# Global-operator perturbation theory for a self-interacting boson system

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We consider a single-mode self-interacting boson system with an arbitrary interaction. The Van Vleck-Primas operator perturbation theory can be used to obtain the perturbative solutions to any desired order in closed form. In contrast to ordinary perturbation theory, which deals with each state individually, the present method is global and treats all the states in the spectrum collectively. The solution process involves the systematic application of four basic rules.

We consider a single-mode self-interacting boson system with the following Hamiltonian:

$$H=H_0(N)+\sum_{ji}\lambda^j[f_{ji}(N)a^i+\text{H.c.}] \ , \tag{1}$$

where only a finite number of the functions $f_{ji}$ are nonzero, $a$ and $a^\dagger$ are the annihilation and creation operators, and $N\equiv a^\dagger a$ is the number operator. The often-studied problem of the anharmonic oscillator and the recently studied model Hamiltonian by Takeda and Ui[1] with special cubic and quartic self-interactions, both in the weak-coupling and strong-coupling limits, as well as many higher-order self-interacting systems, all fall into the category of Hamiltonians that can be represented by Eq. (1). Specifically for the quartic anharmonic oscillator, we have

$$H_0^{\text{AO}}=N \ , \tag{2a}$$

$$f_{10}^{\text{AO}}=\tfrac{3}{4}(2N^2+2N+1) \ , \tag{2b}$$

$$f_{12}^{\text{AO}}=\tfrac{1}{2}(2N+3) \ , \tag{2c}$$

$$f_{14}^{\text{AO}}=1 \ , \tag{2d}$$

and the rest of the $f_{ij}$'s are zero. For the model Hamiltonian studied by Taked and Ui,[1] the Hamiltonian is

$$H^{\text{TU}}=(a^\dagger+\eta a^\dagger a^\dagger)(a+\eta aa) \ . \tag{3}$$

In the weak-coupling limit ($\eta\to 0$), $\lambda=\eta$, and

$$H_0^{\text{TU},W}=N \ , \tag{3a}$$

$$f_{11}^{\text{TU},W}=N \ , \tag{3b}$$

$$f_{20}^{\text{TU},W}=N(N-1) \ . \tag{3c}$$

In the strong-coupling limit ($\eta\gg 1$), $\lambda=1/\eta$, and

$$H_0^{\text{TU},S}=\eta^2(N^2-N) \ , \tag{4a}$$

$$f_{11}^{\text{TU},S}=N \ , \tag{4b}$$

$$f_{20}^{\text{TU},S}=N \ . \tag{4c}$$

The rest of the $f_{ij}$'s are zero. Thus a study of the general solution to the Hamiltonian in Eq. (1) would be of interest in the study of a wide range of problems, ranging from atomic and molecular physics to particle physics.

I would like to show that a global perturbative solution to the Hamiltonian in Eq. (1) can be written down in closed form to any arbitrary order by the application of the Van Vleck[2]–Primas[3] operator perturbation theory (VVP OPT). This procedure involves the repeated application of four rules: (i) normal ordering, (ii) contraction, (iii) computation of commutators, and (iv) solution to operator equations in closed forms.

VVP OPT (Refs. 2–4) seeks perturbative solutions to the Van Vleck operator $U$ that takes the unperturbed state to the perturbed state and to the operator $g$ that maps the unperturbed energy to the perturbed energy. Whereas the ordinary Rayleigh-Schrödinger perturbation theory deals with each state in the spectrum individually, VVP OPT is global and treats the whole spectrum collectively. Moreover, it does not even require knowledge of the unperturbed wave functions. Let $H_0$ and $H=H_0+\sum_i\lambda^i H_i$, where only a finite number of $H_i$'s are nonzero, denote the unperturbed and total Hamiltonians of a system and let $(\psi_0, E_0)$ and $(\psi,E)$ denote the corresponding eigenfunctions and eigenvalues. Then $(\psi_0, E_0)$ and $(\psi,E)$ are related through the mappings

$$\psi=U\psi_0 \ , \tag{5}$$

and

$$E=g(E_0) \ . \tag{6}$$

$U$, $H$, and $g=g(H_0)$ are related by

$$UgU^\dagger=H \ . \tag{7}$$

$U$ is unitary and one can define a Hermitian matrix $\Lambda$ such that

$$U=\exp(i\Lambda) \ . \tag{8}$$

The perturbation expansions of $\Lambda$ and $g$ have the form

$$\Lambda=\sum_{k=1}^{\infty}\lambda^k\Lambda_k \ , \tag{9}$$

$$g=\sum_{j=0}^{\infty}\lambda^j g_j \ . \tag{10}$$

On substituting Eqs. (9) and (10) into Eq. (8), we obtain

$$\sum_{\mu=0}^{\infty}\lambda^\mu\sum_{n=0}^{\mu}\Gamma_{n\mu}=H_0+\sum_{i=1}^{\infty}\lambda^i H_i \ , \tag{11}$$

where

$$\Gamma_{n\mu}\equiv\frac{1}{n!}\sum_{j_{n-1}=n-1}^{\mu-1}\cdots\sum_{j_0=0}^{j_1-1}[i\Lambda_{\mu-j_{n-1}},[\cdots[i\Lambda_{j_1-j_0},g_{j_0}]]] \ , \tag{12}$$

 

and

$$\Gamma_{0\mu}=g_\mu \ . \tag{13}$$

Equation (11) can be rewritten in the hierarchical form

$$g_0=H_0 \ , \tag{14a}$$

$$g_1+[i\Lambda_1,g_0]=H_1 \ , \tag{14b}$$

and for $k\geq 2$,

$$g_k+[i\Lambda_k,g_0]=H_k-\sum_{j=1}^{k-1}[i\Lambda_j,g_{k-j}]-\sum_{j=2}^{k}\Gamma_{jk} \ . \tag{14c}$$

We immediately note the following: (1) The operator equations in the hierarchy are linear. (2) The right-hand side (RHS) of the $k$th-order equation is known once the equations earlier in the hierarchy are solved. (3) The $k$th-order equation is similar in form to the first-order equation except that the effective first-order perturbation involves more terms; however, because of the linearity of the operator equation, this presents no difficulty, in principle. (4) The solution to $g_k$ is obtained by taking the diagonal part of the $k$th-order equation. (5) $\Lambda_k$ is determined up to an additive function of operators that commute with $H_0$. Its uniqueness can be fixed by the requirement that this additive function be zero.[3,4] We now turn to the general solution of the $k$th-order equation:

$$g_k+[i\Lambda_k,H_0]=V_k^D+V_k^0 \ , \tag{15}$$

where we have decomposed the RHS of Eq. (14c) into a diagonal part $V_k^D$ and an off-diagonal part $V_k^0$. According to remark (4) above,

$$g_k=V_k^D \ , \tag{16}$$

and $\Lambda_k$ is obtained by the solution to the linear operator equation:

$$[i\Lambda_k,H_0]=V_k^0 \ , \tag{17}$$

where Eq. (14a) has been used. The solution for $\Lambda_k$ to Eq. (17) is given by[5,6]

$$\Lambda_k=\lim_{\epsilon\to 0+}\int_0^\infty \exp(iH_0t)\,V_k^0\exp(-iH_0t-\epsilon t)\,dt \ . \tag{18}$$

With $g_k$ and $\Lambda_k$ thus obtained, one then moves to the $(k+1)$th-order equation and so on up the hierarchy until singular behaviors show up in Eq. (18). If this situation never develops, then in principle VVP OPT can be used to solve bound-state perturbation problems globally to any given order.

In practice, this integral in Eq. (18) is not easy to evaluate. However, for the class of Hamiltonians represented by Eq. (1), the solutions to the operator equation (15) are most easily obtained by taking advantage of the Lie structure[3] among the operators $a$, $a^\dagger$, and $N\equiv a^\dagger a$. The entire solution process for each equation in the hierarchy involves the systematic application of four rules.

Rule I: All operators need to be normal ordered according to the relations

$$a^n f(N)=f(N+n)a^n \tag{19a}$$

and

$$f(N)a^{\dagger m}=a^{\dagger m}f(N+m) \ . \tag{19b}$$

Rule II: All operators involving the simultaneous appearance of $a$'s and $a^\dagger$'s must be contracted (for $m\geq n$) according to the relations

$$a^{\dagger m}f(N)a^n=(a^\dagger)^{m-n}\frac{N!}{(N-n)!}f(N-n) \tag{20a}$$

and

$$a^{\dagger n}f(N)a^m=\frac{N!}{(N-n)!}f(N-a)a^{m-n} \ . \tag{20b}$$

Rule III: After normal ordering and contraction have been performed, all of the commutators encountered can be computed as given below (for $m\geq n$),

$$[a^{\dagger m}f(N),a^{\dagger n}g(N)]=(a^\dagger)^{m+n}[f(N+n)g(N)-f(N)g(N+m)] \ , \tag{21a}$$

$$[f(N)a^n,g(N)a^m]=[f(N)g(N+n)-f(N+m)g(N)]a^{n+m} \ , \tag{21b}$$

$$[f(N)a^n,a^{\dagger m}g(N)]=(a^\dagger)^{m-n}\left[\frac{(N+m)!}{(N+m-n)!}f(N+m-n)g(N)-\frac{N!}{(N-n)!}f(N-n)g(N-n)\right] \ , \tag{21c}$$

and

$$[f(N)a^m,a^{\dagger n}g(N)]=\left[\frac{(N+m)!}{(N+m-n)!}g(N+m-n)f(N)-\frac{N!}{(N-n)!}g(N-n)f(N-n)\right]a^{m-n} \ . \tag{21d}$$

In Eqs. (20) and (21), the factorial sign is conveniently used for

$$\frac{(N+m)!}{(N+m-n)!}=\prod_{j=0}^{n-1}(N+m-j) \ . \tag{22}$$

Rule IV: After the RHS of Eq. (14c) has been computed according to rule III, it will appear as a sum of normal-ordered terms. Because of the linearity of Eq. (14c), its solution is the sum of the solutions corresponding to each normal-ordered term on the RHS which appears only in one of two forms and the corresponding solution can be obtained as follows:

$$[A,g(N)]=f(N)a^m \rightleftarrows A=f(N)[g(N+m)-g(N)]^{-1}a^m \tag{23a}$$

and

$$[B,g(N)]=a^{\dagger m}f(N) \rightleftarrows B=-a^{\dagger m}f(N)[g(N+m)-g(N)]^{-1} \ . \tag{23b}$$

Thus, the solution to each equation in the hierarchy can

be obtained by the systematic application of rules I to IV. On examining Eq. (14), we note that the unperturbed Hamiltonian $H_0$ corresponds to the function $g(N)$ that appears in Eq. (23). Hence, if $H_0(N)$ exhibit degeneracy, that is, if there exists a pair of numbers $(n,n+m)$, where both $n$ and $m$ are positive such that $H_0(n)$ and $H_0(n+m)$ are equal, the solutions to $A$ and $B$ in Eq. (23) may be singular. However, if $f(n)$ vanishes [it is not necessary that $f(n+m)$ vanishes] the singularity may be avoided. The model Hamiltonian of Takeda and Ui in the strong-coupling limit is such an example. We now apply the present technique to the quartic anharmonic oscillator and the Takeda-Ui model Hamiltonian.

*Example I: The quartic anharmonic oscillator.*[7] The perturbative solutions to the Van Vleck operator and the level shift operator are calculated via Eqs. (14) and rules I–IV. We state the results to second order:

$$g_1^{AO}=\tfrac{3}{4}(2N^2+2N+1) \ , \tag{24a}$$

$$g_2^{AO}=\tfrac{1}{8}(2N+1)(17N^2+17N+21) \ , \tag{24b}$$

$$\Lambda_1^{AO}=\frac{i}{16}[a^{\dagger 4}+4a^{\dagger 2}(2N+3)]+\text{H.c.} \ , \tag{24c}$$

and

$$\Lambda_2^{AO}=i\left(\frac{a^{\dagger 6}}{48}-\frac{3}{32}a^{\dagger 4}(2N+5)-\frac{3}{32}a^{\dagger 2}(22N^2+66N+57)\right)+\text{H.c.} \tag{24d}$$

For the case of the ground state ($N=0$), the first- and second-order energy shifts are in agreement with the Bender-Wu calculations.[8] Hence VVP OPT appears to face the same convergence difficulty associated with the quartic anharmonic oscillator.

*Example II: The model Hamiltonian of Takeda and Ui [Eq. (3)] for a single-mode self-interacting boson system in the weak-coupling limit.* We substitute Eqs. (3a)–(3c) in the hierarchy of Eqs. (14), and obtain the results to second order:

$$g_1^{TU,W}=0 \ , \tag{25a}$$

$$g_2^{TU,W}=-2N^2 \ , \tag{25b}$$

$$\Lambda_1^{TU,W}=i(a^{\dagger}N-Na) \ , \tag{25c}$$

and

$$\Lambda_2^{TU,W}=0 \ . \tag{25d}$$

These results are in harmony with those of Takeda and Ui.

*Example III: The Hamiltonian in example II in the strong-coupling limit.* Here, the energy shift operator vanishes for the first, second, and third orders. We substitute Eqs. (4a)–(4c) in the hierarchy of Eqs. (14). We state the results for the shift operator to fourth order and for the Van Vleck operator to third order:

$$g_i^{TU,S}=0 \ \text{ for } i=1,2,3 \ , \tag{26a}$$

$$g_4^{TU,S}=\frac{1}{8}\frac{N(N-1)}{(2N+1)(2N-3)} \ , \tag{26b}$$

$$\Lambda_1^{TU,S}=\frac{i(a^{\dagger}-a)}{2} \ , \tag{26c}$$

$$\Lambda_2^{TU,S}=\frac{-i}{8}[a^{\dagger}(2N^2+1)^{-1}-(2N+1)^{-1}a^2] \ , \tag{26d}$$

and

$$\Lambda_3^{TU,S}=\frac{i}{16}\{a^{\dagger 3}[(2N+3)(2N+1)]^{-1}-a^{\dagger}(N-1)[(2N+1)(2N-1)]^{-1}\}+\text{H.c.} \tag{26e}$$

Our result for $g_4$ agrees with that of Takeda and Ui.[1] It is interesting to observe that for this model Hamiltonian, the perturbation does not exceed the unperturbed term in the asymptotic region (when written in terms of $x$ and $p$) in contrast to the anharmonic oscillator. Thus, one has good reasons to expect that the perturbation expansion for the energy is a convergent one. The present method provides a convenient way to calculate this energy perturbatively.

The three examples presented in this Brief Report represent certain particular choices for the functions $H_0(N)$ and $f_{ij}(N)$ in Eq. (1). The possible choice for these two functions is, of course, limitless. However, the rules for carrying out the perturbation calculation have been clearly laid out. As the examples given in this paper have shown, we just require the systematic applications of rules I–IV given in Eq. (19)–(23).

Extension to higher order is straightforward in all cases. The present method can be extended to multiboson systems with mutual and self-interactions. If the interactions introduced do not couple among degenerate states, it is simple to develop the rules analogous to rules I–IV for the multiboson systems, especially when the unperturbed Hamiltonian for the multiboson system is a well-behaved function of the number operators of the individual single-boson systems. The resulting rules can definitely be applied to any nondegenerate states of the multiboson system even though the system exhibits degeneracy.

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[1] G. Takeda and H. Ui, Prog. Theor. Phys. 69, 1146 (1983).
[2] J. H. Van Vleck, Phys. Rev. 33, 467 (1929).
[3] H. Primas, Rev. Mod. Phys. 35, 710 (1963).
[4] A. M. Arthurs and P. D. Robinson, Proc. R. Soc. London A301, 507 (1967).
[5] P. D. Robinson, J. Chem. Phys. 47, 2319 (1967).
[6] J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Addison-Wesley, Reading, MA, 1955), Chap. 7.
[7] A convergent perturbation result for the ground-state energy of the quartic anharmonic oscillator has been given by C. K. Au, G. W. Rogers, and Y. Aharonov in Phys. Lett. 95A, 287 (1983).
[8] C. M. Bender and T. T. Wu, Phys. Rev. Lett. 27, 462 (1971).