Rescaled Perturbation Theory

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A non-perturbative method which can go beyond the weak coupling perturbation theory is introduced. Essential idea is to formulate a set of exact differential equations as a function of the coupling strength g. Unlike other resummation in which information of the higher order terms is necessary, we only need a leading order perturbative formula in every step to reach the large value of g. The method is applied to the quantum anharmonic oscillator and quantum double well potential in one dimension. Both are known to have divergent series in the weak coupling perturbation and the latter is not Borel summable. Our method is shown to work well from the weak coupling to the strong coupling for the energy eigenvalues and the wave functions. The method is also applied successfully to the system with time-dependent external field.

In quantum many-body problems and in quantum field theories, there are many systems where one needs to study phenomena over broad range of the coupling strength.[1)] Typical examples are the BEC-BCS crossover in ultracold atoms where the coupling strength is changed by utilizing the Feschbach resonance,[2),3)] hadron-quark transitions in dense QCD (quantum choromodynamics) where the coupling runs with the baryon density,[4)] and the quark-gluon plasma near the critical temperature where the coupling runs with temperature.[5)] So far a number of techniques have been developed to resum naive perturbative series or to produce better behaved series under the names of resummed perturbation, optimized perturbation, variational perturbation and so on. (For reviews, see e.g. Refs.6), 7).)

In this Letter, we introduce a novel method which can go beyond the weak coupling perturbation theory: we test its applicability to quantum mechanical examples such as the anharmonic oscillator and double well potential. Instead of resumming the perturbation series, we iterate the lowest order perturbation through the rescaling of the coupling strength, so that the method gives a global coupling dependence of eigenvalues and eigenvectors simultaneously. The basic formula has formal resemblance to the exact renormalization group method (ERG, see e.g. Ref.9) for a review) if we replace the cutoff scale of ERG by the coupling strength in the present approach.

Let us consider a quantum system such that the Hamiltonian is

$$\mathcal{H}(g) = \mathcal{H}_0 + g\mathcal{H}_{\rm int} \ , \tag{1}$$

where g is a dimensionless coupling strength and $\mathcal{H}_0$ is assumed to be solved exactly. Our goal is to obtain $E_n(g)$ and $|\psi_n(g)\rangle$ satisfying

$$\mathcal{H}(g)|\psi_n(g)\rangle = E_n(g)|\psi_n(g)\rangle \ . \tag{2}$$

To simplify the discussion, we consider a non-degenerate $\mathcal{H}_0$. Generalization to the degenerate case is straightforward. Suppose we know $E_n(g)$ and $|\psi_n(g)\rangle$, then we can

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calculate $E_n(g+\delta g)$ and $|\psi_n(g+\delta g)\rangle$ as long as $\delta g \ll 1$ by using the leading order Rayleigh-Schrödinger perturbation theory (RSPT) for $\mathcal{H}(g+\delta g) = \mathcal{H}(g) + \delta g \mathcal{H}_{\rm int}$,

$$E_n(g+\delta g) = E_n(g) + \delta g \langle\psi_n(g)|\mathcal{H}_{\rm int}|\psi_n(g)\rangle \ , \tag{3}$$

$$|\psi_n(g+\delta g)\rangle = |\psi_n(g)\rangle + \delta g \sum_{n\neq i} \frac{\langle\psi_i(g)|\mathcal{H}_{\rm int}|\psi_n(g)\rangle}{E_n(g)-E_i(g)}|\psi_i(g)\rangle \ . \tag{4}$$

Then we can set up differential equations for the eigenvalues, matrix elements $\mathrm{H}^{ij}_{\rm int}(g) = \langle\psi_i(g)|\mathcal{H}_{\rm int}|\psi_j(g)\rangle$ and the wave functions as

$$\frac{\mathrm{d}}{\mathrm{d}g}E_i(g) = \mathrm{H}^{ii}_{\rm int}(g) \ , \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}g}\mathrm{H}^{ij}_{\rm int}(g) = \sum_{i\neq k} \frac{\mathrm{H}^{ik}_{\rm int}(g)\mathrm{H}^{kj}_{\rm int}(g)}{E_i(g)-E_k(g)} + \sum_{j\neq k} \frac{\mathrm{H}^{ik}_{\rm int}(g)\mathrm{H}^{kj}_{\rm int}(g)}{E_j(g)-E_k(g)} \ , \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}g}|\psi_i(g)\rangle = \sum_{i\neq k} \frac{\mathrm{H}^{ki}_{\rm int}(g)}{E_i(g)-E_k(g)}|\psi_k(g)\rangle \ . \tag{7}$$

Note that we have no approximation to obtain the right hand sides of these equations, so that they are exact equations. We take $\langle\psi_i(0)|\psi_i(g)\rangle = \langle\psi_i(0)|\psi_i(0)\rangle = 1$ as a normalization of the state vector, so that the norm of eigenvectors are conserved i.e. $\frac{\mathrm{d}}{\mathrm{d}g}\langle\psi_i(g)|\psi_i(g)\rangle = 0$. Coupled differential equations (5), (6) and (7) can be solved with the initial conditions, $E_i(0)$, $\mathrm{H}^{ij}_{\rm int}(0)$ and $|\psi_i(0)\rangle$, and one may go to arbitrary large values of g in principle.

Let us now apply this method to the one-dimensional quantum anharmonic oscillator (AHO):

$$\mathcal{H}_{\rm AHO}(g) = \frac{1}{2}p^2 + \frac{1}{2}x^2 + gx^4 \ . \tag{8}$$

This is a typical example that RSPT leads to a divergent series but is Borel summable. (See e.g. Ref.6), 8) for reviews.) Using $c_{ij}(g) = \langle\psi_j(0)|\psi_i(g)\rangle$, we can rewrite eq.(7) as

$$\frac{\mathrm{d}}{\mathrm{d}g}c_{ij}(g) = \sum_{i\neq k} \frac{\mathrm{H}^{ki}_{\rm int}(g)}{E_i(g)-E_k(g)}c_{kj}(g) \ . \tag{9}$$

The initial conditions at $g=0$ read,

$$E_i(0) = i + 1/2 \ , \tag{10}$$

$$\mathrm{H}^{ij}_{\rm int}(0) = \frac{1}{\sqrt{\pi 2^{i+j} i! j!}} \int \mathrm{d}x \ \mathrm{e}^{-x^2} x^4 H_i(x) H_j(x) \ , \tag{11}$$

$$c_{ij}(0) = \delta_{ij} \ , \tag{12}$$

where $H_i(x)$ is the i-th Hermite polynomial. In actual calculation, we solve the coupled differential equations for the states $i = 0, 1, \cdots N-1$. For g up to 10, taking $N = 50$ is accurate enough to have the eigenvalues of the low-lying states as shown in Table I. Here, we compare our results with those given in Ref.10) by the diagonalization method.

Table I. Comparison of the lowest three eigenvalues of AHO. The upper numbers are obtained from the present method and the lower numbers from Ref.10).

g	E_0	E_1	E_2
0.1	0.55914633	1.7695026	3.1386243
	0.55914633	1.7695026	3.1386243
0.5	0.69617582	2.3244064	4.3275250
	0.69617582	2.3244064	4.3275250
1.0	0.80377065	2.7378923	5.1792917
	0.80377065	2.7378923	5.1792915
5.0	1.2245874	4.2995081	8.3179758
	1.2245870	4.2995017	8.3179605
10	1.5049814	5.3216308	10.348359
	1.5049724	5.3216080	10.347056

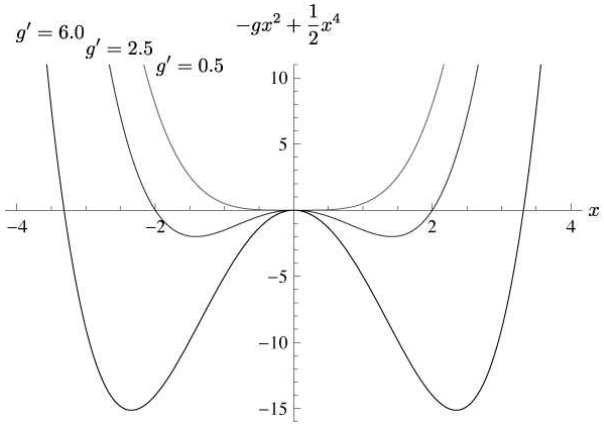

Fig. 1. The double well potential $V(x) = -gx^2 + \frac{1}{2}x^4$ as a function of several values of $g' = g - 1/2$.

Next, we study the quantum double well potential (DWP) with the Hamiltonian,

$$\mathcal{H}_{\rm DWP}(g) = \frac{1}{2}p^2 - gx^2 + \frac{1}{2}x^4 \ \ (g > 0), \tag{13}$$

where the RSPT also breaks down and is known to be Borel non-summable. (See e.g. Ref.6), 8) for reviews.) To make a firm connection between DWP and AHO in our approach, we rewrite the Hamiltonian as

$$\mathcal{H}'_{\rm DWP}(g') = \Big(\frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{2}x^4\Big) - g'x^2 \tag{14}$$

$$= \mathcal{H}_{\rm AHO} - g'\mathcal{H}_{\rm int} \ , \tag{15}$$

so that the un-perturbed Hamiltonian at $g' = 0$ becomes AHO. Note that the system changes from AHO for $g' < 1/2$ to DWP for $g' > 1/2$. In Fig. 1, the shape of the potential is shown for several different values of g'.

Using the results of the previous AHO for $N = 50$, we calculate the energy eigenvalues of this system as a function of g'. The differential equations are the

same as Eqs.(5), (6) and (9), where $|\psi_i(0)\rangle$ is the eigenvector of AHO in the present case. The initial conditions read,

$$E_i(0) = E_i^{\rm AHO}(\frac{1}{2}) \ , \tag{16}$$

$$\mathrm{H}_{\rm int}^{ij}(0) = \langle\psi_i(0)| - \hat{x}^2|\psi_j(0)\rangle \tag{17}$$

$$= \sum_{k,l=0}^{49} c_{ik}^{\rm AHO}(\frac{1}{2}) c_{jl}^{\rm AHO}(\frac{1}{2}) \frac{1}{\sqrt{\pi 2^{k+l} k!l!}} \int \mathrm{d}x \ \mathrm{e}^{-x^2}(-x^2) H_k(x) H_l(x) \ ,$$

$$c_{ij}(0) = \delta_{ij} \ . \tag{18}$$

Here i, j runs from 0 through $N-1$, and N is taken to be 50 as before. This is good enough again for low-lying eigenvalues as shown in Table II where comparison to the high accuracy eigenvalues given in Ref.11) by the diagonalization method is shown.

Table II. Comparison of the lowest two eigenvalues for the DWP. The upper numbers are calculated by our method, while the lower numbers are taken from Ref.11).

g'	E_0	E_1
0.50	0.53018104538	1.8998365150
	0.53018104524	1.8998365149
1.0	0.32882650295	1.4172681012
	0.32882650260	1.4172681011
5.5	-10.316788242	-10.316773352
	-10.316788351	-10.316773442
8.0	-25.420689499	-25.420692377
	-25.420693642	-25.420693642

In Fig. 2, we show g' dependence of the lowest six energy eigenvalues from the weak coupling to the strong coupling. As g' increases, the degeneracy of the even-n and odd-n eigenstates takes place starting from the low energy state. This can be seen clearly by looking at the probability distributions of the lowest two states as shown in Fig. 3. Depending on g', the energy eigenstate changes from a single oscillator to the superposition of double (left and right) oscillators.

The present method can be generalized to the time-dependent Schrödinger equation with non-adiabatic time-depending potential:

$$i\partial_t|\psi(t)\rangle = \mathcal{H}(t)|\psi(t)\rangle \ , \tag{19}$$

where $\mathcal{H}(t) = \mathcal{H}_0 + g(t)\mathcal{H}_{\rm int}$. We expand the state vectors by the adiabatic basis:

$$|\psi(t)\rangle = \sum_n \ a_n(t)|n(t)\rangle \ , \tag{20}$$

$$\mathcal{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle \ , \tag{21}$$

where $E_n(t)$ and $|n(t)\rangle$ are instantaneous eigenvalues and eigenvectors with their time dependence implicitly through the coupling $g(t)$. We perform a unitary transformation:

$$a_n(t) = \alpha_n(t)\mathrm{e}^{-i\Theta_n(t)} \ , \tag{22}$$

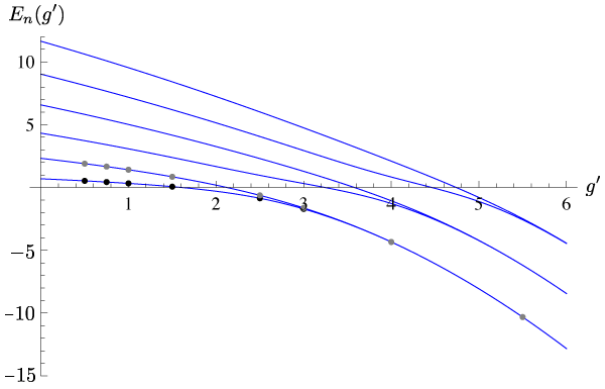

Fig. 2. The lowest six energy eigenvalues for the DWP with $N = 50$. Filled circles are high accuracy numerical results given in Ref.11).

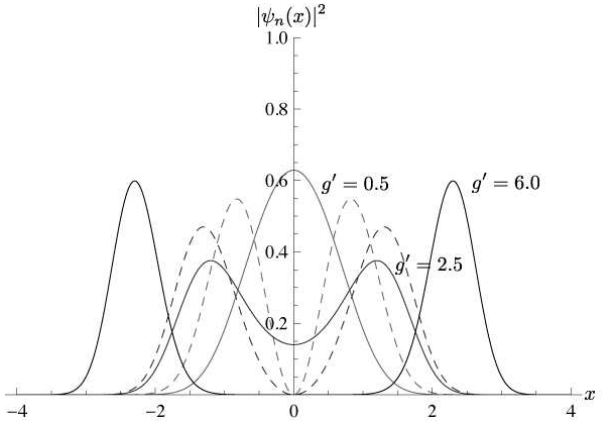

Fig. 3. Probability distributions for the lowest two states for the DWP with $N = 50$. The solid line is for the ground state and the dashed line is for the first excited state. The lighter gray line is for $g' = 0.5$, the gray line is for $g' = 2.5$ and the black line is for $g' = 6.0$.

$$\Theta_n(t) = \int_0^t \mathrm{d}t' \; E_n(t') \; , \tag{23}$$

and obtain

$$\partial_t \alpha_n(t) = -\sum_m \; \alpha_m(t) \langle n(t)|\partial_t|m(t)\rangle \mathrm{e}^{i(\Theta_n(t)-\Theta_m(t))} \; . \tag{24}$$

Although $g(t)$ is an arbitrary smooth function of t, one may always introduce a set of time intervals, so that $g(t)$ is a monotonic function of t. Then, within each interval, we have

$$\partial_g \alpha_n(g) = -\sum_m \; \alpha_m(g) \langle n(g)|\partial_g|m(g)\rangle \mathrm{e}^{i(\Theta_n(g)-\Theta_m(g))} \; , \tag{25}$$

$$\Theta_n(g) = \int_0^g \mathrm{d}\bar{g} \; \frac{1}{\dot{\bar{g}}} E_n(\bar{g}) \; , \tag{26}$$

where $\dot{g}$ implies the time derivative of coupling strength. Assuming that $\mathcal{H}_0$ is not degenerate, we obtain the following equations from (5), (6) and (7):

$$\partial_g \alpha_n(g) = \sum_{m \neq n} \frac{\mathrm{H}_{\mathrm{int}}^{nm}(g)}{E_n(g) - E_m(g)} \alpha_m(g) \mathrm{e}^{i(\Theta_n(g) - \Theta_m(g))} \ , \tag{27}$$

$$\partial_g \Theta_n(g) = \frac{1}{\dot{g}} E_n(g) \ . \tag{28}$$

To calculate the evolution of $\alpha_n(g)$ and $\Theta_n(g)$, we need the coupling dependence of $E_n(g)$ and $\mathrm{H}_{\mathrm{int}}^{nm}(g)$, which is directly obtained from our approach, so that we can trace the flows of $E_n(g)$, $\alpha_n(g)$ and $\Theta_n(g)$ simultaneously through the flows of $\mathrm{H}_{\mathrm{int}}^{nm}(g)$.

Here, we solve the differential equations numerically in the case that a coupling strength depends linearly on time (i.e. $g = vt$) and obtain the transition probabilities to adiabatic states $|\alpha_n(t)|^2$. In Fig. 4, taking the ground state of AHO as an initial condition, we show the transition probabilities as a function of time for the DWP with the Hamiltonian: $\mathcal{H}'_{\mathrm{DWP}}(g'(t) = vt)$ in eq.(14). Because of the parity conservation, the transition probability for odd n becomes zero. If we change the potential slowly as the dashed lines ($v = 0.1$) in Fig 4, instantaneous basis at $n = 0$ is mostly occupied at any time. On the other hand, if we change the potential suddenly as the solid lines ($v = 3.0$), higher instantaneous states are excited with mutual oscillations.

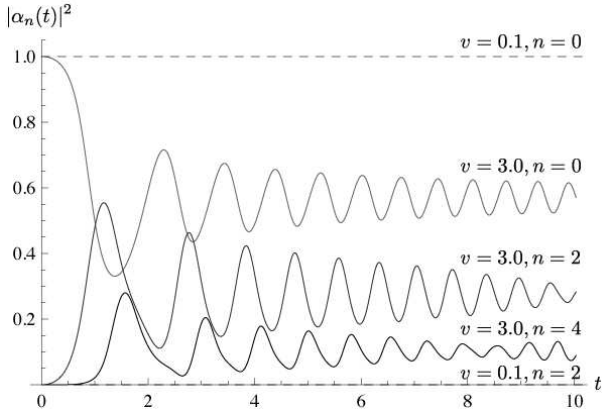

Fig. 4. The lowest three even transition probabilities $|\alpha_n(t)|^2$ ($n = 0, 2, 4$) in DWP for $N = 50$. The lighter gray line is for $n = 0$, the gray line is for $n = 2$ and the black line is for $n = 4$. The dashed line is for $v = 0.1$ and the solid line is for $v = 3$.

In summary, we introduced a non-perturbative method applicable to large values of the coupling strength g. Essential idea is to formulate a set of exact differential equations as a function of g, so that they can be solved with appropriate known initial conditions to reach large values of g. Unlike resummation methods in which information of the higher order terms in the naive perturbation series is necessary, we only need a leading order perturbative formula in every step. This is similar to the situation in the exact renormalization group method. In the present method, all the eigenvalues and eigenstates can be calculated simultaneously and accurately

as a function of g as long as we prepare large enough dimension N of the Hilbert space. Note here that we do not need to diagonalize the $N \times N$ Hamiltonian; instead we trace the flows of eigenvalues and eigenvectors starting from the solvable $N \times N$ Hamiltonian. We have applied our method to the quantum anharmonic oscillator and quantum double well potential in one dimension. Both are known to have divergent series in RSPT and the latter is not even Borel summable. We found that our method works well from the weak coupling to the strong coupling for the energy eigenvalues and wave functions. Furthermore, because of the flow equations of the energy eigenvalues and the matrix elements $\mathrm{H}_{\mathrm{int}}^{ij}(g)$, we could solve even the time-dependent Schrödinger equation for the potential with non-adiabatic variation in time.

The basic idea of the present method can be also generalized to the quantum field theory and quantum statistical mechanics. In these cases, one can derive a differential equation for the partition function $Z[J,g]$ as functions of the external field J and the coupling strength g,

$$\frac{\mathrm{d}}{\mathrm{d}g}Z[J,g] = \mathrm{S}_{\mathrm{int}}(\frac{\delta}{\delta J})Z[J,g] \ , \tag{29}$$

where the initial condition $Z[J,0]$ is assumed to be solvable. Similarly, we can also apply the idea to the generalization of the linear response theory to derive a formula:

$$\frac{\mathrm{d}}{\mathrm{d}g}\langle\hat{O}\rangle[t;g] = i\int_{t_0}^{t}\mathrm{d}t' \ \mathrm{Tr}\Big(\rho(t_0)[\mathcal{H}_{\mathrm{int}}^{h}(t';g),\hat{O}^{h}(t)]\Big) \ . \tag{30}$$

Here A is a external filed and j is a conjugate quantity, and h denotes Heisenberg picture in terms of $\mathcal{H}[t;g] = \mathcal{H}_0 + g\hat{j}A(t)$. Applications of these equations to physical systems will be discussed in the forthcoming publications.

After the completion of this work, we became aware that similar differential equations as ours are discussed in Appendix C of Ref.12) although the equations are applied in rather different context from ours. The author would like to thank Tetsuo Hatsuda, Kyogo Kawaguchi and Haruki Watanabe for useful discussions and suggestions.

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