\infty; \varepsilon) \) is unitary. Therefore as a matter of course, we can describe the bound state by \( U(t, -\infty; \varepsilon) \). But perhaps we can not expect this possibility for \( \mathbb{B} \).
This is caused by the implicit assumption that the operand of $V(t)$ is not singular for $\varepsilon \to 0$.\textsuperscript{5}

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