Quantum mechanics in the general quantum systems (V): Hamiltonian eigenvalues

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We derive out a complete series expression of Hamiltonian eigenvalues without any approximation and cut in the general quantum systems based on Wang’s formal framework [1]. In particular, we then propose a calculating approach of eigenvalues of arbitrary Hamiltonian via solving an algebra equation satisfied by a kernel function, which involves the contributions from all order perturbations. In order to verify the validity of our expressions and reveal the power of our approach, we calculate the ground state energy of a quartic anharmonic oscillator and have obtained good enough results comparing with the known one.

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I. INTRODUCTION

To determine the Hamiltonian eigenvalues is a basic problem in quantum mechanics. As is well known, the exact solution of the Schrödinger equation can be obtained only in some special cases, i.e., for several elementary systems like the hydrogen atom, the $H_2^+$ molecule, or the harmonic oscillator. In the majority of cases, approximation techniques have to be employed in calculation of the Hamiltonian eigenvalues in the general quantum systems, and the precision and computability become focus.

Perturbation theory is one of the few principal methods of approximating solutions to eigenvalue problems in quantum mechanics. The formalism of Rayleigh-Schrödinger perturbation expansion expresses an eigenvalue as a formal power series of the coupling constant $\lambda$:

$$E^{\text{total}}_\lambda = \sum_{m=0}^{\infty} c_m \lambda^m$$  \hspace{1cm} (1)

At the 4th order perturbation level, the explicit form of $c_4$ has appeared a little complicated. Nevertheless, for a given $n$th order perturbation, one can obtain, in principle, the form of $c_n$ according to Kato’s [2] or Bloch’s [3] formal expression.

The normal perturbation theory frequently meets two problems: one is about whether the power series is convergent in some neighborhood of $\lambda = 0$ or it is only asymptotic as $\lambda \to 0$; another is about the strong coupling regime. While the problems of strong coupling is usually overcome with various kinds of renormalization techniques, for example, the renormalization scheme recently used by Čížek and Vrscay [4, 5], summation techniques are employed to give a divergent perturbation series any meaning beyond a mere formal expansion [6].

In our point of view, these problems closely connects with the whole and deep knowledge about the expansion (1) because the perturbation series is inherently multiple in the general quantum systems. In mathematics, a reasonable rearrangement of a multiple series is often significant when a cut approximation needs to be introduced. Consequently, we wonder whether the expansion as a power series of the coupling constant is a unique choice, and whether a more explicit expression of total Hamiltonian eigenvalues exists. Moreover, we would like to find a systematical and new approach for the calculation of Hamiltonian eigenvalues in the general quantum systems.

More than three year ago, An Min Wang, one of authors in this article, presented his research on a formal framework of quantum mechanics in the general quantum systems [1, 7, 8] and made a conjecture about the total Hamiltonian eigenvalues. Just based on Wang’s works, a complete series expression of Hamiltonian eigenvalues in a general quantum system without any approximation and cut is explicitly obtained by using some skills in mathematics and physics. This expression is simply not a power series of perturbed parameter, but a series of power of a kernel function as well as its derivatives that involves the contributions from all order perturbation. No cut and approximation are introduced, and the general term is given out. In special, our kernel function as well as its derivative is equal to $O(\lambda^2)$. It implies that our series is obviously improved in its approximation content not only involving the higher order contributions

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but also being more suitable to cut up to some given nth term since its decrease is more rapidly than the series in the normal theory. Of course, if expanding our expression of the total Hamiltonian according to the perturbed parameter, our expression is consistent with one in the normal perturbation theory. However, our expression really shows the physics nature because it directly comes from the law of quantum dynamics, but not a transcendent input–expansion according to the power of perturbed parameter which covers up a fact that perturbation series is inherently multiple in the general quantum systems. Moreover, it will be seen that the new conclusion can be obtained by our expression.

It is worthy to point out that it is inevitable and acceptable that the complete expression of Hamiltonian eigenvalues, just like ours, is an infinite series, because that a general quantum system has usually no a compact solution without any approximation. More importantly and interestingly, from our expression we further present a practical approach to find the total Hamiltonian eigenvalues only through solving an algebra equation satisfied by our kernel function, which is specially suitable to calculation in a computer. In order to verify the validity of expression of Hamiltonian eigenvalues and check the accuracy of calculation of Hamiltonian eigenvalues using our approach, we study, as an example, a quartic anharmonic oscillator in the normalization, which is frequently used as a test-stone of new methods of calculating the eigenvalues.

This article is organized in this way: in section II we give an overview on how to get our expression of the total Hamiltonian eigenvalues in the general quantum systems. The detail is put in four appendixes; in section III we present how to obtain the total Hamiltonian eigenvalues by solving a given algebraic equation; in section IV we calculate the ground state energy of the quartic anharmonic oscillator for different coupling constants; in section V, we make the summary.

II. DERIVATION: HAMILTONIAN EIGENVALUES

In the section, we would like to derive out an explicit expression of Hamiltonian eigenvalues in a general quantum system. Actually, our purpose is just to prove Wang’s conjecture proposed in his theoretical framework of quantum mechanics in the general quantum systems. In Wang’s work, the complete series expression of time evolution operator or transition amplitude in a solvable representation \( (H_0|\Psi^\gamma) = E_\gamma|\Psi^\gamma) \) is presented as

\[
E_\gamma = \sum_{l=0}^{\infty} A_l^{\gamma\gamma'} e^{-iE_\gamma t} \delta_{\gamma\gamma'} + E_\gamma t \prod_{k=1}^{l+1} \frac{E_{\gamma_{k+1}} - E_{\gamma_k}}{E_{\gamma_k}} \prod_{j=1, j \neq i}^{l+1} \delta_{\gamma_{j}, \gamma_{i}} e^{-iE_{\gamma_{j}} t}
\]

(2)

where

\[
A_0^{\gamma\gamma'} = e^{iE_{\gamma} t} \delta_{\gamma\gamma'}
\]

(3)

\[
A_l^{\gamma\gamma'} = \sum_{\gamma_1, \gamma_2, \ldots, \gamma_{l+1}} \delta_{\gamma_{l+1}} e^{-iE_{\gamma_{l+1}} t} \prod_{j=1, j \neq i}^{l+1} (E_{\gamma_{j}} - E_{\gamma_{i}}) \prod_{k=1}^{l} g_{\gamma_k \gamma_{k+1}}
\]

(4)

It is clear that Wang’s expression can be thought of to be exact in the sense that this series involves contributions from all order perturbations and has no any approximation. In above expression, for simplicity, we have not considered the degenerate cases. It is important that here we have used the following subtle method of dividing Hamiltonian matrix in the solvable \( H_0 \) representation

\[
\{H\} = \{H_0\} + \{H_1\} = \begin{pmatrix}
E_0 & E_1 & \cdots & E_\gamma & \cdots \\
E_1 & g^{01} & g^{02} & \cdots & g^{0\gamma} & \cdots \\
\vdots & g^{12} & g^{13} & \cdots & g^{1\gamma} & \cdots \\
E_\gamma & \vdots & \vdots & \ddots & \vdots & \vdots \\
\cdots & \cdots & \cdots & \ddots & g^{\gamma \gamma-1} & \cdots \\
\end{pmatrix} = \begin{pmatrix}
0 & g^{01} & g^{02} & \cdots & g^{0\gamma} & \cdots \\
g^{10} & 0 & g^{12} & \cdots & g^{1\gamma} & \cdots \\
g^{20} & g^{21} & 0 & \cdots & \vdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \cdots \\
g^{10} & g^{11} & \cdots & g^{\gamma \gamma-1} & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \ddots & \cdots \\
\end{pmatrix}
\]

(5)

Such an expression has separated the total Hamiltonian matrix into diagonal part and off-diagonal part, rather than nonperturbative part and perturbative part, which is marked with the coupling constant in the normal perturbation theory. It is never trivial in our derivations. Breaking the accustomed mentality in the normal perturbation theory and using the more formalized expansion form of time evolution operator are advantages of Wang’s theory, and they bring us successfully to arrive at our purpose.
Obviously, there are many apparent singular points in the expression \( A_{i}^{\gamma} \) of \( A_{i}^{\gamma} \), but they are fake in fact. In Wang’s paper [1] this problem has been fixed by finding their limitations in terms of contraction and anti-contraction of energy summation indexes. Here, we will theorize Wang’s method and further prove Wang’s conjecture about the eigenvalues of Hamiltonian.

A key trick using here is that we start from the partition function and rewrite it by using Wang’s expression (2)

\[
\sum_{\gamma} e^{-iE_{\gamma}t} = \sum_{\gamma} A_{i}^{\gamma}
\]

where \( E_{\gamma} \) are just the total Hamiltonian eigenvalues that we would like to find. It is largely helpful for removing the unexpected “fake” singular points in Wang’s framework, which can be seen in Appendix A. Another key skill is that we use the contraction and anti-contraction of energy summation indexes developed in [1]. It makes all the apparent singular points in the partition function expressed by Wang’s framework are neatly removed, which can be seen in Appendix A. It is interesting that, based on the proof in Appendix A by particularly analyzing, skillfully recombining the summations over energy indexes and perturbed order indexes, we arrive at

\[
\sum_{\gamma} A_{i}^{\gamma} = \sum_{\gamma} e^{-iE_{\gamma}t} \left\{ 1 + (-it)^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)!} \left[ \frac{\partial^m}{\partial z^m} \left( e^{izt} R_{\gamma}^{m+1}(z) \right) \right]_{z=0} \right\}
\]

where

\[
R_{\gamma}(z) = \sum_{l=1}^{\infty} \sum_{\gamma_1,\gamma_2,\ldots,\gamma_l \neq \gamma} \frac{g^{\gamma_1} g^{\gamma_2} \cdots g^{\gamma_l}}{(E_{\gamma} - E_{\gamma_1} - z)(E_{\gamma} - E_{\gamma_2} - z) \cdots (E_{\gamma} - E_{\gamma_l} - z)}
\]

\( R_{\gamma}(z) \) is a kernal function that involves contributions from all order perturbations, and plays a key role in our expression. It is clear that \( R_{\gamma}^{m+1}(z) \) and \( \partial^m R_{\gamma}^{m+1}(z)/\partial z^m \bigg|_{z=0} \) have the same order of magnitude of perturbed parameter \( \lambda \), but \( R_{\gamma}^{m+1}(z)/R_{\gamma}^{m}(z) \) and \( (\partial^{m+1} R_{\gamma}^{m+2}(z)/\partial z^{m+1} \bigg|_{z=0})/(\partial^m R_{\gamma}^{m+1}(z)/\partial z^m \bigg|_{z=0}) \) is equal to \( O(\lambda^2) \). This implies that the approximation ability of this series is obviously improved and then it is more suitable to cut up to some given the \( m \)th term since it decreases more rapidly with \( \lambda \).

However, more importantly and interestingly, we obtain

\[
\sum_{\gamma} e^{-iE_{\gamma}t} = \sum_{\gamma} \exp \left\{ -i \left( E_{\gamma} + \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)!} \left[ \frac{\partial^m}{\partial z^m} R_{\gamma}^{m+1}(z) \right]_{z=0} \right) t \right\}
\]

It is proved in the Appendix D by expending the partition function in Eq. (7) into the time power series and verifying the coefficient power relation. In fact, the form of Eq. (9) has its physics origin rather than the mathematics arbitrariness, and it is valid in the general quantum systems independent of the form of Hamiltonian. Therefore, we think that the complete series expression of Hamiltonian eigenvalues in the general quantum systems as below

\[
\tilde{E}_{\gamma} = E_{\gamma} + \Delta E_{\gamma} = E_{\gamma} + \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)!} \left[ \frac{\partial^m}{\partial z^m} R_{\gamma}^{m+1}(z) \right]_{z=0} t
\]

Obviously, it is simply not a summation over the perturbed parameter, but a series of power of the kernal function \( R_{\gamma}(z) \) as well as its derivative at \( z = 0 \). It is completely different from the normal perturbation theory in its thoughtway. In particular, when a cut is introduced in a practical calculation, a higher \( \lambda^2 \) term than the last term of cut part is dropped, but not a higher \( \lambda \) term than the last term of cut part is dropped in the normal perturbation theory.

It is easy to verify that our result is consistent with one in the normal perturbation theory if one expands our expression (10) according to the order of perturbed parameter for the known lower order forms in the textbook and refs. However, our expression involves the contribution from all order perturbation and has a neat form of general term. Rearranging summation in our expression is helpful for theoretical derivation and practical calculation since its completeness, orderliness and clearness. In particular, it provides a physical reason how to chose part contributions from higher order perturbations, which is able to simplify the calculation and lead the result more precision. An example has been presented in Ref. 3. In fact, our reassignment summation is reasonable because it reveals the mathematical beauty and then physical nature. Moreover, its new content, at least, to surprise us, will be obtained in the following section.

Of course, our expression of the total Hamiltonian eigenvalues can be thought of to be exact in the sense that this series involves the contributions from all order perturbations and has no any approximation and cut in form, as well as the general term is obtained.
Although the complete series expression of total Hamiltonian eigenvalues in the general quantum system arrives at our theoretical aspiration and we believe that it is interesting and important in the formulism of quantum mechanics, we have to admit that this expression is probably too complicated to be practical. It is inevitable and acceptable that the complete expression of Hamiltonian eigenvalues is an infinite series, because a general quantum system has usually no a compact solution without any approximation. It seems to be not convenient in the calculation the th order derivative of , but because that is such a function with a product form , such a difficulty is not serious. However, except for a reasonable rearrangement summation and a neat general term to reasonably involve the higher order contributions, what is more in our expression than one in the normal perturbation theory for the calculation of total Hamiltonian eigenvalues. In this section, our purpose is just designed to answer this problem.

Actually, we find that the difference between ‘s and quantums’s eigenvalues is such a function with a product form. Therefore the Laurent series of can be expanded as a Taylor’s series at , that is

\[ F_\gamma(z) = \frac{\ln(1 + R_\gamma(z))}{z} \]  

(11)

It is easy to proved. In fact, setting , we can rewrite \[ F_\gamma(z) = R_\gamma(z) \ln(1 + u)/u. \] Obviously, the limit of \( \ln(1 + u)/u \) when \( u \to 0 \) is 1. Thus it means that \( \ln(1 + u)/u \) can be expanded as a Taylor’s series at \( u = 0 \), that is

\[ F_\gamma(z) = R_\gamma(z) \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} u^{k-1} = \sum_{k=0}^{\infty} \frac{(-1)^{k} R_{\gamma}^{k+1}}{k+1} z^{k} \]  

(12)

Again note that can be expanded as a Taylor’s series at \( z = 0 \), we finish the proof of our above conclusion.

Now our task is to seek an explicit form of Laurent series of \( F_\gamma(z) \). We first set \( \alpha_\gamma \) is a solution of following equation

\[ R_\gamma(\alpha_\gamma) = -\alpha_\gamma \]  

(13)

When \( \alpha_\gamma \) is finite, from above equation it follows that \( R_\gamma(z) \) can be expanded as

\[ R_\gamma(z) = R_\gamma(\alpha_\gamma) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[ \frac{d^{n}}{d\alpha_\gamma^{n}} R_\gamma(\alpha_\gamma) \right] (z - \alpha_\gamma)^{n} = -\alpha_\gamma + \overline{R}_\gamma(z) \]  

(14)

Then, we rewrite

\[ F_\gamma(z) = z \ln \left[ 1 - \frac{\alpha_\gamma}{z} + \overline{R}_\gamma(z)/z \right] = z \ln \left[ 1 - \frac{\alpha_\gamma}{z} \right] + z \ln \left[ 1 + \frac{\overline{R}_\gamma(z)}{(z - \alpha_\gamma)} \right] \]  

(15)

Since \( \overline{R}_\gamma(z)/(z - \alpha_\gamma) \) is canonical at \( z = \alpha_\gamma \) from Eq.\( (13) \) for a finite \( \alpha_\gamma \), the second term in above equation does not involve \( z \)’s 0th power part. Actually, this is a reason why to set Eq.\( (13) \). While the first term in Eq.\( (14) \) can be expanded as

\[ z \ln \left[ 1 - \frac{\alpha_\gamma}{z} \right] = -\sum_{k=1}^{\infty} \frac{z}{k} \left( \frac{\alpha_\gamma}{z} \right)^{k} \]  

(16)

Therefore the Laurent series of \( F_\gamma(z) \) has its coefficient of \( z \)’s 0th power to be \( -\alpha_\gamma \). It implies that we obtain

\[ E_\gamma = E_\gamma + \Delta E_\gamma = E_\gamma - \alpha_\gamma \]  

(17)

This conclusion is so interesting because it tells us that the total Hamiltonian eigenvalues in the general quantum system can be calculated through solving an algebra equation

\[ R_\gamma(-\Delta E_\gamma) = \Delta E_\gamma \]  

(18)

and then adding its solution \( \Delta E_\gamma \) to the \( H_0 \)’s eigenvalues \( E_\gamma \). More obviously, the total Hamiltonian eigenvalues \( \tilde{E}_\gamma \) is a solution of following algebra equation

\[ \sum_{l=1}^{\infty} \sum_{\gamma_1, \gamma_2, \ldots, \gamma_l \neq \gamma} \frac{g^{\gamma_1} g^{\gamma_2} \ldots g^{\gamma_l}}{(E_\gamma - E_{\gamma_1})(E_\gamma - E_{\gamma_2}) \cdots (E_\gamma - E_{\gamma_l})} = 1 \]  

(19)
This conclusion distinctly reveals the advantages of Wang’s formal framework and goes to an extent that we have ever not researched using the known other theory. It must be emphasized that the contributions from higher order even all order perturbation are naturally involved in such an algebra equation. The difference between our approach and usual one has been clearly seen here because that we give up the accustomed calculation method order by order in the normal perturbation theory.

IV. AN EXAMPLE: QUARTIC ANHARMONIC OSCILLATOR

In this section, we attempt to verify the validity of expression of Hamiltonian eigenvalues and check the accuracy of calculation of Hamiltonian eigenvalues using our method. As an example, we study a quartic anharmonic oscillator in the normalization, which is frequently used as a test-stone of new methods of calculating the eigenvalues. Harmonic oscillators and their anharmonic counter parts are extremely important model systems in all branches of quantum physics and particularly in quantum field theory. Even order anharmonic oscillators defined by

$$H^{(m)} = p^2 + x^2 + \lambda x^{2m}, \ m = 2, 3, 4 \cdots \tag{20}$$

were studied in Bender and Wu’s seminal work [9, 10, 11], and then Simon made a rigorous analysis of the mathematical property in [12]. The perturbation expansions of the anharmonic oscillators diverge strongly for the coefficients $c_m$ in Eq. (11) always grow factorially. Therefore anharmonic oscillators are frequently used to test new approximation techniques.

Let us begin to consider a quartic anharmonic oscillator. Its Hamiltonian reads

$$H = -\frac{d^2}{dx^2} + x^2 + \lambda x^4 \tag{21}$$

Obviously, the primary task is to write out our kernel function $R_\gamma$. But, as it is defined, $R_\gamma$ is the summation of an infinite series. Thus, a certain cut approximation should be made, that is, some terms of this series need to be omitted. So, what strategy should be adopted when trying to distinguish those of importance from trivial terms? One may think of the tactics when making perturbation approximation, we just pick those terms of low powers of the coupling constant, and drop the higher powers. We are going to point out that such a tactic won’t be very proper here, for the two reasons below. First, the usual perturbation expansion is a power series of the coupling constant, but, our expression has no longer been simply a power series of coupling constant. Second, even though we admitted that the longer the term the smaller the value, the the longer the term, the bigger the number of such terms. So, we propose a new one, according to the fact that the states nearby exert larger impact than the states faraway in our expression, we drop the terms reflecting the effect of the states far away from the initial one.

To put our idea into reality, we choose such some terms that the summations over $\gamma_1, \gamma_2, \cdots, \gamma_l$ has a maximum value $n$ and define them as a new series

$$R^c_\gamma(z, n) = \sum_{l=1}^{\infty} \sum_{\gamma_1, \gamma_2, \cdots, \gamma_l \neq \gamma_{\max}} \frac{g^{\gamma_1 \gamma_2} g^\gamma}{(E_\gamma - E_{\gamma_1} - z)(E_\gamma - E_{\gamma_2} - z) \cdots (E_\gamma - E_{\gamma_l} - z)} \tag{22}$$

Thus, we can rewrite the kernel function $R_\gamma$ as the summation of $R^c_\gamma(z, n)$ over $n$ as below

$$R_\gamma(z) = \sum_{n=1}^{\infty} R^c_\gamma(z, n) \tag{23}$$

In the calculation of the ground state energy of quartic anharmonic oscillator we make the cut approximation to $N$

$$R_\gamma(z) \approx \sum_{n=1}^{N} R^c_\gamma(z, n) \tag{24}$$

To justify our approximation scheme, we’ve made some numerical calculation as shown in Table. II And our result of the ground state energy of quartic anharmonic oscillator for different coupling constants is shown in Table. III These results are good enough comparing with the known one in [13].
TABLE I: The value of $R_0^c(0, n)$.

| $\lambda$ | $n$ = 3 | $n$ = 5 | $n$ = 11 | $n$ = 21 | $n$ = 51 | $n$ = 101 | $n$ = 199 |
|-----------|---------|---------|---------|---------|---------|---------|---------|
| 0.1       | -9.1837e-003 | -4.5775e-004 | -1.4406e-007 | -5.0107e-012 | -8.129e-024 | -2.8911e-041 | -4.3465e-068 |
| 0.2       | -3.1034e-002 | -3.516e-004 | -8.6467e-007 | -3.0709e-010 | -6.5572e-034 | -4.4807e-057 |
| 1.0       | -3.4615e-001 | -2.128e-002 | -8.6467e-007 | -1.5403e-006 | -6.5085e-013 | -4.5152e-022 | -3.4768e-040 |
| 2.0       | -8.1818e-001 | -1.204e-001 | -8.6467e-007 | -1.5403e-006 | -6.5085e-013 | -4.5152e-022 | -3.4768e-040 |
| 10.0      | -4.7872e+000 | -1.5066e+000 | -2.0541e-001 | -5.5894e-004 | -2.8380e-006 | -4.8053e-012 | -1.2683e-020 |
| 20.0      | -9.7826e+000 | -3.4221e+000 | -1.5066e+000 | -7.2278e-001 | -1.3054e-003 | -3.1365e-008 | -1.8263e-014 |
| 100.0     | -4.9779e+001 | -1.8999e+001 | -3.0893e+001 | -1.2912e+001 | -4.2734e+002 | -3.6783e-002 | -5.2184e-006 |

TABLE II: The value of the ground state energy of quartic anharmonic oscillator, using the summation of the first $n R_0^c(z, i)$ ($i = 1, 2, \cdots, n$) as the approximation of $R_0(z)$.

| $\lambda$ | $n$ = 10 | $n$ = 20 | $n$ = 30 | $n$ = 50 | $n$ = 100 | $n$ = 200 | $n$ = 500 |
|-----------|---------|---------|---------|---------|---------|---------|---------|
| 0.1       | 1.06528550957781 | 1.06528550957275 | 1.06528550957275 | 1.065285509571137 | 1.065285509571137 | 1.065285509571137 |
| 0.2       | 1.1189265444366 | 1.1189265444366 | 1.1189265444366 | 1.1189265444366 | 1.1189265444366 | 1.1189265444366 |
| 1.0       | 1.39235164312960 | 1.39235164312960 | 1.39235164312960 | 1.39235164312960 | 1.39235164312960 | 1.39235164312960 |
| 2.0       | 1.60754130400797 | 1.60754130400797 | 1.60754130400797 | 1.60754130400797 | 1.60754130400797 | 1.60754130400797 |
| 10.0      | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 |
| 20.0      | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 |
| 100.0     | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 | 3.00994481555778 |

Here, the value denoted by “known” from Ref. [13].

V. SUMMARY

In this article, we proposed a new approach calculating the Hamiltonian eigenvalues in the general quantum systems. In theoretical form, we obtain a complete series expression of total Hamiltonian eigenvalues without any approximation and cut. In practical calculation, we present an algebra equation satisfied by the total Hamiltonian eigenvalues. These conclusions is based on Wang's framework of quantum mechanics in the general quantum system. Consequently we can say that Wang’s formulism of quantum mechanics in the general quantum systems is useful. In fact, the revised Fermi’s gold rule as well as its calculation [8] also accounts for Wang’s theory has itself advantages.

Although only the non-degeneracy and discrete case is considered here, but our derivation can be extended to the continuous and/or degeneracy case.

It must be emphasized that an accustomed mentality that expands the series according to the perturbed parameter in the normal perturbation theory is given up, the contributions from all order perturbation is involved via a kernel function, which plays a key role in our theoretical expression and our calculation approach. The advantages of
our kernal function have been mentioned in the previous sections. The calculation about this kernal function is an important task. However, it only involves a product of matrices, and then it can be efficiently calculated by using a computer. So in the computability and usability, our approach is not weaker. In formal beauty, please see our concrete expressions, no more words need to say.

Perhaps, our expression is thought of a rearrangement of perturbation series. However, such a rearrangement summation in form is never trivial, it really shows the physics nature because it directly comes from the law of quantum dynamics, but not a transcendent input – expansion according to the power of perturbed parameter. In mathematics, the reasonable rearrangement of a multiply series is often significant if a cut approximation is needed. We think that the rearrangement summation in our expression make us reasonably involve the contributions from part higher even all order perturbations from our derivation. In fact, our expression is more neat, more explicit and more deep than the known Kato’s \cite{2} and Bloch’s \cite{3}. This should be a reason why it can lead to an interesting conclusion – the total Hamiltonian eigenvalues can be calculated by solving an algebra equation.

Our approach to calculate the total Hamiltonian eigenvalues also gives up the accustomed way order by order, it makes the calculation to be simplified, but still involves the contributions from important part higher order perturbations when a cut approximation is introduced. Actually, it is similar to choose the important parts in higher order (equal to or more than the fourth order) contributions based on some physics reasons. Specially, our equation about the total Hamiltonian eigenvalues can more naturally and conveniently involve the contributions from higher even all order perturbations, and it is easy to be solved numerically in a computer. Therefore, our approach is able to remarkably simplify the calculation as well as advance the precision.

As an example, we applied our approach in the calculation of the ground state energy of a quartic anharmonic oscillator. The highly accurate results for the energies of the ground state energy of quartic anharmonic oscillators of different coupling ranging from 0.1 to 100 are yielded. Something we should mention is that the factorial divergence in the usual perturbation expansion of even order anharmonic oscillators no longer appears in our expansion, and our way of “summing” expansion, which should be owed to the fact that our expression is complete, is rather simple and neat in form and also proved to be effective. On the basis of the results presented in this article, one can expect that our new method should also give good enough results in some other quantum mechanical problems, and we’ll proceed our work in the near future.

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**APPENDIX A**

This appendix is focus on a derivation of the first expression of partition function \cite{1} based Wang’s formal framework \cite{1}.

Note that the $H_1$ matrix is able to be taken as off-diagonal based on Wang’s proof \cite{1}, from Eq. \ref{eq:3} it follows

\[
A_i^{\gamma} = \sum_{\gamma_1, \gamma_2} \sum_{i=1}^{2} \frac{e^{-iE_{\gamma_i}t}}{(E_{\gamma_1} - E_{\gamma_2})} g^{\gamma_1\gamma_2} \delta_{\gamma_11} \delta_{\gamma_22} = 0 \tag{A1}
\]

It implies that the contraction and anti-contraction of off-diagonal elements skill using in \cite{1} is largely simplified when $H_1$ matrix is taken as an off-diagonal form.

Since the existing the factor $\delta_{\gamma_11} \delta_{\gamma_2l+1}$ in the $A_i^{\gamma}$ expression \cite{3} it leads to that $E_{\gamma_1} = E_{\gamma_{l+1}} = E_\gamma$ after summation. It implies that there is, at least, an obvious singular point among the beginning and ending terms in the summation over $i$ from 1 and $l + 1$ for a fixed $l > 1$. To remove it, we can combine this two terms, and introduce an infinite small
\[\begin{align*}
&\left\{ \frac{e^{-iE_{\gamma_1}t}}{l+1} \prod_{j=2}^{l+1} (E_{\gamma_j} - E_{\gamma_1}) + \frac{e^{-iE_{\gamma_i+1}t}}{l} \prod_{j=1}^{l} (E_{\gamma_i+1} - E_{\gamma_j}) \right\} \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_i+1} \\
&= \lim_{\varepsilon \to 0} e^{-iE_{\gamma_1}t} \left\{ \frac{1}{l} \prod_{i=2}^{l} \frac{1}{(E_\gamma - E_{\gamma_i})} \left( i\varepsilon \right) + \frac{e^{-\varepsilon t}}{(-i\varepsilon)} \prod_{i=2}^{l} (E_\gamma - E_{\gamma_i} - i\varepsilon) \right\} \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_i+1} \\
&= -e^{-iE_{\gamma_1}t} \frac{d}{dz} \left[ e^{izt} \prod_{i=2}^{l} \frac{1}{(E_\gamma - E_{\gamma_i} - z)} \right] \bigg|_{z=0} \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_i+1}. \tag{A2}
\end{align*}\]

The last step has directly used the definition of derivative.

Furthermore, let us first consider how to deal with the terms in the summation over \(i\) from \(i = 2\) to \(i = l\) of Eq.\((3)\). By summing the index \(\gamma_1\) and \(\gamma_{i+1}\) we have

\[\begin{align*}
&\sum_{\gamma_1, \gamma_2, \ldots, \gamma_{i+1}} \sum_{l=2}^{l} \frac{e^{-iE_{\gamma_1}t}}{l+1} \prod_{j=1, j \neq i}^{l+1} (E_{\gamma_j} - E_{\gamma_1}) \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_i+1} \prod_{i=1}^{l} g_{\gamma_{i+1}} = \sum_{\gamma_{i+2}} \frac{e^{-iE_{\gamma_{i+2}}t}}{(E_{\gamma_{i+2}} - E_{\gamma_1})^2} g_{\gamma_{i+2}} g_{\gamma \gamma_{i+1}} \delta_{\gamma_1 \gamma} \\
&+ \sum_{\gamma_1, \gamma_2, \gamma_3} \left[ \frac{e^{-iE_{\gamma_1}t}}{(E_{\gamma_2} - E_{\gamma_1})^2} + \frac{e^{-iE_{\gamma_3}t}}{(E_{\gamma_3} - E_{\gamma_1})^2} \right] g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_{i+1}} \\
&+ \theta(l-4) \sum_{\gamma_1, \gamma_2, \ldots, \gamma_i} \sum_{l=2}^{l} \left[ \frac{e^{-iE_{\gamma_i}t}}{(E_{\gamma_i} - E_{\gamma_1})^2} \prod_{j=2}^{l-1} (E_{\gamma_j} - E_{\gamma_i}) \prod_{k=i+1}^{l} (E_{\gamma_k} - E_{\gamma_i}) \right] g_{\gamma_1} \prod_{i=2}^{l} g_{\gamma_{i+1}} \tag{A3}
\end{align*}\]

where \(\theta(x) = 1\) if \(x \geq 0\), otherwise \(\theta(x) = 0\).

The simplest case is that \(l = 2\). Only there is the first term in above equation (A3). Interchanging the dummy index \(\gamma \leftrightarrow \gamma_2\), we have

\[\begin{align*}
&\sum_{\gamma_{i+2}} \frac{e^{-iE_{\gamma_{i+2}}t}}{(E_{\gamma_{i+2}} - E_{\gamma_1})^2} g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} = \sum_{\gamma_{i+2}} e^{-iE_{\gamma_{i+2}}t} \left[ e^{izt} \frac{d}{dz} \left( \frac{1}{(E_{\gamma_{i+2}} - E_{\gamma_1} - z)} \right) \right] \bigg|_{z=0} g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} \tag{A4}
\end{align*}\]

Similarly, for \(l = 3\), we set \{\(\gamma_2, \gamma_3, \gamma\)\} \(\to\) \{\(\gamma, \gamma_2, \gamma_3\)\} for \(i = 2\), and \{\(\gamma_3, \gamma, \gamma_2\)\} \(\to\) \{\(\gamma, \gamma_2, \gamma_3\)\} for \(i = 3\). Thus

\[\begin{align*}
&\sum_{\gamma_1, \gamma_2, \gamma_3} \sum_{l=2}^{3} \frac{e^{-iE_{\gamma_1}t}}{4} \prod_{j=1, j \neq i}^{3} (E_{\gamma_j} - E_{\gamma_1}) \delta_{\gamma_1 \gamma} \delta_{\gamma \gamma_{i+1}} \prod_{i=1}^{3} g_{\gamma \gamma_{i+1}} \\
&= \sum_{\gamma_1, \gamma_2, \gamma_3} \left[ \frac{e^{-iE_{\gamma_1}t}}{(E_{\gamma_2} - E_{\gamma_1})^2} + \frac{e^{-iE_{\gamma_2}t}}{(E_{\gamma_3} - E_{\gamma_1})^2} \right] g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} \\
&= \sum_{\gamma_1, \gamma_2, \gamma_3} \frac{1}{(E_{\gamma_2} - E_{\gamma_1})^2} (E_{\gamma_2} - E_{\gamma_1}) + \frac{1}{(E_{\gamma_3} - E_{\gamma_1})^2} (E_{\gamma_3} - E_{\gamma_1}) \right] g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} \\
&= \sum_{\gamma_1, \gamma_2, \gamma_3} e^{-iE_{\gamma_1}t} \left[ e^{izt} \frac{d}{dz} \left( \frac{1}{(E_{\gamma_2} - E_{\gamma_1} - z)(E_{\gamma_3} - E_{\gamma_1} - z)} \right) \right] \bigg|_{z=0} g_{\gamma \gamma_{i+2}} g_{\gamma \gamma_{i+1}} \tag{A5}
\end{align*}\]
The skill of dummy index transformations can be continuously used when \( l \geq 4 \). For \( i = 2 \) and to \( i = l \), they are respectively \( \{ \gamma_2, \gamma_3, \ldots, \gamma_l, \gamma_l \} \to \{ \gamma, \gamma_2, \ldots, \gamma_l, \gamma_l \} \) and \( \{ \gamma_l, \gamma_1, \gamma_2, \ldots, \gamma_l-1 \} \to \{ \gamma, \gamma_2, \ldots, \gamma_l \} \). For the other \( i \) \( (l - 1 \geq i \geq 3) \), our dummy index transformations are taken as \( \{ \gamma_i, \gamma_{i+1}, \ldots, \gamma_l, \gamma_l \} \to \{ \gamma, \gamma_2, \ldots, \gamma_l \} \). It is easy to prove that, under above index transformations, \( g^{\gamma_\gamma_2}g^{\gamma_\gamma_3}\ldots g^{\gamma_\gamma} \) is invariant in form. Obviously, \( i = 2 \) and \( i = l \) terms are transformed as following form

\[
\begin{align*}
\frac{e^{-iE_\gamma t}}{(E_{\gamma_2} - E_{\gamma})^2 \prod_{k=3}^{l} (E_{\gamma_2} - E_{\gamma_k})} & \to \frac{e^{-iE_\gamma t}}{(E_{\gamma} - E_{\gamma_i})^2 \prod_{k=2}^{l-1} (E_{\gamma} - E_{\gamma_k})} \left[ (E_{\gamma} - E_{\gamma_i})^2 \right] \\
\frac{e^{-iE_\gamma t}}{(E_{\gamma} - E_{\gamma_i})^2 \prod_{k=2}^{l-1} (E_{\gamma} - E_{\gamma_k})} & \to \frac{e^{-iE_\gamma t}}{(E_{\gamma} - E_{\gamma_i})^2 \prod_{k=3}^{l} (E_{\gamma} - E_{\gamma_k})}
\end{align*}
\] (A6)

While the other \( i \) from 3 to \( l - 1 \) \( (l \geq 4) \), our dummy index transformations lead to

\[
\begin{align*}
\sum_{i=3}^{l-1} \frac{e^{-iE_\gamma t}}{(E_{\gamma_i} - E_{\gamma})^2 \prod_{j=2, j \neq i}^{l} (E_{\gamma_i} - E_{\gamma_j})} & \to \sum_{i=3}^{l-1} \frac{e^{-iE_\gamma t}}{(E_{\gamma} - E_{\gamma_i})^2 \prod_{j=2, j \neq i}^{l} (E_{\gamma} - E_{\gamma_j})}
\end{align*}
\] (A7)

Thus, when \( l \geq 4 \)

\[
\begin{align*}
\sum_{l=4}^{\infty} \sum_{\gamma_1, \ldots, \gamma_{l+1}} \sum_{i=2}^{l} e^{-iE_\gamma t} \prod_{j=1, j \neq i}^{l+1} \frac{1}{(E_{\gamma_i} - E_{\gamma_j})} \prod_{k=1}^{l} g^{\gamma_k \gamma_{k+1}} \delta_{\gamma_{1i}} \delta_{\gamma_{l+1}} \\
= \sum_{l=4}^{\infty} \sum_{\gamma_1, \ldots, \gamma_{l+1}} e^{-iE_\gamma t} \left\{ \prod_{j=2}^{l-1} \frac{1}{(E_{\gamma} - E_{\gamma_j})} (E_{\gamma} - E_{\gamma_i})^2 \prod_{j=2, j \neq i}^{l} \frac{1}{(E_{\gamma} - E_{\gamma_j})} \right\} \\
+ \frac{1}{(E_{\gamma} - E_{\gamma_2})^2 \prod_{k=3}^{l} (E_{\gamma} - E_{\gamma_k})} \left[ \prod_{i=2}^{l-1} g^{\gamma_i \gamma_{i+1}} \right] g^{\gamma_\gamma} \\
= \sum_{l=4}^{\infty} \sum_{\gamma_1, \ldots, \gamma_{l+1}} e^{-iE_\gamma t} \left\{ e^{izt} \frac{d}{dz} \left[ \prod_{j=2}^{l} \frac{1}{(E_{\gamma} - E_{\gamma_j} - z)} \right] \right\} \bigg|_{z=0} \left[ \prod_{i=2}^{l-1} g^{\gamma_i \gamma_{i+1}} \right] g^{\gamma_\gamma}
\end{align*}
\] (A8)

Substituting eqs. (A1) (A2) (A4) (A5) (A9) into the expression of partition function, we obtain

\[
\sum_{\gamma} \frac{A^{\gamma}}{\gamma} = \sum_{\gamma} e^{-iE_{\gamma} t} + \sum_{l=2}^{\infty} \sum_{\gamma_1, \ldots, \gamma_l} e^{-iE_{\gamma} t} g^{\gamma_\gamma} g^{\gamma_2 \gamma_3} \ldots g^{\gamma_\gamma} \\
\times \left\{ \frac{d}{dz} \left[ -e^{izt} \prod_{j=2}^{l} \frac{1}{(E_{\gamma} - E_{\gamma_j} - z)} \right] + e^{izt} \frac{d}{dz} \left[ \prod_{j=2}^{l} \frac{1}{(E_{\gamma} - E_{\gamma_j} - z)} \right] \right\} \bigg|_{z=0} \\
= \sum_{\gamma} e^{-iE_{\gamma} t} \left[ 1 + \sum_{l=1}^{\infty} \sum_{\gamma_1, \ldots, \gamma_l} (-it) g^{\gamma_\gamma} g^{\gamma_2 \gamma_3} \ldots g^{\gamma_\gamma} \prod_{j=1}^{l} \frac{1}{(E_{\gamma} - E_{\gamma_j})} \right]
\] (A9)

in which, we have reset the summation indexes.
APPENDIX B

In this section, we would like to further remove all apparent singular points in the expression of partition function. It is clear that there are still the singular points in the expression (A10) although they are fake. In fact, these singular points as well as the relevant terms in form are similar to those have been removed in Appendix A except for the delta function factors. Consequently, to further deal with these unexpected singular points, we need to pick out the terms when \( E_\gamma = E_{\gamma j} \). Its method is just like the things that the ref. [1] has ever done, that is, we start from the identity in the sense of summation:

\[
1 = \delta_{\gamma \gamma_1} + \eta_{\gamma \gamma_1}
\]

and rewrite a summation as

\[
\sum_{\gamma_i} f [x_\gamma, x_{\gamma j}] = \sum_{\gamma_i} f [x_\gamma, x_{\gamma j}] \delta_{\gamma_i \gamma_1} + \sum_{\gamma_i} f [x_\gamma, x_{\gamma j}] \eta_{\gamma_i \gamma_1}
\]

The first summation of right side of above equation is picked out, in which, \( \delta \) is the delta function action, but each in the other terms.

Similar to the skill used in Appendix A, we rewrite it as \( \prod_{j=1}^l (E_\gamma - E_{\gamma j})^{-1} \) we product it by \( \bar{\delta}_{\{p^l\}_m \gamma} \) so that there are, at least, \( m \) obvious singular points within it since \( g^{\gamma \gamma} = 0 \) has been taken here. This result leads to that the number of subset \( \{p^l\}_m \) element with contribution is not larger than \( \lfloor (l+1)/2 \rfloor \). However, in form, we can keep these vanishing terms.

In order to pick out the singular terms from the summation \( \sum_{\gamma_1, \ldots, \gamma_l} \prod_{j=1}^l (E_\gamma - E_{\gamma j})^{-1} \) we product it by \( \bar{\delta}_{\{p^l\}_m \gamma} \) so that there are, at least, \( m \) obvious singular points within it since \( \bar{\delta}_{\{p^l\}_m \gamma} \) contains \( m \) delta functions. Obviously, \( m = 0 \) case is not needed to considered since there is no the singular point.

Similar to the skill used in Appendix A, we rewrite it as \( \prod_{j=1}^l (E_\gamma - E_{\gamma j})^{-1} \) we product it by \( \bar{\delta}_{\{p^l\}_m \gamma} \) so that there are, at least, \( m \) obvious singular points within it since \( \bar{\delta}_{\{p^l\}_m \gamma} \) contains \( m \) delta functions. Obviously, \( m = 0 \) case is not needed to considered since there is no the singular point.

In order to remove the fake singularity, we introduce \( m \) infinite small numbers \( \varepsilon_m (m = 1, 2, \ldots, l) \) so that \( E_\gamma - E_{\gamma m} = \)
The last summation term appears only when $m$ belonging to $i_q$ where we have denoted the $\varepsilon$. Now let us prove the following equation

Firstly, we calculate the limitation $\lim_{\varepsilon \to 0} \sum_{k=0}^{m} B_k \delta_{\{p'\}}_{\varepsilon_{m\gamma}}$

where we have denoted the $q'_{j} \in \{q'\}_m (j = 1, 2, \ldots, t - m)$, rewrite the summation or production over the index belonging to $\{q'\}_m$ (or $\notin \{p'\}_m$) as from $q'_1$ to $q'_{l-m}$, and also define $B_k$ by

Now let us prove the following equation

Firstly, we calculate the limitation $\lim_{\varepsilon \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}}_{\varepsilon_{m\gamma}} = \lim_{\varepsilon \to 0} \left[ \sum_{k=0}^{m} B_k \right] \delta_{\{p'\}}_{\varepsilon_{m\gamma}}$

The last summation term appears only when $m \geq 2$. Actually, by setting

$$f_{lm}^{k}(x) = \frac{1}{\prod_{i=k}^{m} (\varepsilon_i - x) \prod_{j=1}^{l-m} (E_{\gamma} - E_{\gamma_{ij}} - ix)}$$

(B14)
next doing its Taylor expansion

\[ f_{lm}^k(x) = f_{lm}(0) + \left[ \frac{d}{dx} f_{lm}(x) \right]_{x=0} x + \frac{1}{2!} \left[ \frac{d^2}{dx^2} f_{lm}(x) \right]_{x=0} x^2 + O(x^3) \]

\[ = \frac{1}{m} \prod_{i=k}^{l+m} (E - E_l) \left[ \frac{1}{m} \prod_{i=k}^{l} (E - E_l) + \frac{1}{m} \prod_{i=k}^{l} (E - E_l - ix) \right]_{x=0} + \frac{1}{2!} \frac{d^2}{dx^2} \left[ \frac{1}{m} \prod_{i=k}^{l} (E - E_l) + \frac{1}{m} \prod_{i=k}^{l} (E - E_l - ix) \right]_{x=0} x^2 + O(x^3) \]  \hspace{1cm} (B15)

and then substituting \( k = 2 \) result into Eq. (B13), we arrive at

\[ \lim_{\varepsilon_1 \to 0} \left( \sum_{k=0}^{m} B_k \right) = (-1) \frac{d}{d\varepsilon_1} \left[ \frac{1}{m} \prod_{i=2}^{l-\varepsilon_1} (E - E_l) + \frac{1}{m} \prod_{i=2}^{l-\varepsilon_1} (E - E_l - i\varepsilon_1) \right]_{\varepsilon_1=0} \]

\[ + \sum_{k=2}^{m} \frac{1}{\varepsilon_k^2} \prod_{i=2, i \neq k}^{m} (\varepsilon_i - \varepsilon_k) \prod_{j=1}^{l-\varepsilon_1} (E - E_l - j\varepsilon_k) \]  \hspace{1cm} (B16)

From the definition of derivative of a function, it is easy to see

\[ \lim_{\varepsilon_1, \varepsilon_2 \to 0} \left( \sum_{k=0}^{m} B_k \right) = \lim_{\varepsilon_2 \to 0} \left[ (-1) \frac{d}{d\varepsilon_1} \left[ f_{lm}^2(\varepsilon_1) \right]_{\varepsilon_1=0} + \frac{1}{\varepsilon_2} \left[ f_{lm}^3(\varepsilon_2) \right]_{\varepsilon_2=0} \right] \]

\[ - \sum_{k=3}^{m} \frac{1}{\varepsilon_k^3} \prod_{i=3, i \neq k}^{m} (\varepsilon_i - \varepsilon_k) \prod_{j=1}^{l-\varepsilon_1} (E - E_l - j\varepsilon_k) \]  \hspace{1cm} (B17)

where \( f_{lm}^k(x) \) is defined by Eq. (B14). From

\[ (-1) \frac{d}{d\varepsilon_1} \left[ f_{lm}^2(\varepsilon_1) \right]_{\varepsilon_1=0} = -\frac{1}{\varepsilon_2} f_{lm}^3(0) - \frac{1}{\varepsilon_2} \frac{d}{d\varepsilon_1} \left[ f_{lm}^3(\varepsilon_1) \right]_{\varepsilon_1=0} \]  \hspace{1cm} (B18)
and Eq. (B15), but taking $k = 3$, it follows that

$$
\lim_{\varepsilon_1, \varepsilon_2 \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}_{m \gamma}} = \left( -\frac{1}{2} \right)^n \frac{d^n}{d\varepsilon_n^n} \left[ f^{n+1}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} \frac{d}{d\varepsilon_2} \left[ \frac{1}{\varepsilon_1 - \varepsilon_2} \right] \frac{e^{-\varepsilon_2 t}}{\prod_{j=1}^{l} (E - E_{\gamma_{j}'} - i\varepsilon_2)} \delta_{\{p'\}_{m \gamma}}
$$

In particular,

$$
\lim_{\varepsilon_1, \varepsilon_2 \to 0} \left( \sum_{k=0}^{2} B_k \right) \delta_{\{p'\}_{2 \gamma}} = \left( -\frac{1}{2} \right)^n \frac{d^n}{d\varepsilon_n^n} \left[ f^{n+1}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} \frac{d}{d\varepsilon_2} \left[ \frac{e^{-\varepsilon_2 t}}{\prod_{j=1}^{l} (E - E_{\gamma_{j}'} - i\varepsilon_2)} \right] \delta_{\{p'\}_{2 \gamma}}
$$

Analyzing the above derivation, we have seen the fact that the singular points are able be removed by finding limitations step by step. Every limitation calculation increases one order of derivative in the first term and decreases a term in the last summation. When all limitations are calculated, this expression becomes a pure $m$ order derivative. Without loss of generality, for $n \leq (m - 2)$ we assume that

$$
\lim_{\varepsilon_1, \varepsilon_2 \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}_{m \gamma}} = \left( -\frac{1}{2} \right)^n \frac{d^n}{d\varepsilon_n^n} \left[ f^{n+1}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} \delta_{\{p'\}_{m \gamma}}
$$

we can have

$$
\lim_{\varepsilon_1, \varepsilon_2 \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}_{m \gamma}} = \lim_{\varepsilon_{n+1} \to 0} \left\{ \left( -\frac{1}{2} \right)^n \frac{d^n}{d\varepsilon_n^n} \left[ f^{n+1}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} \right\} \frac{d}{d\varepsilon_2} \left[ \frac{e^{-\varepsilon_2 t}}{\prod_{j=1}^{l} (E - E_{\gamma_{j}'} - i\varepsilon_2)} \right] \delta_{\{p'\}_{m \gamma}}
$$

Using the fact that

$$
\frac{d^n}{d\varepsilon_n^n} \left[ f^{n+1}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} = \sum_{j=0}^{n} \frac{n!}{j!} \frac{d^j}{d\varepsilon_n^j} \left[ f^{n+2}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0}
$$

we have

$$
\frac{d^n}{d\varepsilon_n^n} \left[ f^{n+2}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0} = \sum_{j=0}^{n} \frac{n!}{j!} \frac{d^j}{d\varepsilon_n^j} \left[ f^{n+2}_{lm}(\varepsilon_n) \right] |_{\varepsilon_n = 0}
$$
we have

$$\lim_{\varepsilon_n \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}_m} = \left( -1 \right)^{n+1} \frac{1}{(n+1)!} \left[ \frac{d^{n+1}}{d\varepsilon_{m+1}^{n+1}} f_{m+2}^{\varepsilon_{n+1}} (\varepsilon_{n+1}) \right]_{\varepsilon_{n+1} = 0} \delta_{\{p'\}_m}$$

$$+ \left[ \sum_{k=n+2}^{m} \frac{1}{m!} \left( \sum_{l=n+1}^{m} \prod_{i=n+1, i \neq k}^{l} (\varepsilon_i - \varepsilon_k) \prod_{j=1}^{l-m} (E_{\gamma} - E_{\gamma_j} - i\varepsilon_k) \right) e^{-\varepsilon_k t} \right] \delta_{\{p'\}_m} \tag{B25}$$

Finally, set \( n = m - 1 \) and then use the same method we can finish the proof of Eq. (B12). Obviously

$$\lim_{\varepsilon_m \to 0} \left( \sum_{k=0}^{m} B_k \right) \delta_{\{p'\}_m} = \left( -1 \right)^{m-1} \frac{1}{(m-1)!} \left[ \frac{d^{m-1}}{d\varepsilon_{m-1}^{m-1}} f_{m-1}^{\varepsilon_{m-1}} (\varepsilon_{m-1}) \right]_{\varepsilon_{m-1} = 0} + \left( -1 \right)^{m} \frac{1}{m!} \left[ \prod_{j=1}^{l-m} (E_{\gamma} - E_{\gamma_j} - i\varepsilon_m) \right] \delta_{\{p'\}_m}$$

$$= \left( -1 \right)^{m} \frac{d^{m}}{d\varepsilon^{m}} \left[ \prod_{j=1}^{l-m} (E_{\gamma} - E_{\gamma_j} - i\varepsilon) \right]_{\varepsilon = 0} \delta_{\{p'\}_m} \tag{B26}$$

Substituting it into Eq. (B19) and setting \( i\varepsilon = z \) follow the conclusion Eq.(B12).

When the set \( \{q'\}_1 \) is not an empty set, the product or summation over this set is well-defined. Usually, in the formal expressions, the product over an empty is thought of 1 and the summation over an empty is thought of 0. At the above sense, \( m \) still can take \( l \). But \( g^{\gamma_1} = 0 \) has been taken, thus

$$g^{\gamma_1} g^{\gamma_2} \cdots g^{\gamma_l} \delta_{\{p'\}_1} = 0 \tag{B27}$$

Finally, we arrive at

$$\sum_{\gamma} A_{\gamma} = \sum_{\gamma} e^{-iE_{\gamma} t} + \sum_{l=1}^{\infty} \sum_{m=0}^{l} \sum_{\gamma_{1}\gamma_{2}\cdots\gamma_{l}} (-it)e^{-iE_{\gamma} t} \left( -1 \right)^{m} \frac{d^{m}}{(m+1)!} \left[ \prod_{j=1}^{l-m} (E_{\gamma} - E_{\gamma_j} - z) \right]_{z = 0}$$

$$g^{\gamma_1} g^{\gamma_2} \cdots g^{\gamma_l} \delta_{\{p'\}_m} \tag{B28}$$

It must be emphasized that all obvious singular points have been removed in above form.

**APPENDIX C**

Now, our task is to continue to derive out the final expression of partition function that is written as a series of power of a kernal function as well as its derivative.

It is clear that \( \{p'\}_m \) is a subset of \( \mathcal{L} = \{1, 2, \cdots, l\} \), and has, at most, \( l-1 \) elements. Its every element can be taken as an end point so that \( \mathcal{L} \) is divided into \( m+1 \) subsets \( \mathcal{L}_n = \{p_{n-1}^l+1, p_{n-2}^l+2, \cdots, p_n^l\} \) \( (n = 1, 2, \cdots, m+1) \) except for \( p_m = l \) case. But this exceptional case does not really appear since \( g^{\gamma_{m+1}} \delta_{\{p'\}_m} = g^{\gamma_{m+1}} \delta_{\{p'\}_m} = 0 \) by using the fact that \( g^{\gamma_{m+1}} \) has been taken as off diagonal, but in form, we simply set \( \mathcal{L}_{m+1} \) to be an empty set.

Obviously, the cardinal numbers of \( \mathcal{L}_n \) are respectively \( l_n = p_{n-1}^l - p_{n-2}^l \), in which \( p_0^l = 0 \) and \( p_{m+1}^l = l \) are defined. For unify the denotation we need to define the subsets that do not contain the \( p_i^l \), they are \( \mathcal{L}_n' = \mathcal{L}_n - p_i^l \) and in the
exceptional case when $p_m = l$, $L'_{m+1} = \emptyset$. Their cardinal numbers are respectively $l'_n = l_n - 1$. But in the exceptional case when $p_m = l$, we still set $l'_{m+1} = 0$.

After summing all delta functions within $\delta_{(p')_{m}\gamma}$ and grouping the relevant terms, we have

$$
\sum_{\gamma_1, \cdots, \gamma_{l_n}} \delta_{(p')_{m}\gamma} g^{\gamma_1 \gamma_2} \cdots g^{\gamma_{l_n}} \prod_{i=1, i \notin \{p'\}_m}^l \frac{1}{(E_\gamma - E_{\gamma_i} - z)}
$$

$$
= \prod_{n=1}^{m+1} \left[ \sum_{\gamma_{p'_{n-1}+1}}^m g^{\gamma_{p'_{n-1}+1} \gamma \gamma_{p'_{n-1}}+1} g^{\gamma_{p'_{n-1}+1} \gamma_{p'_{n-1}+2} \gamma_{p'_{n-1}}+1} \cdots \frac{\eta_{\gamma \gamma_{p'_{n-1}}}}{(E_\gamma - E_{\gamma_i} - z)} \right]
$$

(C1)

(C2)

It must be emphasized that $l'_n = 0$ will lead to appear the factor $g^{\gamma_{p'_{n+1}} \gamma_{p'_{n+2}}} \delta_{\gamma_{p'_{n+1}} \gamma_{p'_{n+2}}} = g^{\gamma_{p'_{n+1}} \gamma_{p'_{n+2}}} \delta_{\gamma_{p'_{n+1}} \gamma_{p'_{n+2}}} = 0$, and no any $\frac{\eta_{\gamma_{p'_{n+1}}}}{(E_\gamma - E_{\gamma_i} - z)}$ is grouped into the square bracket. Note that the dummy indexes can be changed according to the given rules, we define

$$
R_{(p')}^{(l_n)}(z) = \sum_{\gamma_1, \cdots, \gamma_{l_n}} g^{\gamma_1 \gamma_2} \cdots g^{\gamma_{l_n}} \prod_{i=1}^l \frac{\eta_{\gamma \gamma_{p'_{n-1}}}}{(E_\gamma - E_{\gamma_i} - z)}
$$

(C3)

and then

$$
\sum_{\gamma_1, \cdots, \gamma_{l'_n}} \delta_{(p')_{m}\gamma} g^{\gamma_1 \gamma_2} \cdots g^{\gamma_{l'_n}} \prod_{i=1, i \notin \{p'\}_m}^l \frac{1}{(E_\gamma - E_{\gamma_i} - z)} = \prod_{n=1}^{m+1} R_{(p')}^{(l'_n)}(z)
$$

(C4)

Again substituting it into Eq. (B28), we arrive at

$$
\sum_{\gamma} A^{\gamma \gamma} = \sum_{\gamma} e^{-iE_\gamma t} + \sum_{\gamma} \sum_{i=1}^\infty \sum_{m=0}^\infty (-it)e^{-iE_\gamma t} \left( \frac{(-1)^m}{(m+1)!} \frac{d^m}{dz^m} \left[ \prod_{n=1}^{m+1} R_{(p')}^{(l'_n)}(z)e^{izt} \right] \right)_{z=0}
$$

(C5)

The summations over all set $\{p'\}_m$ can be changed into the summations over $l'_1, l'_2, \cdots, l'_m$, but there is a limitation that $\sum_{n=1}^m l'_n \leq l$. Interchanging the summations over $l$ and $m$, then $l$ begins at $m+1$, setting $l'_{m+1} = l - m$, and noting $t_{m+1}$ can be taken up to infinity, every $l'_n$ ($n = 1, 2, \cdots, m$) also can be taken up to infinity. Therefore

$$
\sum_{\gamma} A^{\gamma \gamma} = \sum_{\gamma} e^{-iE_\gamma t} + \sum_{\gamma} \sum_{m=0}^\infty \sum_{l'_1, \cdots, l'_{m+1}=1}^{l'_1 \leq l'_2} \left( -it \right) e^{-iE_\gamma t} \left( \frac{(-1)^m}{(m+1)!} \frac{d^m}{dz^m} \left[ \prod_{n=1}^{m+1} R_{(p')}^{(l'_n)}(z)e^{izt} \right] \right)_{z=0}
$$

(C6)

where we define the function $R_{(p')}^{(l'_n)}(z)$ by

$$
R_{(p')}^{(l'_n)}(z) = \sum_{l'_1=1}^{\infty} R_{(p')}^{(l'_1)}(z) = \sum_{\gamma} \sum_{l'_1=1}^{\infty} \left( \frac{(-1)^m}{(m+1)!} \frac{d^m}{dz^m} \left[ R_{(p')}^{(l'_n+1)}(z)e^{izt} \right] \right)_{z=0}
$$

(C7)

It is a kernel function in our approach and expressions.

**APPENDIX D**

Furthermore, we can expand the partition function as the power series of time $t$.

$$
\sum_{\gamma} A^{\gamma \gamma} = \sum_{\gamma} e^{-iE_\gamma t} \left[ 1 + \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} C^{\gamma \gamma}_n \right]
$$

(D1)
where the coefficient of $(-it)^n$ is as below:

$$C_n^\gamma = \sum_{m=n-1}^{\infty} \frac{n(-1)^{m-n+1}}{(m+1)(m-n+1)!} \left[ \frac{d^{m-n+1}_z}{dz^{m-n+1}} R^{m+1}_\gamma(z) \right] \bigg|_{z=0}$$

(D2)

It is easy to prove by expanding $e^{it\xi}$ and noting the derivative at $z = 0$.

From the definition of partition function, we also have

$$\sum_{\gamma} \hat{A}_{\gamma} = \sum_{\gamma} e^{-i\hat{E}_\gamma t} = \sum_{\gamma} e^{-i(E_\gamma + \Delta E_\gamma)t} = \sum_{\gamma} e^{-iE_\gamma t} \left[ 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} (\Delta E_\gamma)^n \right]$$

(D3)

Here, we have rewritten the Hamiltonian eigenvalues as

$$\bar{E}_\gamma = E_\gamma + \Delta E_\gamma$$

(D4)

After finishing the proof of the following relation

$$C_n^\gamma = (C_1^\gamma)^n$$

we can obtain

$$\sum_{\gamma} e^{-i\hat{E}_\gamma t} = \sum_{\gamma} e^{-i(E_\gamma + C_1^\gamma)t}$$

(D6)

Obviously

$$C_1^\gamma = \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)!} \left[ \frac{d^m}{dz^m} R^{m+1}_\gamma(z) \right] \bigg|_{z=0}$$

(D7)

Now let us begin our task. It is clear that if $C_{n+1}^\gamma = (C_1^\gamma) \times C_n^\gamma$ is verified then Eq.(D3) is proved. From the definition of $C_n^\gamma$, we see that,

$$C_n^\gamma \times C_1^\gamma = \left\{ \sum_{m=0}^{\infty} \frac{n(-1)^{m-n+1}}{(m+1)(m-n+1)!} \left[ \frac{d^{m-n+1}_z}{dz^{m-n+1}} R^{m+1}_\gamma(z) \right] \bigg|_{z=0} \right\} \times \left\{ \sum_{m=0}^{\infty} \frac{(-1)^m}{(m+1)!} \left[ \frac{d^m}{dz^m} R^{m+1}_\gamma(z) \right] \bigg|_{z=0} \right\}$$

$$= \sum_{M=n}^{M-n} (-1)^{M-n} \sum_{m=0}^{\infty} \frac{n}{(M-m)(M-m-n)!} \left[ \frac{d^{M-n-m}_z}{dz^{M-n-m}} R^{M-m}_\gamma(z) \right] \left[ \frac{d^m}{dz^m} R^{m+1}_\gamma(z) \right] \bigg|_{z=0}$$

(D8)

The last step has used the index transformations $M \rightarrow m_1 + m_2 + 1$ and $m_2 \rightarrow m$. While, we also know that

$$C_{n+1}^\gamma = \sum_{M=n}^{\infty} (-1)^{M-n} \frac{(n+1)}{(M+1)(M-n)!} \left[ \frac{d^{M-n}_z}{dz^{M-n}} R^{M+1}_\gamma(z) \right] \bigg|_{z=0}$$

(D9)

So, to prove Eq.(D5), we should prove the equation below (where $n \geq 1$).

$$\frac{d^{M-n}_z}{dz^{M-n}} R^{M+1}_\gamma(z) = \sum_{m=0}^{M-n} \frac{n}{n+1} \frac{M+1}{M-m} \frac{(M-n)!}{(m+1)!(M-m-n)!} \left( \frac{d^{M-n-m}_z}{dz^{M-n-m}} R^{M-m}_\gamma(z) \right) \left( \frac{d^m}{dz^m} R^{m+1}_\gamma(z) \right)$$

(D10)

Or for simplicity, set $M - n = k$

$$\frac{d^k}{dz^k} R^{k+1}_\gamma(z) = \sum_{m=0}^{k} \frac{n}{n+1} \frac{k+n}{k+m} \frac{k!}{(m+1)!(k-m)!} \left( \frac{d^{k-m}_z}{dz^{k-m}} R^{k+1}_\gamma(z) \right) \left( \frac{d^m}{dz^m} R^{m+1}_\gamma(z) \right)$$

(D11)
Note that it is not Leibnitz’ rule for the $n$th derivative of a product since the differential functions connect with the summation index. It is clear that when $k = 1$, we can directly verify Eq. (D11) is valid. That is

$$\sum_{m=0}^{1} \frac{n}{n+1} \frac{1}{n-m} \frac{1}{(m+1)!} \left( \frac{d^{1-m}}{dz^{1-m}} R_{\gamma}^{1+n-m}(z) \right) \left( \frac{d^{m}}{dz^{m}} R_{\gamma}^{m+1}(z) \right)$$

$$= (n+2) R_{\gamma}^{n+1}(z) \frac{d}{dz} R_{\gamma}(z) = \frac{d}{dz} R_{\gamma}^{n+1}(z)$$

(D12)

Assume up to a given $l$ Eq. (D11) is correct, and then, in the case of $l+1$, we can also prove it is correct as below. After the one order differential, using the Leibnitz’ rule for high order derivative of a product, it follows that

$$\frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1+n+1} = (l+n+2) \sum_{j=0}^{l} \frac{l!}{j!(l-j)!} \left[ \sum_{m=0}^{l-j} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{\frac{d^{l-j-m}}{dz^{l-j-m}} R_{\gamma}^{l-m}}{\sum_{m=0}^{l-j}} \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \right]$$

(D13)

Since Eq. (D11) is assumed to be correct up to a given $l$, Eq. (D11) is valid up to $M = l+n \ (n \geq 1)$. Thus we can make use of Eq. (D10) to replace the $(l-j)$th derivative in above equation except for $j = 0$.

$$\frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1+n+1} = \sum_{m=0}^{l} \frac{(l+n+2)}{(l-m)} \left( \begin{array}{c} \frac{l+1}{l-m} \frac{1}{(m+1)!} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \right)$$

$$= \sum_{j=1}^{l} \frac{l!}{j!(l-j)!} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right)$$

(D14)

Interchanging the summations over $j$ and $m$, we have

$$\frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1+n+1} = \sum_{m=0}^{l} \frac{(l+n+2)}{(l-m)} \left( \begin{array}{c} \frac{l+1}{l-m} \frac{1}{(m+1)!} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \right)$$

$$= \sum_{j=1}^{l} \frac{l!}{j!(l-j)!} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right)$$

(D15)

Specially, the terms in the square bracket can be simplified as

$$= \sum_{j=1}^{l} \frac{l!}{j!(l-j)!} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right) \frac{d^{l-j}}{dz^{l-j}} \left( \begin{array}{c} \frac{R_{\gamma}^{m}}{d^{m}} \\ \frac{d^{m}}{dz^{m}} \end{array} \right)$$

(D16)
\[ \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1+n} = \sum_{m=0}^{l-1} \frac{n}{n+1} \frac{l+1+n+1}{l+1+n-m} \frac{(l+1)!}{(m+1)!((l+1)-m)!} \left( \frac{d^{l+1-m}}{dz^{l+1-m}} R_{\gamma}^{l+1+n-m}(z) \right) \left( \frac{d^{m}}{dz^{m}} R_{\gamma}^{m+1}(z) \right) \]

\[ + \sum_{m=0}^{l-1} \frac{1}{n+1} \frac{l+1+n+2}{l+1+n-m} \frac{(l+1)!}{(m+1)!((l+1)-m)!} \left( \frac{d^{l+1-m}}{dz^{l+1-m}} R_{\gamma}^{l+1-n-m}(z) \right) \left( \frac{d^{m}}{dz^{m}} R_{\gamma}^{m+1}(z) \right) \]

\[ + \frac{l+n+2}{n+1} \left( \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1} \right) \frac{d}{dz} R_{\gamma}^{n+1} \]

Now, the problem is changed into the proof that the below expression is zero.

\[ \frac{1}{l+2} \left( \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+2} \right) R_{\gamma}^{n} + (n-1) \left( \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1} \right) \frac{d}{dz} R_{\gamma}^{n+1} \]

\[ - \sum_{m=0}^{l-1} \frac{1}{l+1+m} \frac{l+1+1-1}{l+1+n-m} \frac{(l+1)!}{(m+1)!((l+1)-m)!} \left( \frac{d^{l+1-m}}{dz^{l+1-m}} R_{\gamma}^{l+1-m}(z) \right) \left( \frac{d^{m}}{dz^{m}} R_{\gamma}^{m+1}(z) \right) \]

\[ + (l+1) \left( \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1} \right) \frac{d}{dz} R_{\gamma} \]

Similar to deal with Eq. (D10), that is, carrying out derivation like Eq. (D17), we can obtain the \((l+1)\)th the derivative in the first term.

\[ \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+2} = \sum_{m=0}^{l-1} \frac{l+2}{l+1} \frac{(l+1)!}{l+1+n-m} \frac{(l+1)!}{(m+1)!((l+1)-m)!} \left( \frac{d^{l+1-m}}{dz^{l+1-m}} R_{\gamma}^{l+1-m} \right) \left( \frac{d^{m}}{dz^{m}} R_{\gamma}^{m+1}(z) \right) \]

\[ + (l+2) \left( \frac{d^{l+1}}{dz^{l+1}} R_{\gamma}^{l+1} \right) \frac{d}{dz} R_{\gamma} \]

Substitute it into Eq. (D18), we immediately see the expression (D18) is zero. It means that (D11) is proved to be correct for \(l+1\). Therefore, we have proved Eq. (D5)

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