Time Scale and its Application in Perturbation Theory

S. Olszewski
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Z. Naturforsch. 46a, 313–320 (1991); received January 7, 1991

A circular scale of time is proposed and applied to the calculation of the Rayleigh-Schrödinger perturbation energy for a non-degenerate state.

1. Introduction

In physics, time is – in principle – a coordinate: in a non-relativistic theory this coordinate may vary independently of the spatial coordinates, whereas in a relativistic case the time coordinate is coupled with its spatial counterparts. This situation holds equally for classical and quantum physics. A scale of time is then assumed in which the time coordinate may vary from a minus infinity called the “past” to a plus infinity called the “future”. A time scale of this kind we call linear, see Figure 1.

One of the applications of a time scale is perturbation theory. In reality, the perturbation calculation based on a linear scale of time is quite complicated: we construct the time-dependent vacuum amplitude for a given perturbation order, then calculate its logarithm and differentiate with respect to time, see e.g. [1]. Going with the time variable, corrected by an imaginary infinitesimal part, to infinity we find all the components of the perturbation series. The procedure is not straightforward, especially because there exists a diagrammatical representation for the vacuum amplitude but not for the limit of the logarithmic time derivative, exhibiting some lack in the diagrammatical representation for the individual terms of the perturbation series.

The purpose of the present paper is to indicate that a time scale which is different from linear may be – at least in some cases – also of use. This is done for the perturbation calculation of a non-degenerate and non-relativistic quantum-mechanical energy state. The applied scale is topologically equivalent to a circle, which means that the end point and the beginning point on the scale merge, see Figure 2. A scale of this kind may occur also to be more natural for some classical systems, for example a perfect harmonic oscillator: since there is no physical parameter in such an oscillator which enables us to distinguish between one and another oscillation periods, the same should apply to the time variable.

2. Rayleigh-Schrödinger One-Particle Perturbation Theory

The non-relativistic Rayleigh-Schrödinger (RS) perturbation theory can be useful even to a high perturbation order, see e.g. [2]. As mentioned above, the perturbation energy \(\Delta E\) of a one-particle system in state \(n\) can be represented with the aid of the time-dependent quantum vacuum amplitude \(R(t)\) for this system [1]. This amplitude is the sum of probability amplitudes for all various ways, the system can start from its initial (unperturbed) state, scatter on a perturbation potential \(V(r)\) zero, one, or more times and return to the unperturbed state. The linked-cluster
theorem gives
\[ \Delta E = \lim_{t \to -\infty} i \frac{d}{dt} \ln R(t) \]
\[ = \lim_{t \to -\infty} i \frac{d}{dt} \left\{ (-1)^n \int_0^t i G_\infty(n,t_1-t) + \sum_{p+n} (-1)^p V_{np} V_{pn} \int_0^1 i \int_0^t i G_\infty(p,t_2-t_1)i G_\infty(n,t_1-t_2) \right\} \]

where \( \eta \) is an infinitesimal, yet positive number; for an unperturbed energy state \( E_k \) we have
\[ G_\infty(k,t_2-t_1) = \Theta_{t_2-t_1} \exp \{ -i E_k(t_2-t_1) \}, \] (2)
\[ = i \quad \text{for} \quad t_2 = t_1; \]
\[ G_\infty^*(k,t_2-t_1) = -i \frac{d}{dt} \Theta_{t_2-t_1} \exp \{ -i E_k(t_2-t_1) \}, \] (3)
\[ = 0 \quad \text{for} \quad t_2 = t_1; \]
\[ \Theta_{t_2-t_1} = 1 \quad \text{if} \quad t_2 > t_1, \]
\[ = 0 \quad \text{if} \quad t_2 < t_1, \] (4)

\( V_{np}, V_{pn}, \ldots \) are the matrix elements between the unperturbed one-particle wave functions and the perturbation potential. A graphical representation of (1) is

\[ \Delta E = \lim_{t \to -\infty} i \frac{d}{dt} \left[ + \right] \]

where in the square brackets we have the 1st, 2nd, 3rd, 4th... order diagrams. The representation corresponds to a sequence of scattering events \( t_1, t_2, t_3, t_4 \ldots \) which can be arranged, however, in different ways. For example, for a fourth perturbation order, the scattering events – beyond \( t_1 \) – can be arranged as
\[ t_2, t_3, t_4, \]
\[ t_4, t_2, t_3, t_2, \]
\[ t_4, t_2, t_3, t_4, \]
\[ t_3, t_2, t_4, t_3, \]
\[ t_3, t_2, t_4, t_3, \]
which exhausts all linked diagrams of order 4 which enter representation (5). In effect, the number \( L_N \) of the linked diagrams of order \( N \) entering (5) is
\[ L_N = (N-1)! \] (7)

This is not a satisfactory situation since, in fact, the number of terms which are given, for example, by the Brueckner-Huby bracketing technique [3, 4] and enter

apply some postulates concerning the sequence of scattering events on a circular time scale. On the second step we show for this scale that the same combination of the scattering events which leads to \( \Delta E \) gives also corresponding diagrams for the RS terms.

3. Time Scale and the Main Term of the RS Theory

Similarly to Sect. 2 we assume the \( N \)-th order perturbation to be connected with \( N \) time intervals
\[ \{ t' \} : \quad t_{(01)} < t' < t_{(1)} , \quad n \to p, \]
\[ \{ t'' \} : \quad t_{(02)} < t'' < t_{(2)} , \quad p \to q, \]
\[ . . . . . . . . . . . . . . . \]
\[ \{ t^{(N)} \} : \quad t_{(0N)} < t^{(N)} < t_{(N)} , \quad z \to n \] (10)
during which a system from its initial state \( n \) comes back to this state. During the first interval \( n \) is scattered to \( p \), during the second one \( p \) is scattered to \( q \), in
the last interval $z$ is scattered back to $n$; for $N = 1$ we have obviously the $n \rightarrow n$ scattering. [The superscripts of $t$ in (10) for time intervals further than the third one will be written in Roman style.] We postulate that a part of $\Delta E$ which corresponds to $N$, called $\Delta E^{(N)}$, is

$$\Delta E^{(N)} = \sum_c \Delta E^{(N)}_c,$$

where the sum is extended over all allowed sequence (cycles) of the time intervals for a given $N$. Any $\Delta E^{(N)}_c$ contributed by a cycle is obtained from the equation

$$\Delta E^{(N)}_c \cdot \tau^{(N)}_c = 0 \int dt + \int dt \psi^*_c(r, t) \hat{V}(r) \psi_c(r, t),$$

(11)

where $\tau^{(N)}_c$ is the length of the last time interval in a cycle.

$$\psi_c(r, t) = \exp \{-iE_c t\} \varphi_c(r),$$

(12)

$$\psi^*_c(r, t) = \exp \{-iE^{(N)}_c t\} \varphi^*_c(r),$$

(12a)

($h = 1$) and the symbol $S$ means that integrations have to be performed in (11) over all time intervals in a given cycle. Because of (12) and (12a) the integration over $r$ and $t$ in (11) can be separated. The integral over $r$ extended over the whole space we call the static part of the matrix element (11), whereas the integral over $t$ is a kinetic part of this element. The static part gives a constant, whereas the kinetic part is a value dependent on the limits of the time interval. We see from (10) that $\psi_c(r, t)$ of a given time interval is equal to $\psi^*_c(r, t)$ of a preceding interval. Moreover, $\psi_c(r, t) = \psi_{N}(r, t)$ for any $t$ belonging to $\{t^{(N)}\}$, the last time interval in each cycle. During any of the time intervals $\{t^{(1)}\}, \{t^{(2)}\}, \ldots \{t^{(N)}\}$ the space-dependent perturbation potential does not change its form, so

$$V(r') = V(r),$$

$$V(r'') = V(r),$$

$$\ldots \ldots$$

$$V(r^{(N)}) = V(r).$$

(13)

Putting $\beta = p$, the first component in (11) is [see (10) and (13)]

$$\int dt' \int dt'' \exp \{iE' t'\} \varphi^*_c(r') V(r') \exp \{-iE' t''\} \varphi_c(r'')$$

$$= U_{np}(E_n - E_p)^{-1} \cdot \exp \{i(E_n - E_p) \cdot \tau^{(1)}\} - \exp \{i(E_n - E_p) \cdot \tau^{(01)}\},$$

(14)

where

$$U_{np} = \int \varphi^*_n(r') V(r') \varphi_p(r') dr' \equiv \langle n | V | p \rangle.$$ (15)

We assume the upper limit of $\{t''\}$ to be a definite number, but the lower limit is an undefined number. Therefore, the second term within the square brackets in (14) oscillates, giving an average value tending to zero. This will apply to the value at the lower limit of any integral over $t$, the example of which is represented in (14). On the other hand, we postulate that the upper limit $\tau^{(1)}$ becomes within the second time interval $\{t''\}$ equal to the variable $t''$, viz.

$$\tau^{(1)} \Rightarrow t''$$

(16)

so the integration over the intervals $\{t^{(1)}\}, \{t^{(2)}\}$ together with that performed over $r'$, $r''$ gives

$$U_{np} \frac{1}{E_n - E_p} \int dt'' \int dt''^* \exp \{iE_p t''\} \varphi^*_p(r'') V(r'') \exp \{-iE_p t''^*\} \varphi_p(r'') \exp \{i(E_n - E_p) t''\} \exp \{i(E_n - E_n) t''^*\}$$

$$= U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} \exp \{i(E_n - E_q) \cdot \tau^{(1)}\}$$

(17)

on the condition that the reasoning concerning the limits of $\{t'\}$ presented below (15) is applied also in the case of the limits of $\{t''\}$. The calculation procedure can be extended to an arbitrary number of intervals (10) accompanied by the integration done over the corresponding space variable and the potential (13). In case $\{t^{(1)}\}$ is a last interval in a cycle we obtain as total result of the integration over $\{t^{(1)}\}, \{t^{(2)}\}, \ldots \{t^{(N)}\}$ and those over $r'$, $r''$, $r'''$:

$$U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} \int dt''' \int dt''^* \exp \{iE_p t'''\} \varphi^*_p(r''') V(r''') \exp \{-iE_p t''^*\} \varphi_p(r''')$$

$$= U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} U_{q e} \int dt''^* \exp \{i(E_n - E_q) \cdot \tau^{(3)}\}$$

(18)

where – similarly to (16) – we have put under the integral

$$\tau^{(3)} \equiv t''.$$
Expression (18) substituted into (11) gives $\Delta E^{(3)}_c = \Delta E^{(3)}_m$, which we call the main term of $\Delta E^{(3)}$. Similarly $\Delta E^{(N)}_m$ can be obtained for any $N$ in the way indicated above, which means that the upper limit $t(N-1)$ of an interval $\{t^{(v-1)}\}$ enters the next interval $\{t^{(v)}\}$ as a variable $t^{(v)}$.

4. Elimination principle for equal times

Our purpose is now to get the remainder of $S_N - 1$ terms $\Delta E^{(N)}_i$ which enter $\Delta E^{(N)}$ beyond $\Delta E^{(N)}_m$. A guide to find the cycles for the components of the perturbation series other than $\Delta E^{(N)}_m$ is the elimination principle. In the calculations of Sect. 3, (10), we assumed tacitly that the time variable in any interval is larger than in a preceding interval:

$$\{t'\} < \{t''\} < \{t'''\} < \ldots < \{t^{(N-1)}\} < \{t^{(N)}\}. \quad (20)$$

The elimination principle assumes that the sequence given in (20) — except for the last inequality $\{t^{(N-1)}\} < \{t^{(N)}\}$ — may be violated. For example, for $N = 4$ we may have the following time contractions:

$$\{t'\} = \{t''\}, \quad (21)$$
$$\{t''\} = \{t'''\}, \quad (21a)$$
$$\{t'\} = \{t'''\}, \quad (21b)$$

and

$$\{t'\} = \{t''\} = \{t'''\}. \quad (21c)$$

We shall demonstrate that any of the allowed contractions represent a term of the RS series; in effect, for $N = 4$ the contractions (21) – (21c) together with the main term represented by the sequence

$$\{t'\} < \{t''\} < \{t'''\} < \{t^{IV}\} \quad (20a)$$

(and calculated according to Sec. 3) give the total number

$$S_4 = \frac{(2 * 4 - 2)!}{4! (4-1)} = \frac{6!}{4! 3!} = 5 \quad (22)$$

of the perturbation terms of order 4. The allowed contractions can be chosen according to the following topological rule. Let us set consecutively $N$ time intervals on a circular scale of time beginning from some point $v$ which is also the end point on the scale; see Figure 3. If all $N-1$ points beyond $v$ representing the interval ends are projected to any other point different from $v$ in the way that projection lines do not cross we...
obtain the time contractions for all terms of the RS series of order $N$. The examples of corresponding allowed diagrams are represented in Figs. 4 and 5; an example of a forbidden diagram is represented on Figure 6. In the present Section we show how contractions may give the perturbation terms. First we postulate that a contraction between two intervals which have the end points say $p$ and $q$, see (10), leads to an equality

$$\exp\{-iE_p t'\} \phi_p(r') = \exp\{-iE_q t''\} \phi_q(r'')$$  \hspace{1cm} (23)

for any $t'$, $t''$, $r'$, and $r''$, so

$$E_p = E_q;$$ \hspace{1cm} (23a)

a similar contraction between $p$ and $r$ would mean

$$\exp\{-iE_p t'\} \phi_p(r') = \exp\{-iE_r t''\} \phi_r(r''),$$ \hspace{1cm} (24)

$$E_p = E_r;$$ \hspace{1cm} (24a)

e tc. We apply (23)–(23a) and (23)–(24a), respectively, in the calculation of the RS terms represented by (21) and (21 b). The first interval of time gives, see (14) and inferences below (15),

$$U_{np}(E_n - E_p)^{-1} \exp\{i(E_n - E_p) t_{(1)}\},$$ \hspace{1cm} (14a)

$$U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} \int \frac{d(r' = r''')}{{(t' = t''; \ t_{(1)} = t_{(3)})}} \int \frac{d(t' = t'')}{{(t' = t''; \ t_{(1)} = t_{(2)})}} \cdot \exp\{-i(E_p = E_q)(t'' = t''')\} \phi_{r = q}(r' = r'') \exp\{i(E_n - E_q)(t'' = t''')\} = U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} U_{qp} \frac{1}{E_n - E_p} \cdot \exp\{i(E_n - E_q) t_{(2)} = t_{(3)}\},$$ \hspace{1cm} (26)

whereas for the case of (21 b) we have

$$U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} \int \frac{d(r' = r''')}{{(t' = t''; \ t_{(1)} = t_{(3)})}} \int \frac{d(t' = t'')}{{(t' = t''; \ t_{(1)} = t_{(2)})}} \cdot \exp\{-i(E_r = E_p)(t' = t''')\} \phi_{r = p}(r = r'') \exp\{i(E_n - E_q)(t' = t''')\} = U_{np} \frac{1}{E_n - E_p} U_{pq} \frac{1}{E_n - E_q} U_{qp} \frac{1}{E_n - E_p} \cdot \exp\{i(E_n - E_p)(t_{(1)} = t_{(3)})\},$$ \hspace{1cm} (27)

In case of the contraction (21 c) we apply – on the first step – the result for (21) given in (25). We have

$$U_{np}(E_n - E_p)^{-2} U_{pp} \int \frac{d(r' = r''')}{(t' = t'''; \ t_{(1)} = t_{(3)})} \int \frac{d(t' = t'')}{{(t' = t''; \ t_{(1)} = t_{(2)})}} \cdot \exp\{-i(E_r = E_p)(t' = t''')\} \phi_{r = p}(r' = r'') \exp\{i(E_n - E_p)(t' = t''')\} \cdot \exp\{i(E_n - E_p)(t_{(1)} = t_{(3)})\} \cdot \exp\{i(E_n - E_p)(t_{(2)} = t_{(3)})\}.$$ \hspace{1cm} (28)
Fig. 7. Diagrams for the perturbation orders from $N = 1$ to $N = 6$; the beginning-end point is represented by $v$; arrows above the point symbols are omitted; the contractions on the scale are represented by colons. The diagram for the main term of order $N$ is labeled by $O_N$. 
where again in the last term under the integral the substitution (19) is taken into account together with (21c).

In order to get the integral over the whole cycle, expression (25) has to be integrated over $t''', r'''$ and $t''$, $r''$, whereas (26), (27) and (28) solely over $t''$, $r''$. This is done according to the rules given in Section 3. We obtain from (25):

$$U_{np}(E_n - E_p)\cdot U_{pp}(E_n - E_p)\cdot U_{rn} \cdot \tau_{(4)};$$

from (26):

$$U_{np}(E_n - E_p)\cdot U_{pq}(E_n - E_q)\cdot U_{qn} \cdot \tau_{(4)};$$

from (27):

$$U_{np}(E_n - E_p)\cdot U_{pq}(E_n - E_q)\cdot U_{pm} \cdot \tau_{(4)};$$

and from (28):

$$U_{np}(E_n - E_p)\cdot U_{pp} U_{pp} U_{pm} \cdot \tau_{(4)}.$$  

5. Postulate concerning the static part and the sign of $\Delta E_c^{(N)}$

The static part of $\Delta E_c^{(N)}$ is essentially a product of the matrix elements $U_{np}$, the number of which is equal to $N$. For example, the static part of the main term for $N = 4$ is

$$U_{np} U_{pq} U_{qr} U_{rn};$$

see Section 3. Time contractions make that some indices entering the main static part given in (33) repeat more than twice whereas other indices are cancelled. For example the time contractions (21), (21a), (21b), and (21c) discussed in Sect. 4 give respectively

$$U_{np} U_{pp} U_{pp} U_{rn},$$

$$U_{np} U_{pq} U_{qq} U_{qq},$$

$$U_{np} U_{pq} U_{qp} U_{pm},$$

$$U_{np} U_{pp} U_{pp} U_{pm}.$$  

Any contraction gives a loop, or loops, on a diagram representing a given cycle of time intervals, and we postulate that the static part corresponding to any loop should be: (i) independent of the position of this loop in a cycle; (ii) equal to the static part of the same loop when it represents a separate cycle. For example, $U_{pp}$ in (34) comes from the loop with only one point on the loop, and we postulate that this static part should be equal to $U_{nn}$, which is a static part for the loop of the same kind making a cycle for its own; the same concerns the loop giving $U_{qq}$ (34a), and two loops giving $U_{pp} U_{pp}$, (34c). On the next step the product, $U_{pq} U_{qp}$ in (34b) comes from a loop which has two
Table I. The correspondence between the diagrams of Fig. 7 and the Brueckner-Huby terms for the RS perturbation series for energy of a non-degenerate state. Perturbation orders from \( N = 1 \) to \( N = 6 \) are examined. The points on diagrams in which 2, 3, 4... loops touch give, respectively, \( P^2 \), \( P^3 \), \( P^4 \), ... and the arcs on the loops between the points are represented by \( V \).

<table>
<thead>
<tr>
<th>( N )</th>
<th>( \langle V \rangle )</th>
<th>( \langle VP^2 \rangle )</th>
<th>( \langle VP^3 \rangle )</th>
<th>( \langle VP^4 \rangle )</th>
<th>( \langle VP^5 \rangle )</th>
<th>( \langle VP^6 \rangle )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( O_1 )</td>
<td>( I_1 )</td>
<td>( II_1 )</td>
<td>( III_1 )</td>
<td>( IV_1 )</td>
<td>( V_1 )</td>
</tr>
<tr>
<td>2</td>
<td>( O_2 )</td>
<td>( I_2 )</td>
<td>( II_2 )</td>
<td>( III_2 )</td>
<td>( IV_2 )</td>
<td>( V_2 )</td>
</tr>
<tr>
<td>3</td>
<td>( O_3 )</td>
<td>( I_3 )</td>
<td>( II_3 )</td>
<td>( III_3 )</td>
<td>( IV_3 )</td>
<td>( V_3 )</td>
</tr>
<tr>
<td>4</td>
<td>( O_4 )</td>
<td>( I_4 )</td>
<td>( II_4 )</td>
<td>( III_4 )</td>
<td>( IV_4 )</td>
<td>( V_4 )</td>
</tr>
<tr>
<td>5</td>
<td>( O_5 )</td>
<td>( I_5 )</td>
<td>( II_5 )</td>
<td>( III_5 )</td>
<td>( IV_5 )</td>
<td>( V_5 )</td>
</tr>
<tr>
<td>6</td>
<td>( O_6 )</td>
<td>( I_6 )</td>
<td>( II_6 )</td>
<td>( III_6 )</td>
<td>( IV_6 )</td>
<td>( V_6 )</td>
</tr>
</tbody>
</table>

where any term, or product of terms, which begins and ends with the subscript \( n \) corresponds to one loop. This procedure can be extended to any cycle. For example, for \( N = 6 \) we have one (main) cycle represented by one loop and 41 cycles having diagrams composed of more than one loop. The diagrams for \( N = 1, 2, ..., 6 \) are represented on Figure 7. With the aid of the postulate given above any of the diagrams gives some \( \Delta E^{(N)} \) which is equal to some Brueckner-Huby (BH) term. A full list representing the correspondence between diagrams and the BH terms for \( N = 1, 2, ..., 6 \) is given in Table 1. Any bracket

\[
\langle VP^2 VP^3 VP^4 ... V \rangle
\]

represents one loop. The sequence \( VVV ... V \) within the bracket is an abbreviated formula for

\[
U_{np} U_{pq} U_{qr} ... U_{zn},
\]

whereas the sequence \( P^2 P^3 P^4 ... \) is for

\[
(E_n - E_p)^{-3} (E_n - E_q)^{-2} (E_n - E_p)^{-1} ...
\]

In a final result for the RS series any sum over \( p, q, r ... \) is done separately for each loop. The sign of \( \Delta E^{(N)} \) is defined by the number \( l \) of loops in the diagram by the formula

\[
(-1)^{l+1}.
\]

This formula completes the representation of the RS series with the aid of \( \Delta E^{(N)} \).

Acknowledgement

I am grateful to T. Kwiatkowski for his assistance in preparing the manuscript and to Dr. P. Modrak for his comments.