The Hydrogen Atom in Strong Electric Fields:
Summation of the Weak Field Series Expansion

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ABSTRACT

The order dependent mapping method, its convergence has recently been proven for the energy eigenvalue of the anharmonic oscillator, is applied to re-sum the standard perturbation series for Stark effect of the hydrogen atom. We perform a numerical experiment up to the fiftieth order of the perturbation expansion. A simple mapping suggested by the analytic structure and the strong field behavior gives an excellent agreement with the exact value for an intermediate range of the electric field, $0.03 \leq E \leq 0.25$. The imaginary part of the energy (the decay width) as well as the real part of the energy is reproduced from the standard perturbation series.
Quite often the perturbation series in quantum theory is not only divergent but even non-Borel summable [1]. Such a non-Borel summability is sometimes known to have its physical origin. For quantum mechanics with an unstable potential or degenerated potential minima the tunneling (barrier penetration) effect gives the Borel singularity [2]. For a uniform electric field in QED, it can explicitly be shown [3] that the instability of the vacuum state causes the non-Borel summability. One may even conjecture [3] that the Borel singularity in QED and QCD is an indication of the instability of the perturbative vacuum.

The above observations in turn suggest a possibility that for certain case the standard perturbation series has enough information on the quantum tunneling (or the vacuum instability) that is usually regarded as “non-perturbative” effect.

Recently Kleinert [4] has made an interesting observation that the decay width (imaginary part of the energy eigenvalue) for an unstable potential (anharmonic oscillator (AHO) with the negative coupling $g < 0$) can precisely be reproduced only by using the perturbation series of the energy eigenvalue of AHO, hence explicitly implemented the above possibility. His method is based on the so-called delta expansion [5] (variational perturbation method) that is a special case of the order dependent mapping method (ODM) [6,7]. The convergence of the method for AHO has later been rigorously proven [8] for $|g| \geq g_0$ ($g_0$ is the radius of convergence of the strong coupling expansion $g_0 \sim 0.1$). The proof itself [8] is applicable for other quantum systems if one has enough information on the analyticity and the strong coupling behavior of the interested quantity.

In this article, we take a simple quantum mechanical system for which the perturbation expansion exhibits the Borel singularity on the positive real axes and apply ODM to re-sum the standard perturbative expansion. The physical origin of the non Borel summability in this system is the instability of the “vacuum.”

We consider the ground state energy of the hydrogen atom in a uniform electric
field (Stark effect),

\[
\left( -\frac{\hbar^2}{2m_e} \nabla^2 - \frac{e^2}{r} - eEZ \right) \Psi = \mathcal{E} \Psi. \tag{1}
\]

This system is unstable due to quantum tunneling (or spontaneous ionization) and thus the energy eigenvalue of the quasi-ground state has the imaginary part \((= -\Gamma/2)^*\).

On the other hand, the standard weak field expansion of the “ground state” energy reads†

\[
\mathcal{E}(E) \sim \sum_{n=0}^{\infty} a_n E^{2n}, \tag{2}
\]

where the first several coefficients are

\[
\begin{align*}
& a_0 = -1/2, \quad a_1 = -9/4, \quad a_2 = -3 \, 555/64, \\
& a_3 = -2 \, 512 \, 779/512, \quad a_4 = -13 \, 012 \, 777 \, 803/16 \, 384, \\
& a_5 = -25 \, 497 \, 693 \, 122 \, 265/131 \, 072.
\end{align*} \tag{3}
\]

(An economical way to compute the higher order coefficients \(a_n\) is summarized in Appendix.) The simple (truncated) sum of the series is of course real for \(E\) real. Note all the coefficients have the same sign. In what follows we will apply ODM [6,7] to this standard weak field expansion and see how the exact energy eigenvalue (that is complex) emerges.

As was emphasized in [8], knowledge on the analytical property and the strong coupling (field) behavior of the physical quantity are crucial for applying ODM.

* In what follows, the energy \(\mathcal{E}\) and the field strength \(E\) are measured respectively by, \(2(\text{Ry}) = m_e e^4/\hbar^2 = 27.21\text{(eV)}\) and \(1(\text{a.u.}) = m_e^2 e^5/\hbar^4 = 5.142 \times 10^9(\text{V/cm})\). Under a realistic condition in laboratory, the maximum strength of the electric field is \(E \sim 2 \times 10^{-4}(\text{a.u.})\), and practically is in the validity region of the standard perturbation theory and WKB approximation. The aim of this article is thus somewhat academic and to investigate how one can extract information from a badly divergent (and non-Borel summable) perturbation series.

† Since the perturbation hamiltonian has an odd parity, only the even powers of the electric field survives in the expansion for the ground state energy.
For the quasi-ground state of (1): i) The energy eigenvalue $\mathcal{E}(E)$ is analytic on the cut $E$ plane at least in the vicinity of the origin and the cut is along positive real axis of $E$, as well as the negative axis, due to the quantum tunneling [9]. $\mathcal{E}(E)$ is analytic on cut $-E^2$ plane (at least in the vicinity of the origin), only the negative real axis being the cut. ii) The discontinuity along the cut is given by the WKB formula (for $E > 0$)

$$\text{Im} \mathcal{E}(E) = -\frac{2\sqrt{2}}{1 + \sqrt{2}} e^{\sqrt{2} - \pi/4} E^{-1} e^{-2/(3E)} (1 + O(E)) \sim -2E^{-1} e^{-2/(3E)}. \quad (4)$$

The above two properties in turn give the large order behavior of the perturbation coefficients in (2) [10]

$$a_n \sim -\frac{4}{\pi} \left(\frac{3}{2}\right)^{2n+1} (2n)!. \quad (5)$$

Corresponding to the instability of the ground state, the series is non-Borel summable. iii) The strong field behavior [10] is given by

$$\arg \mathcal{E} \sim -\pi/3 + O((\ln E)^{-1}),$$

$$|\mathcal{E}| \sim 2^{-5/3} E^{2/3} (\ln E)^{2/3} + \frac{2^{4/3}}{3} E^{2/3} (\ln \ln E) (\ln E)^{-1/3} + O(E^{2/3} (\ln E)^{-1/3}). \quad (6)$$

This is an asymptotic expansion in contrast to the convergent strong coupling expansion in AHO case.

In ODM [6,7], one first map the coupling constant $E$ to another variable $\lambda$ by some function $F(\lambda)$

$$E = \rho F(\lambda), \quad F(\lambda) = \lambda + O(\lambda^2), \quad (7)$$

and factorize the original function with some prefactor function $f(\lambda)$

$$\mathcal{E}(E) = f(\lambda) \Psi(\lambda), \quad (8)$$

and expand $\Psi(\lambda)$ with respect to $\lambda$. The parameter of the mapping $\rho$ is determined order by order by some condition. The choice of $F(\lambda)$ and $f(\lambda)$ is crucial for the
convergence property of the method, and is constrained by the analytic property
and the strong field behavior of $\mathcal{E}(E)$ [6,7,8].

In the case of AHO [6,8], the (known) best choice of the mapping is equivalent
to the delta expansion [5] which starts from a decomposition of the hamiltonian

$$H = -\frac{1}{2}\rho^2 + \frac{\Omega^2}{2} q^2 + \delta \left( \frac{\omega^2 - \Omega^2}{2} q^2 + \frac{g}{4} q^4 \right),$$

and the expansion with respect to $\delta$ (and finally $\delta = 1$). The variational parameter
$\Omega$ (which corresponds to $\rho$ in ODM) is determined order by order of the expansion
by some condition. It can be shown [8] that the sequence obtained in this way
converges to the exact energy eigenvalue for a wide range of complex $g$.

As our first choice of the mapping in the present problem we may therefore
start from a decomposed hamiltonian:

$$H = -\frac{1}{2} \nabla^2 - \frac{Z}{r} + \delta \left( \frac{Z - 1}{r} - Ez \right),$$

where in the spirit of the delta expansion, we have introduced a variational pa-
parameter $Z$. The expansion is done with respect to $\delta$ (and finally $\delta = 1$) and $Z$ is
determined order by order by some condition. As for AHO [6], it is easy to see the
expansion is equivalent to a mapping

$$E = \rho \frac{\lambda}{(1 - \lambda)^3},$$

and a factorization

$$\mathcal{E}(E) = \frac{1}{(1 - \lambda)^2} \Psi(\lambda).$$

The relation of parameters in both methods is given by (setting $\delta = 1$)

$$\lambda = 1 - \frac{1}{Z}, \quad \rho = \frac{E}{Z^2(Z - 1)}.$$
The expansion of $\Psi(\lambda)$ up to $N$th order reads

$$\Psi_N(\lambda) = \sum_{n=0}^{N} b_n(\rho)\lambda^n$$  \hfill (14)

where

$$b_0(\rho) = a_0, \quad b_1(\rho) = -2a_0, \quad b_2(\rho) = a_0 + a_1\rho^2,$$

$$b_n(\rho) = \frac{[n/2]}{(n-2m)!(6m-3)!} a_m\rho^{2m}, \text{ for } n \geq 3. \hfill (15)$$

As the condition to fix $\rho$ order by order, we use \cite{6,7},

$$\Psi_N(\lambda) - \Psi_{N-1}(\lambda) = 0,$$  \hfill (16)

and pick up the real positive solution for $\rho$ \cite{6,8}. We may use the other condition such as \cite{5} \(\partial((1 - \lambda)^{-2}\Psi_N)/\partial\rho = 0\) as well. In the case of AHO, the convergence property is known to be insensitive \cite{8} to such a choice of the condition.

At first sight, the choice in (11) and (12) seems to be well suited to the strong field behavior of $\mathcal{E}$ (6): For $|E|$ large, $\lambda \sim 1$ and $E \sim (1 - \lambda)^{-3}$ from (11), so the prefactor in (12), $(1 - \lambda)^{-2} \sim E^{2/3}$ reproduces the correct power in (6). The logarithm in (6) cannot be reproduced in the present simple mapping.

We have done a numerical experiment based on the mapping (11) and (12) to $N = 50$. For an actual calculation of the perturbation coefficients $a_n$, see Appendix. For a wide range of $E$, we observed a violating oscillating behavior such that $\text{Re}\mathcal{E}(E) > 0$ for $E = 0.25$ from the first several orders. The mapping (11) and (12) completely fails.

The failure of the mapping (11) and (12) that is equivalent to a naive delta expansion like method (10), should clearly be related to the incompatibility of the mapping (11) and the analytic structure of $\mathcal{E}(E)$. As was shown for AHO \cite{8} the mapping should be chosen to be compatible with the analytic structure. In this sense, the surprising success of the delta expansion for AHO was somewhat
accidental. In ODM on the other hand we have a wide freedom to choose the form of the mapping and the decomposition\footnote{Of course it is quite possible that our choice of the variational parameter in (10) is not good enough to simulate the effect of the electric field. One may introduce more complicated form of the variational Hamiltonian. Note however that for such a general choice, a connection with the standard perturbation series is lost and hence the advantage of the delta expansion is too.}. In fact according to i) above the analogy with AHO case, for which the cut is only along the negative real axis, is not hold.

This observation suggests a use of \(-E^2\) instead of \(E\) as the fundamental variable for which the cut exists only along the negative real axis (at least in the vicinity of the origin). As the second choice therefor we take

\[-E^2 = \rho \frac{\lambda}{(1 - \lambda)^{\alpha}}, \tag{17}\]

and

\[E = \frac{1}{(1 - \lambda)^{\alpha/3}} \Psi(\lambda). \tag{18}\]

The form of the prefactor in (18) has been chosen to reproduce the \(E^{2/3}\) behavior in (6). Here we again abandon to reproduce the correct logarithmic behavior in (6) and hence we expect the present mapping fails for a large \(E\) anyway\footnote{Of course it is quite possible that our choice of the variational parameter in (10) is not good enough to simulate the effect of the electric field. One may introduce more complicated form of the variational Hamiltonian. Note however that for such a general choice, a connection with the standard perturbation series is lost and hence the advantage of the delta expansion is too.}. The coefficients \(b_n(\rho)\) in (14) now read

\[b_n(\rho) = \sum_{m=0}^{n} (-1)^m \frac{\Gamma(n + (\alpha - 1)m - \alpha/3)}{(n - m)!\Gamma(\alpha m - \alpha/3)} a_m \rho^m. \tag{19}\]

For the value of \(\alpha\), we do not have any criteria at present (see below) and the choice is a sort of guesswork. We examined \(\alpha = 3/2, 2, 5/2, 3, 7/2, 4\) and \(9/2\). We have again done numerical experiments up to \(N = 50\). The \(\rho\) is determined again by the condition (16) and the real solution for \(\rho\) is taken.

For \(\alpha = 3/2\), we observed a tendency of a slow convergence to a wrong answer, for example for \(E = 0.25\), \(\text{Re} E \rightarrow -0.63\) and \(\text{Im} E \rightarrow 0.1\). For \(\alpha = 2\), the sequence
again converges but to a wrong answer, namely $\text{Re} \mathcal{E} \to -0.54$ and $\text{Im} \mathcal{E} \to 0.05$. $\alpha = 4$ and $\alpha = 9/2$ cases do not work (slowly divergent). Among the above values, $\alpha = 5/2$, $\alpha = 3$, $\alpha = 7/2$ seems work and $\alpha = 3$ seems to give the fastest convergence. Therefore we will only report the result for $\alpha = 3$ in the following.

In Fig. 1, we have plotted the value of $\rho$ determined in this way. A numerical fitting gives a scaling on the order $N$:

$$\rho \sim 0.2851 N^{-1.686}. \quad (20)$$

In Figs. 2a and 2b, the relative error to the exact value of the energy (obtained by a numerical integration of the Schrödinger equation [11]) is depicted for a fixed value of the field strength $E = 0.25$ (2a for the real part and 2b for the imaginary part). A tendency of the fast convergence to $N = 50$ is observed.

Observing this convergent behavior, in Figs. 3a and 3b, we plotted $\text{Re} \mathcal{E}(E)$ and $\text{Im} \mathcal{E}(E)$ by ODM and the exact values [11] (full squares) in the intermediate range of the field strength. We see a surprisingly good agreement for the imaginary part as well as the real part.

As was mentioned above, for a strong field regime, we expect the method fails because the present mapping can only reproduce the correct power behavior in (6) but not the logarithmic corrections. To see this we have plotted $\text{Re} \mathcal{E}(E)$ and $\text{Im} \mathcal{E}(E)$ by ODM and the asymptotic behavior (6) (broken line) in Figs. 4a and 4b.

On the other hand, the experience in AHO case [8] suggest the method also fails to reproduce the imaginary part for the weak field region. In Table 1, the imaginary part obtained by WKB approximation (4) (which is a good approximation within this regime) and ODM are compared. It can be seen that ODM completely fails for $E < 0.025^*$.  

* For the real part of the energy, ODM gives an excellent result in this weak field regime.
In summary we have numerically observed that, at least for an intermediate range of the field strength, we can extract an accurate value of the imaginary part from the standard perturbation series by suitably choosing the mapping in ODM.

In spite of this success, the convergence proof of [8] cannot directly be applied to the present case: First of all, $\alpha = 3$ is a dangerous case in the view point of the proof [8] because the negative real of $-E^2$ is mapped to $\lambda$ with $|\lambda| < 1$ which obstructs the direct application of the proof. One have to extend the “contour” [8] to the outside of $|\lambda| > 1$ but this requires some knowledge on the analyticity on the higher Riemann sheet of $-E^2$ that is lacking at present.

Secondly the prefactor $(1 - \lambda)^{-1}$ (for $\alpha = 3$) in (18) is not sufficient to make $\Psi(\lambda)$ finite as $\lambda \to 1$, because of the logarithmic correction in (6). The boundedness of $\Psi(\lambda)$ at $\lambda = 1$ was another necessity condition for the convergence proof in [8].

Finally the fact that the observed power in (20) is larger than $-2$ is rather strange. Repeating the analysis of [8], the error of the method caused by the divergence of the perturbation series ($R_N^{(A)}$ part in [8]) is estimated as

$$|R_N^{(A)}| \sim \frac{2}{\pi} \left(\frac{3}{2}\right)^{2N+1/2} \frac{|\lambda|^N}{|1 - \lambda|^N} \rho^N N \Gamma(2N + 1)(1 + O(1/N))$$

which diverges if the scaling (20) retaines for $N \to \infty$ and is in fact $\sim 156$ for $N = 50$ and $E = 0.25$ (The relative error $\sim 26300\%$). This clearly contradicts with the observed fast convergence in Figs 2a and 2b. The convergence mechanism in [8] therefore cannot be applied in the present case. We need some new explanation such as a cancellation among $R_N^{(A)}$ part and $R_N^{(B)}$ part in [8]. The fact that $\Psi(\lambda)$ is not bounded at $\lambda = 1$ also suggests this possibility.

Obviously more theoretical study is needed to explain the empirical success of the mapping (17) with $\alpha = 3$. Nevertheless we believe our observation gives another concrete support for the possibility that one can in practice reproduce the exact property (tunneling or decay in the present case) of the physical quantity only relying on the standard perturbation series.
It is possible to reproduce the correct logarithmic behavior in (6) by using more complicated mapping such as the one in [7]. Although we do not try in this article, it is crucial if one wants an accurate value for a large $E$.

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**APPENDIX**

It is well known [12] that the Schrödinger equation (1) has a separated form in the parabolic coordinate $x = \sqrt{\lambda \mu} \cos \varphi$, $y = \sqrt{\lambda \mu} \sin \varphi$ and $z = (\lambda + \mu)/2$. The problem is then reduced to one-dimensional and we may apply the recursion formula technique in [13]. Setting

$$
\Psi = (\xi \eta)^{m/2} e^{-(\xi + \eta)/2} F(\xi) G(\eta),
$$

(A.1)

($m$ is the magnetic quantum number) where

$$
\xi = \sqrt{-2\varepsilon \lambda}, \quad \eta = \sqrt{-2\varepsilon \mu},
$$

(A.2)

we have

$$
\xi F'' + (m + 1 - \xi) F' - \left( \frac{1}{2} m + \frac{1}{2} - \sigma - \frac{g^2}{4} \xi^2 \right) F = 0,
$$

\[ \xi G'' + (m + 1 - \xi) G' - \left( \frac{1}{2} m + \frac{1}{2} - \tau + \frac{g^2}{4} \xi^2 \right) G = 0. \]

(A.3)

Here $\sigma$ and $\tau$ are the separation constants and the “coupling constant” $g$ is defined by

$$
\sigma + \tau = \frac{1}{\sqrt{-2\varepsilon}}, \quad g = \frac{E}{(-2\varepsilon)^{3/2}}.
$$

(A.4)

In what follows we consider only the case $m = 0$. 

10
We define the “perturbative expansion”

\[ \sigma = \sum_{k=0}^{\infty} \sigma_k g^k, \quad F(\xi) = \sum_{j=0}^{\infty} F_j(\xi) g^j. \quad (A.5) \]

The zeroth order solution is given by \( \sigma_0 = 1/2 \) and \( F_0(\xi) = 1 \). The equation (A.3) has a polynomial solution order by order in \( g \). Hence we further set

\[ F_j(\xi) = \sum_{l=1}^{2j} f_{j,l} \xi^l, \quad \text{for} \quad j \geq 1. \quad (A.6) \]

Eq. (A.3) then becomes a set of recursion relations:

\[ \sigma_j = -f_{j,1}, \quad (A.7) \]

and

\[ (l + 1)^2 f_{j,l+1} - l f_{j,l} + \sum_{k=1}^{j-1} \sigma_k f_{j-k,l} - \frac{1}{4} f_{j-1,l-2} = 0, \quad (A.8) \]

for \( j \geq 1 \) (\( f_{0,0} = 1 \) and \( f_{0,l} = 0 \) for \( l > 0 \)).

We have numerically solved (A.7) and (A.8) by FORTRAN in double precision up to \( \sigma_{100} \). We then have used a symbolic manipulation package MATHEMATICA to invert (A.4) (note \( \tau = \sum_{k=0}^{\infty} (-1)^k \sigma_k g^k \)) for obtaining the perturbation coefficients \( a_n \) in (2) up to \( a_{50} \).

To examine the quality of our numerical value for \( a_n \), we plotted the ratio of \( a_n \) to the asymptotic behavior (5) in Fig. 5.
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Table Caption

Table 1 Comparison of ODM with WKB formula (4) in the weak field region.

Figure Captions

Fig. 1 Scaling of $\rho$ with respect to the order of ODM $N$. $\rho$ is fixed by the condition (16).

Fig. 2 The relative error of ODM (17) with $\alpha = 3$ (2a for the real part, 2b for the imaginary part) with respect to the order $N$.

Fig. 3 The real part (3a) and the imaginary part (3b) of the energy obtained by ODM in the intermediate region of the field strength. The full squares are the exact values [11].

Fig. 4 The real part (4a) and the imaginary part (4b) of the energy obtained by ODM in the strong region of the field strength. The asymptotic behavior (6) is depicted by broken lines.

Fig. 5 The ratio of the perturbative coefficients $a_n$ and the large order behavior (5).
| $E$  | $\text{Im}\,\mathcal{E}$ (WKB) | $\text{Im}\,\mathcal{E}$ (ODM) |
|------|-------------------------------|-------------------------------|
| 0.01 | $-2.44847 \times 10^{-27}$   | $-1.38778 \times 10^{-16}$   |
| 0.0125 | $-1.20942 \times 10^{-21}$   | $+1.09635 \times 10^{-16}$   |
| 0.015 | $-7.30789 \times 10^{-18}$   | $+7.32747 \times 10^{-14}$   |
| 0.0175 | $-3.58320 \times 10^{-15}$   | $+3.27433 \times 10^{-13}$   |
| 0.02  | $-3.66731 \times 10^{-13}$   | $-1.04966 \times 10^{-11}$   |
| 0.0225 | $-1.32341 \times 10^{-11}$   | $-1.66882 \times 10^{-10}$   |
| 0.025 | $-2.30534 \times 10^{-10}$   | $-1.66460 \times 10^{-9}$    |
| 0.0275 | $-2.36688 \times 10^{-9}$    | $-1.11321 \times 10^{-8}$    |
| 0.03  | $-1.63588 \times 10^{-8}$    | $-1.11321 \times 10^{-8}$    |

Table. 1
Fig. 1
Fig. 2a
Fig. 2b
Fig. 3a
Fig. 3b
Fig. 4a
Fig. 4b
