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A time-dependent multi-reference unified cluster cumulant formulation to study the subdynamics of quantum system coupled both to thermal and stochastic bath

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This is to introduce a time-local effective hamiltonian unified cluster cumulant method based on the time-dependent multi-reference cluster cumulant (TDMRCC) and thermal cluster cumulant (TCC) strategy developed by Mukherjee and his coworkers. A factorized ansatz for $U_I P = [U_I]_{ex} [U_I]_M P$ with $P = |\varphi_i> \otimes |0_\beta> \otimes |0_f>$, where $|\varphi_i>$, $|0_\beta>$ and $|0_f>$ denote the purely quantum mechanical vacuum state, the thermal vacuum state, the base state for the solvent degrees of freedom respectively, and $[U_I]_{ex}$ consists of operators admixing the thermally as well as the stochastically projected **model space** functions with that of the **virtual space** outside the model space whose functions govern the time-evolution of $[U_I]_M$ via the time-local effective operator, $V_{eff}[\beta, \xi, t](=<< V_I[U_I]_{ex} >\beta >f)$, where $< \cdots >_\beta$ and $< \cdots >_f$ denote thermal and stochastic averaging respectively. The exponential ansatz is introduced both for $[U_I]_{ex}$ and $[U_I]_M$ and these ansatze are normal ordered with respect to both the thermal and the stochastic variables, i.e. $[U_I]_{ex} = \left\{\left\{e^{S_{m,n}^{p,q,f}}\right\}_\beta\right\}_f$ and $[U_I]_M = \left\{e^{X_{k,k}}\right\}_\beta$, where m, n denotes system boson creation and destructions operators and p, q denotes both boson creation and destructions operators. The averaged evolution operator, $<< U_1(t) >_\beta >_f$ with respect to both the thermal boson variables in thermal equilibrium and the stochastic variables is obtained. Finally, the mathematical expression for the second order cluster cumulant $[X_{0,0}]^{(2)}$ is derived for a quantum particle trapped in a 1-dimensional anharmonic oscillator potential coupled both to the stochastic and thermal baths.

Keywords: .

1. A prelude

It is of great interest to develop microscopic theories for studying the dynamic and thermodynamic properties of quantum systems in the ground and in the excited states with many degrees of freedom often encountered in the experimental situations.

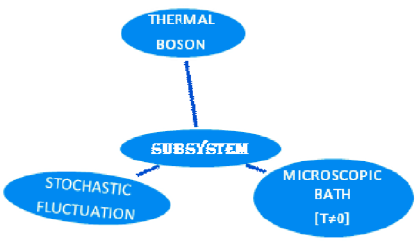

Fig. 1. A schematic diagram of a subsystem interacting with bath (thermal, stochastic/microscopic).

The experimentalists observe a few relevant degrees of freedom called the "subsystem" and its dynamics is a combined interplay of that of subsystem and bath (thermal, stochastic/microscopic). If the time-scale of the subsystem, τ_{SS} is far apart from that of the bath, τ_B then the process is called Markovian process. If, $\tau_{SS} \cong \tau_B$, then the process is called non-Markovian process.

Our interest is to study non-Markovian process where bath makes its presence felt via a time delayed effective interaction (memory effect) whose actual form depends upon the way the bath is averaged out (e.g. microscopic/stochastic/thermal) and which causes quantum interference leading to dissipation, de-phasing, line-shape etc. that experimentalists actually observe. Although the study of such a system is relatively simple for the ground state, the situation for the excited state is nontrivial displaying richness and complexity. It is not possible for us to mention all the theoretical studies in this evenly growing field of research. It is worthy to mention a few of them to begin with. Heller and his coworkers[1,2] developed the time-dependent wave-packet formalism which provide exact solution for Gaussian potential energy surfaces both at zero-temperature and at non-zero temperature. But it is not suitable for non-Gaussian potential energy surfaces as it is usually the case. Some other relevant developments to study the non-Gaussian problems with their specific features are time-dependent self-consistent field (TDSCF) and multi-configurational variants (MCTDSCF)[3], wave-packet-path-integral method[4], matrix-technique of Balian and Berezin[5], the projection operator technique of Nakajima-Zwanzig-Mori[6–8], reduced density-matrix based methods[9], time-path approach of Tanimura *et al.*[10], the path-integral based method of Domcke *et al.*[11,12]. Mukherjee *et al.*[13–15] developed a nonperturbative time-local effective Hamiltonian approach called time-dependent multi-reference coupled cluster method (TDMRCC). The TDMRCC method admits of a factorized ansatz and a normal ordered cluster expansion representation of evolution operator which guarantees the formulation to be size-extensive, scaled linearly with the number of degrees of freedom and allowed a systematic truncation scheme. Some of the ideas of TDMRCC method are exploited along with to develop thermal cluster cumulant (TCC) method[16,17] for computing equilibrium thermal averages in an efficient and systematic manner.

In this paper, a systematic nonperturbative unified cluster cumulant method is developed for studying the dynamic and the equilibrium thermodynamic properties of the quantum systems which are simultaneously coupled to the stochastic and thermal bath. The evolution operator, $U(t)$ is represented by an exponential ansatz to guarantee size extensiveness of the measured averaged propertries and the ansatz is normal ordered with respect to the stochastic and to the thermal variables simultaneously. Substituting the normal ordered ansatz in Heisenberg equation of motion and applying the field theoretic tool like the Wick's reordering theorem, a closed set of Time-dependant Multi-reference Unified Cluster Cumulant (TDMRUCC) equations are obtained. Finally, the formalism is applied for calculating dynamic and spectroscopic properties of a double well potential coupled both with the thermal bath and stochastic bath simultaneously.

2. A unified cluster cumulant formalism to study the averaged sub-dynamics of system-bath composite in the quantum domain

The generic hamiltonian for the system-bath composite system is given by

$$H(t) = H_S(t) + H_B(t) + V_{SB}(t) \tag{1}$$

where $H_S(t)$, $H_B(t)$ and $V_{SB}(t)$ are the hamiltonians of the sub-system, bath and the system-bath interaction respectively. Our task is to solve the Heisenberg equation of motion of the time-evolution operator $U(t)$ which is given by

$$i\frac{\partial U(t)}{\partial t} = H(t)U(t) \tag{2}$$

In the interaction representation, eq. (2) is given by

$$i\frac{\partial U_I(t)}{\partial t} = V_I(t)U_I(t) \tag{3}$$

where $U_I(t) = e^{-iH_0t}\,U(t)$; $V_I(t) = e^{-iH_0t}\,V(t)\,e^{-iH_0t}$, and H_0 is the exactly solvable Hamiltonian.

The general solution of eq. (3) is given by

$$U_I(t) = T\exp\left(-i\int_0^t V_I(t')dt'\right) \tag{4}$$

where T is the ordering operator in time.

The question is: how to obtain thermally and stochastically averaged time-evolution Operator,

$<< U_I(t) >_\beta >_f$ (say) ?

Let us choose **some selected** group of states from which evolution is supposed to take place and define a Model Space Projection Operator, P as a direct product space of these states such that $P = |\varphi_i> \otimes |0_\beta> \otimes |0_f>$, where $|\varphi_i>$, $|0_\beta>$ and $|0_f>$ denote the purely quantum mechanical vacuum state, the thermal vacuum state, the base state for the solvent degrees of freedom respectively. That is, $<< U_I(t) >_\beta >_f \equiv PU_I(t)P$. In the spirit of time-depemdent multireference cluster cumulant (TDMRCC)[13–15] and thermal cluster cumulant (TCC)[16,17] formalism, let us introduce a factorized Ansatz for $PU_I(t)P$ as

$$U_IP = [U_I]_{ex} \cdot [U_I]_M\, P \tag{5}$$

where $[U_I]_{ex}$ consists of operators admixing the thermally as well as the stochastically projected **model space** functions with that of the **virtual space** outside the model space whose functions govern the time-evolution of $[U_I]_M$ via the time-local effective operator given by

$$V_{eff}[\beta, \xi, t] = << V_I[U_I]_{ex} >\beta >f \tag{6}$$

Physically, the situation is equivalent to the formation of a dressed subsystem which is driven by the effective operator, $V_{eff}[\beta, \xi, t]$ which depends on the temperature variable, β [$= (kT)^{-1}$] and on ξ that in turn depends on the anharmonic strength of the system oscillator, the system-bath coupling constant, and the strength of the colored noise.

The time-evolution of $[U_I]_{ex}$ and $[U_I]_M$ is governed by the following equations:

$$i\frac{\partial[U_I]_{ex}}{\partial t} = V_I[U_I]_{ex} - [U_I]_{ex}.V_{eff}[\beta, \xi, t] \tag{7}$$

$$i\frac{\partial[U_I]_M}{\partial t} = V_{eff}[\beta, \xi, t].[U_I]_M \tag{8}$$

In order to maintain size-extensiveness and simplify operator differentiation, let us introduced exponential ansatz both for $[U_I]_{ex}$ and $[U_I]_M$ and make them normal ordered with respect to both thermal and stochastic variables.

$$[U_I]_{ex} = \left\{\left\{e^{S^{p,q,f}_{m,n}}\right\}_\beta\right\}_f \tag{9}$$

$$[U_I]_M = \left\{e^{X_{k,k}}\right\}_\beta \tag{10}$$

where $\{\cdots\}_\beta$ denotes thermal normal ordering with respect to creation/annihilation operators and $\{\cdots\}_f$ denotes normal ordering with respect to the stochastic fluctuation variables, f.

Substituting the above normal ordered eqs. (9) and (10) in the eqs. (5)-(8) and using the techniques of normal ordering and generalized Wick's theorem, the following time-dependent equations for the cluster operators $S^{p,q,f}_{m,n}$ and $X_{m,n}$ is derived

$$i\frac{\partial S^{p,q,f}_{m,n}}{\partial t} = \left[\left\{\left\{\overline{\overline{[V_I]^{p_1,q_1,f}_{m_1,n_1}.\exp\left(S^{p_2,q_2,f}_{m_2,n_2}\right)}}\right\}_\beta\right\}_f\right]^{p,q,f}_{m,n} - \left[\left\{\left\{\overline{\overline{\exp\left(S^{t,l,f}_{r,s}\right).[V_{eff}(\beta, \xi, t)]_{k,k}}}\right\}_\beta\right\}_f\right]^{p,q,f}_{m,n} \tag{11}$$

$$i\frac{\partial X_{k,k}}{\partial t} = \left[\left\{\overline{\overline{[V_{eff}(\beta, \xi, t)]_{l'l'}\exp(X_{l''l''})}}\right\}_\beta\right]_{k,k} \tag{12}$$

where $\left[\left\{\left\{\overline{\overline{[V_I]^{p_1,q_1,f}_{m_1,n_1}.\exp\left(S^{p_2,q_2,f}_{m_2,n_2}\right)}}\right\}_\beta\right\}_f\right]^{p,q,f}_{m,n}$ denotes contractions of system (e.g. $\overline{aa^\dagger}$ and/or $\overline{a^\dagger a}$) and bath (e.g. $\overline{b_k b_k^\dagger}$ and/or $\overline{b_k^\dagger b_k}$) thermal boson variables, and/or contractions of stochastic variables, e.g. $\overline{f.f}$. Since $P\left(i\frac{\partial S^{p,q,f}_{m,n}}{\partial t}\right)P = 0$ in eq. (11) taking the P – Projection from both side, we have

$$\left[\left\{\left\{\overline{\overline{[V_I]^{p_1,q_1,f}_{m_1,n_1}.\exp\left(S^{p_2,q_2,f}_{m_2,n_2}\right)}}\right\}_\beta\right\}_f\right]^{p,q,f}_{m,n} = \left[\left\{\left\{\overline{\overline{\exp\left(S^{t,l,f}_{r,s}\right).[V_{eff}(\beta, \xi, t)]_{k,k}}}\right\}_\beta\right\}_f\right]^{p,q,f}_{m,n} \tag{13}$$

Equating the connected closed component from both sides of eq. (13), we have

$$[V_{eff}(\beta, \xi, t)]_{k,k} = \left[\left\{\left\{\overline{\overline{[V_I]^{p_1,q_1,f}_{m_1,n_1}.\exp\left(S^{p_2,q_2,f}_{m_2,n_2}\right)}}\right\}^{cl}_\beta\right\}^{cl}_f\right]^{\mathrm{cl}}_{k,k} \tag{14}$$

where the superscript "cl" denotes closed component with no thermal and stochastic variables free after contraction.

In fact, we solve for the cluster amplitudes $S^{p,q,f}_{m,n}$ starting with an initial value and also the effective potential, $[V_{eff}[\beta, \xi, t]]_{r',r'}$ which is used to obtain the value of $X_{k,k}$ with $k = 0, 1, 2, \cdots$ by solving eq. (12). The advantage of factorization of U_I into $[U_I]_{ex}$ and $[U_I]_M$ with added normalization is also evident through the ease in taking time-derivative of the exponential of operators and convenient disentanglement of them. The normal ordered representation prevents $\overline{S.S}$ and $\overline{X.X}$ contractions which results in terminating the infinite power series of S and/or X to a finite power in the right-hand side of eqs. (11) and (12).

Finally, the averaged evolution operator with respect to both the thermal boson variables in thermal equilibrium and the stochastic variables

$$<< U_I(t) >_\beta >_f = PU_I(t)\, P$$

$$= P\left\{\left\{e^{S_{m,n}^{p,q,f}}\right\}_\beta\right\}_f \left\{e^{X_{k,k}}\right\}_\beta P \tag{15}$$

where $<< U_I(t) >_\beta >_f$ is exact for system in which the Hamiltonian operators obey "closed" Lie algebra. Otherwise, we have to restrict our computation up to finite rank of cluster operators (here "rank" means the sum of powers of $a^\dagger$ and a operators).

It is worthy to note that the cluster amplitudes $S_{m,n}^{p,q,f}$ and $X_{k,k}$ when propagated in **imaginary-time**, one can calculate the **equilibrium partition function** as

$$< U_I(\beta) >_\beta$$

$$= P\left\{\left\{e^{S_{m,n}^{p,q,f} + \overline{X}_{k,k}}\right\}_\beta\right\}_f P\left\{e^{X_{0,0}}\right\}_\beta = e^{X_{0,0}} \tag{16}$$

where $\overline{X}_{k,k}$ is the operator part of $X_{k,k}$ other than the pure number.

3. Calculations of observable properties

We can calculate the following observable properties :

(i) Survival probabilities, $P_{ii}(t)$:

$$\boldsymbol{P_{ii}(t) = |< i\, |U_I(t)|\, i >|^2} \tag{17}$$

That is,

$$P_{00}(t) = |< 0|U_I(t)|0 >|^2 = |\exp[X_{0,0}(t)]|^2. \tag{18}$$

$$P_{11}(t) = |< 1|U_I(t)|1 >|^2 = |\exp[X_{0,0}(t)](1.0 + X_{1,1}(t))|^2 \tag{19}$$

etc.

where $P_{00}(t)$, $P_{11}(t)$, …. are the survival probabilities of ground, first excited,….. states respectively. One can plot the calculated values of $P_{00}(t)$, $P_{11}(t)$ against time, t to observe the time-variation.

(ii) Transition probabilities, $P_{f\leftarrow i}(t)$:

$$\boldsymbol{P_{f\leftarrow i}(t) = |< f\, |U_I(t)|\, i >|^2} \tag{20}$$

(iii) Power spectra:

The power spectrum can be obtained from the expression given by

$$I(\omega) \propto \int_0^\infty << U_M(t) >_\beta >_f \times e^{i\omega t}\, dt \tag{21}$$

One can plot the calculated values of $I(\omega)$ against the frequency, ω, to observe the spectral pattern.

4. Perturbative solution of TDMRUCC equations

It is instructive to derive the perturbative variant of the TDMRUCC eqs. (11) and (12) in interaction representation. Then, the first order TDMRUCC equation of external cluster cumulant, ${}^{(1)}S_{m,n}^{p,q,f}$ (t) is given by

$$i\frac{\partial\, {}^{(1)}S_{m,n}^{p,q,f}}{\partial t} = \left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{m,n}^{p,q,f} \tag{22}$$

and that of the Cluster Cumulant, ${}^{(1)}X_{k,k}$ (t) is given by

$$i\frac{\partial\, {}^{(1)}X_{k,k}}{\partial t} = \left[\{[V_I(t)]\}_\beta\right]_{k,k} \tag{23}$$

It is worthy to note that in eq. (22) there is no contribution from the second term of eq. (11), i.e.

$$\left[\left\{\left\{\overline{\overline{\exp\left(S_{r,s}^{t,l,f}\right).[V_{eff}(\beta,\xi,t)]_{k,k}}}\right\}_\beta\right\}_f\right]_{m,n}^{p,q,f}$$, because $[V_{eff}(\beta, \xi, t)]_{k,k}$ is itself a closed operator.

Likewise, the second order TDMRUCC equations of external cluster cumulant, ${}^{(2)}S_{m,n}^{p,q,f}$ (t) is given by

$$i\frac{\partial\, {}^{(2)}S_{m,n}^{p,q,f}}{\partial t} = {}^{(2)}\left[\left\{\left\{\overline{\overline{[V_I]_{m_1,n_1}^{p_1,q_1,f}.\exp\left({}^{(1)}S_{m_2,n_2}^{p_2,q_2,f}\right)}}\right\}_\beta\right\}_f\right]_{m,n}^{p,q,f}$$

$$+ {}^{(2)}\left[\left\{\left\{\overline{\overline{[V_I]_{m_1,n_1}^{p_1,q_1,f}.\exp\left({}^{(1)}X_{l,l}\right)}}\right\}_\beta\right\}_f\right]_{m,n}^{p,q,f} \tag{24}$$

$$i\frac{\partial\, {}^{(2)}X_{k,k}}{\partial t} = {}^{(2)}\left[\left\{[V_{eff}(\beta,\xi,t)]_{l'l'}.\exp\left({}^{(1)}X_{l''l''}\right)\right\}_\beta\right]_{k,k} \tag{25}$$

It is worthy to note that the n-th order perturbative cluster cumulants ${}^{(n)}S_{m,n}^{p,q,f}$ (t) and ${}^{(n)}X_{k,k}$ (t) can be obtained by using the value of cluster cumulant of lower orders and subsequent time-integration. This would be more clear while calculating with a simple system.

Finally, the averaged evolution operator up to n-th order can be calculated as

$$^{(n)}[<< U_I(t) >_\beta >_f] = {}^{(n)}[R(t)] = P\,{}^{(n)}[U_I(t)]\,P = e^{(n)X_{k,k}} \quad (26)$$

We shall show explicitly its second order variant, $^{(2)}[R(t)]$, taking a concrete example to illustrate the theory in Section 5.

5. Illustrative application

5.1. The normal ordered working hamiltonian at finite temperature:

Let us consider a model system-bath composite Hamiltonian given by

$$H = \frac{P_s^2}{2} + \frac{1}{2}\omega_s^2 X_s^2 + \in X_s^2 + \eta X_s^4 + \left(\Sigma_k \frac{p_k^2}{2} + \frac{1}{2}\omega_k^2 y_k^2\right)$$

$$+\, g_{stoc.} \times 2E_0\, Cos\,(\omega_0 t) \times f(t) * X_s + \Sigma_k \gamma_k . X_s * y_k \quad (27)$$

where the symbols have their usual meaning k = 1 to N_B, maximum number of both variables and $\boldsymbol{f}\,(\boldsymbol{t})$ is the Ornstein-Uhlenbech colored noise having stationary Gaussian distribution. The stochastic variable $\boldsymbol{f}\,(\boldsymbol{t})$ satisfies the following properties:

$$\langle f(t)\rangle = 0 = \langle f(t_1) \cdots f(t_{2n+1})\rangle, \forall t\,;$$

$$\langle f(t_1).f(t_2)\rangle = F(t_1,t_2) = \left(\frac{\lambda}{2}\right).e^{-\lambda|t_1-t_2|}$$

$$\langle f(t_1) \cdots f(t_{2n})\rangle = \Sigma_{\text{all }(n)\text{pairs}} \Pi\langle f(t_1)\cdot f(t_2)\rangle$$

where $\boldsymbol{\lambda}$ is the coloured noise strength.

In the second quantization representation, the Hamiltonian becomes

$$H = \omega_s\left(a^\dagger a + \frac{1}{2}\right) + \left(\frac{\in}{2\omega_s}\right)(a^\dagger + a)^2$$

$$+ \left(\frac{\eta}{4\omega_s^2}\right)(a^\dagger + a)^4 + \Sigma_k \omega_k \left(B_k^\dagger B_k + \frac{1}{2}\right) +$$

$$+\; \boldsymbol{g'_s} \times f(t) \times \left(a^\dagger e^{-i\omega_0 t} + a e^{-i\omega_0 t}\right)$$

$$+\, \Sigma_k \boldsymbol{\gamma'_k}\left(a^\dagger B_k + a B_k^\dagger\right) \quad (28)$$

where $\boldsymbol{g'_s} = \left(g_{stoc.} \times 2E_0/\sqrt{2\omega_s}\right)$ and $\boldsymbol{\gamma'_k} = \left(\gamma_k/\sqrt{2\omega_s}\sqrt{2\omega_k}\right)$ are the modified coupling constants of the system-stochastic bath and system-thermal bath respectively; $a^\dagger/a$ and $B^\dagger_k/B_k$ are the creation/annihilation operators of the system degree of freedom and $\boldsymbol{k}$-th thermal bath degrees of freedom.

Let us apply the Bogolyubov transformation to the system operators $a^\dagger/a$ leading to $A^\dagger/A$ operators as

$$\boldsymbol{A} = \boldsymbol{N}(a - t_1 a^\dagger);\ \boldsymbol{A}^\dagger = \boldsymbol{N}(a^\dagger - t_1 a)\,; \quad (29)$$

such that $[\boldsymbol{A}^\dagger, \boldsymbol{A}] = \mathbf{1}$, and $\boldsymbol{N} = \dfrac{\mathbf{1}}{\sqrt{(\mathbf{1}-t_1^2)}}$.

This leads to the following transformation

$$a = \boldsymbol{N}(A^\dagger + t_1 A)\,;\ a^\dagger = \boldsymbol{N}(A + t_1 A^\dagger); \quad (30)$$

$$(a^\dagger + a) = \boldsymbol{K}\cdot(A^\dagger + A) \quad (31)$$

$$(a^\dagger a) = \boldsymbol{N}^2\cdot(1 + t_1^2)\,A^\dagger A + \boldsymbol{N}^2\cdot t_1\,(A^{\dagger 2} + A^2) + \boldsymbol{N}^2 t_1^2) \quad (32)$$

$$\text{where } \boldsymbol{K} = \sqrt{\frac{(1+t_1)}{(1-t_1)}}\,. \quad (33)$$

The hamiltonian in eq. (28) in terms of $A^\dagger$ and A becomes

$$H = \omega_s\left[\frac{1+t_1^2}{1-t_1^2}\right].A^\dagger A + \left[\frac{\in}{2\omega_s}K^2\right].(A^\dagger + A)^2$$

$$+ \left[\frac{\eta}{4\omega_s^2}.K^4\right](A^\dagger + A)^4 + \omega_s.\left[\frac{t_1}{1-t_1^2}\right].(A^{\dagger 2} + A^2) +$$

$$+ \left[\frac{\omega_s}{2} + \omega_s.\left(\frac{t_1^2}{1-t_1^2}\right)\right]$$

$$+\, \boldsymbol{g'}_s \times f(t) \times [A^\dagger\cdot(N\cdot e^{-i\omega_0 t} + N\cdot t_1\cdot e^{-i\omega_0 t})]$$

$$+\, \boldsymbol{g'}_s \times f(t) \times [A\cdot(N\cdot t_1\cdot e^{-i\omega_0 t} + N\cdot e^{-i\omega_0 t})]$$

$$+\, \Sigma_k\,\omega_k\left(B_k^\dagger B_k + \tfrac{1}{2}\right) + \Sigma_k\,\gamma'_k\,[N\cdot(A^\dagger B_k + AB_k^\dagger)$$

$$+\, N\cdot t_1\cdot(A^\dagger B_k^\dagger + AB_k)] \quad (34)$$

Let us apply thermal normal ordering operation both on the system part and thermal-bath part of the above hamiltonian (eq. (34)) in the following way

$$(A^\dagger A) = \{A^\dagger A\}_\beta + n;\ (AA^\dagger) = \{A^\dagger A\}_\beta + (n+1);$$

$$\boldsymbol{n} = [\mathbf{e}^{\beta\Omega_M} - \mathbf{1.0}]^{-1} \quad (35)$$

$$(A^\dagger + A) = \{(A^\dagger + A)\}_\beta \quad (36)$$

$$(A^\dagger + A)^2 = \{(A^\dagger + A)^2\}_\beta + (2n + 1) \quad (37)$$

$$(A^\dagger + A)^3 = \{(A^\dagger + A)^3\}_\beta + (6n + 3)\cdot\{(A^\dagger + A)\}_\beta \quad (38)$$

$$(A^\dagger + A)^4 = \{(A^\dagger + A)^4\}_\beta + (12n + 6)\cdot\{(A^{\dagger 2} + A^2)\}_\beta + (24n + 12)\cdot\{A^\dagger A\}_\beta + (12n^2 + 12n + 3) \quad (39)$$

$$\left(B_k^\dagger B_k\right) = \left\{B_k^\dagger B_k\right\}_\beta + n_k;\ \left(B_k B_k^\dagger\right) = \left\{B_k^\dagger B_k\right\}_\beta + (n_k + 1);$$

$$\boldsymbol{n_k = [e^{\beta\omega_k} - 1.0]^{-1}} \quad (40)$$

where Ω_M is the modified optimum Thermal Hartree frequency to be shown in eq. (43).

After the above transformations, the hamiltonian in eq. (34) becomes

$$H = \left[\omega_s \cdot \left(\frac{1+t_1^2}{1-t_1^2}\right) + \left(\frac{\in}{\omega_s}\right).K^2 + \left(\frac{\eta}{\omega_s^2}.K^4\right) \times (6n+3)\right].\{A^\dagger A\}_\beta +$$

$$+\left[\omega_s \cdot \left(\frac{t_1}{1-t_1^2}\right) + \left(\frac{\in}{2\omega_s}K^2\right) + \left(\frac{\eta}{2\omega_s^2}.K^4\right) \times (6n+3)\right].\{A^{\dagger 2}+A^2\}_\beta + \left(\frac{\eta}{4\omega_s^2}.K^4\right).\{(A^\dagger + A)^4\}_\beta +$$

$$+\left[\frac{\omega_s}{2} + \omega_s \cdot \left(\frac{t_1^2}{1-t_1^2}\right)\right] + \omega_s \cdot \left(\frac{1+t_1^2}{1-t_1^2}\right).n + \left(\frac{\in}{2\omega_s}K^2\right).(2n+1) + \left(\frac{3\eta}{4\omega_s^2}.K^4\right).\times(4n^2 + 4n + 1) +$$

$$+ \boldsymbol{g'_s} \times f(t) \times [A^\dagger \cdot (N \cdot e^{-i\omega_0 t} + N \cdot t_1 \cdot e^{-i\omega_0 t})] +$$

$$+ \boldsymbol{g'_s} \times f(t) \times [A \cdot (N \cdot t_1 \cdot e^{-i\omega_0 t} + N \cdot e^{-i\omega_0 t})] +$$

$$+ \sum_k \omega_k \left\{B_k^\dagger B_k\right\}_\beta + \sum_k \omega_k \left(n_k + \frac{1}{2}\right) +$$

$$+ \Sigma_k \gamma'_k [N \cdot (A^\dagger B_k + A B_k^\dagger) + N \cdot t_1 \cdot (A^\dagger B_k^\dagger + A B_k)] \quad (41)$$

Let us define a new parameter $\boldsymbol{\alpha_1 = [(1 - t_1)/(1 + t_1)]}$, that leads to

$$\boldsymbol{K = (1/\sqrt{\alpha_1});\ N = [(1+\alpha_1)^2/2\sqrt{\alpha_1}];\ t_1 = [(1-\alpha_1)/(1+\alpha_1)];}$$

$$\left(\frac{\boldsymbol{1+t_1^2}}{\boldsymbol{1-t_1^2}}\right) = \boldsymbol{[(1+\alpha_1^2)/2\alpha_1]};\ \left(\frac{\boldsymbol{t_1}}{\boldsymbol{1-t_1^2}}\right) = \boldsymbol{[(1-\alpha_1^2)/4\alpha_1]};\ \text{and}$$

$$\left(\frac{\boldsymbol{t_1^2}}{\boldsymbol{1-t_1^2}}\right) = \boldsymbol{[(1-\alpha_1)^2/4\alpha_1]}.$$

The thermal normal ordered Hamiltonian (eq. (41)) in terms of $\boldsymbol{\alpha_1}$ becomes

$$H = \left[\omega_s \cdot \left(\frac{1+\alpha_1^2}{2\alpha_1}\right) + \in.\left(\frac{1}{\omega_s\alpha_1}\right) + \eta.\left(\frac{1}{\omega_s^2\alpha_1^2}\right) \times (6n+3)\right].\{A^\dagger A\}_\beta +$$

$$+\left[\omega_s \cdot \left(\frac{1-\alpha_1^2}{4\alpha_1}\right) + \left(\frac{\in}{2\omega_s\alpha_1}\right) + \left(\frac{\eta}{2\omega_s^2\alpha_1^2}\right).\times(6n+3)\right].\{A^{\dagger 2}+A^2\}_\beta + \left(\frac{\eta}{4\omega_s^2}.K^4\right).\{(A^\dagger + A)^4\}_\beta +$$

$$+\left[\frac{\omega_s}{2} + \omega_s \cdot \left(\frac{(1-\alpha_1)^2}{4\alpha_1}\right)\right] + \omega_s \cdot \left(\frac{1+\alpha_1^2}{2\alpha_1}\right).n + \left(\frac{\in}{2\omega_s\alpha_1}\right).(2n+1) + \left(\frac{3\eta}{4\omega_s^2\alpha_1^2}\right).\times(2n+1)^2 +$$

$$+ \boldsymbol{g'_s} \times f(t) \times \left[A^\dagger.\left(\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}}.e^{-i\omega_0 t} + \frac{(1-\alpha_1)}{2\sqrt{\alpha_1}}.e^{i\omega_0 t}\right)\right] +$$

$$+ \boldsymbol{g'_s} \times f(t) \times \left[A.\left(\frac{(1-\alpha_1)}{2\sqrt{\alpha_1}}.e^{-i\omega_0 t} + \frac{(1+\alpha_1)}{2\sqrt{\alpha_1}}.e^{i\omega_0 t}\right)\right] +$$

$$+ \Sigma_k \omega_k \{B_k^\dagger B_k\}_\beta + \Sigma_k \omega_k \left(n_k + \tfrac{1}{2}\right) +$$

$$+ \Sigma_k \gamma'_k \left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}} \cdot (A^\dagger B_k + A B_k^\dagger) + \frac{(1-\alpha_1)}{2\sqrt{\alpha_1}} \cdot (A^\dagger B_k^\dagger + A B_k)\right] \quad (42)$$

Let us implement "***Thermal Hartree***" condition for which the coefficient of $\{A^{\dagger 2} + A^2\}_\beta$ will be zero and under this condition the coefficient of $\{A^\dagger A\}_\beta$ will be $\boldsymbol{(\omega_s\alpha_1) = \Omega_M}$ **(say)**, where $\boldsymbol{\Omega_M}$ is the modified harmonic frequency corresponding to an optimized Gaussian.

Therefore, the thermally normal ordered Hamiltonian under finite-temperature Hartree condition takes the simplified form given by

$$H = \mathbf{\Omega_M} \cdot \{A^\dagger A\}_\beta + \left[\frac{\eta}{(2\Omega_M)^2}\right] \cdot \{A^{\dagger 4} + A^4 + 4 \times (A^{\dagger 3}A) + 4 \times (A^\dagger A^3) + 6 \times (A^{\dagger 2} A^2)\}_\beta + \left[\left(\frac{g'_s}{\sqrt{\alpha_1}}\right) \times f(t) \times \theta_+(t)\right] \cdot A^\dagger + \left[\left(\frac{g'_s}{\sqrt{\alpha_1}}\right) \times f(t) \times \theta_-(t)\right] \cdot A + \Sigma_k \omega_k \left\{B_k^\dagger B_k\right\}_\beta + \Sigma_k \gamma'_k \left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}} \cdot (A^\dagger B_k + A B_k^\dagger) + \frac{(1-\alpha_1)}{2\sqrt{\alpha_1}} \cdot (A^\dagger B_k^\dagger + A B_k)\right] + \langle \boldsymbol{H} \rangle \quad (43)$$

where

$$\langle H \rangle = \left[\frac{\omega_s}{2} + \omega_s \cdot \left(\frac{1-\alpha_1^2}{4\alpha_1}\right)\right] + \omega_s \cdot \left(\frac{1+\alpha_1^2}{2\alpha_1}\right) \cdot n + \left(\frac{\in}{2\Omega_M}\right) \cdot (2n+1) + \left[\frac{3\eta}{(2\Omega_M)^2}\right] \cdot (2n+1)^2 + \sum_k \omega_k \left(n_k + \frac{1}{2}\right),$$

$$\theta_+(t) = \frac{1}{2} \cdot \left[(1-\alpha_1)\, e^{i\omega_0 t} + (1+\alpha_1)\, e^{-i\omega_0 t}\right] = [\cos(\omega_0 t) - i\,\alpha_1 \sin(\omega_0 t)],$$

$$\theta_-(t) = \frac{1}{2} \cdot \left[(1-\alpha_1)\, e^{-i\omega_0 t} + (1+\alpha_1)\, e^{i\omega_0 t}\right] = [\cos(\omega_0 t) + i\,\alpha_1 \sin(\omega_0 t)]$$

Transforming the above Hamiltonian (eq.(43)) into its interaction representation with respect to both the system's optimized frequency and the thermal-bath frequencies, we have

$$V_I = \Lambda \times \left\{\left(\frac{A_I^{\dagger 4}}{4!}\right) \cdot e^{4i\Omega_M t} + \left(\frac{A_I^4}{4!}\right) \cdot e^{-4i\Omega_M t} + \left(\frac{A_I^{\dagger 3} A_I}{3!1!}\right) \cdot e^{2i\Omega_M t} + \left(\frac{A_I^\dagger A_I^3}{1!3!}\right) \cdot e^{-2i\Omega_M t} + \left(\frac{A_I^{\dagger 2} A_I^2}{2!2!}\right)\right\}_\beta + \left[\left(\frac{g'_s}{\sqrt{\alpha_1}}\right) \times f(t) \times \theta_+(t)\right] \cdot A_I^\dagger \cdot e^{i\Omega_M t} + \left[\left(\frac{g'_s}{\sqrt{\alpha_1}}\right) \times f(t) \times \theta_-(t)\right] \cdot A_I \cdot e^{-i\Omega_M t} + \Sigma_k \left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}} \cdot \gamma'_k\right] \times \left\{\left(A_I^\dagger B_{k,I}\right)\right\}_\beta \cdot e^{i(\Omega_M - \omega_k)t} + \Sigma_k \left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}} \cdot \gamma'_k\right] \times \left\{\left(A_I B_{k,I}^\dagger\right)\right\}_\beta \cdot e^{-i(\Omega_M - \omega_k)t} + \Sigma_k \left[\frac{(1-\alpha_1)}{2\sqrt{\alpha_1}} \cdot \gamma'_k\right] \times \left\{\left(A_I^\dagger B_{k,I}^\dagger\right)\right\}_\beta \cdot e^{i(\Omega_M + \omega_k)t} + \Sigma_k \left[\frac{(1-\alpha_1)}{2\sqrt{\alpha_1}} \cdot \gamma'_k\right] \times \left\{\left(A_I B_{k,I}\right)\right\}_\beta \cdot e^{-i(\Omega_M + \omega_k)t} + \langle H \rangle \quad (44)$$

where Λ = $[\mathbf{24\eta/(2\Omega_M)^2}]$. This is the required normal ordered potential at finite temperature.

5.2. The cluster cumulants upto second order for ground state of the subsystem:

As discussed in Section (4), the second order cluster clumulant for the model space operators of the subsystem, denoted by ${}^{(2)}X_{k,k}(t)$, can be obtained if we know the first order cluster cumulants of the virtual space operator, denoted by ${}^{(1)}S_{m,n}^{p,q,f}(t)$, that being connected to the interaction potential, V_I leading to only the *k* numbers of system creation operators, $A_I^\dagger$ and *equal* numbers of system annihilation operators, A_I. For the ground state problem, the second order cluster cumulant for the model space operator is ${}^{(2)}X_{0,0}(t)$. Let us compute the first order cluster cumulants as follows.

The time-dependent equation for the first order cluster cumulant, ${}^{(1)}S_{4,0}^{0,0,0}(t)$, is given by

$$i\frac{\partial\,{}^{(1)}S_{4,0}^{0,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{4,0}^{0,0,0}=\Lambda\times e^{4i\Omega_M t} \tag{45}$$

Integrating eq. (45), we have

$${}^{(1)}S_{4,0}^{0,0,0}(t)=-\Lambda\times\left(\frac{1}{4\Omega_M}\right)\times(e^{4i\Omega_M t}-1) \tag{46}$$

Similarly, the first order cluster cumulant, ${}^{(1)}S_{0,4}^{0,0,0}(t)$, is given by

$$i\frac{\partial\,{}^{(1)}S_{0,4}^{0,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{0,4}^{0,0,0}=\Lambda\times e^{-4i\Omega_M t} \tag{47}$$

Integrating eq. (47), we have

$${}^{(1)}S_{0,4}^{0,0,0}(t)=\Lambda\times\left(\frac{1}{4\Omega_M}\right)\times(e^{-4i\Omega_M t}-1) \tag{48}$$

For the first order cluster cumulant, ${}^{(1)}S_{3,1}^{0,0,0}(t)$, is given by

$$i\frac{\partial\,{}^{(1)}S_{3,1}^{0,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{3,1}^{0,0,0}=\Lambda\times e^{2i\Omega_M t} \tag{49}$$

Integrating eq. (49), we have

$${}^{(1)}S_{3,1}^{0,0,0}(t)=-\Lambda\times\left(\frac{1}{2\Omega_M}\right)\times(e^{2i\Omega_M t}-1) \tag{50}$$

Similarly, the first order cluster cumulant, ${}^{(1)}S_{1,3}^{0,0,0}(t)$, is given by

$${}^{(1)}S_{1,3}^{0,0,0}(t)=\Lambda\times\left(\frac{1}{2\Omega_M}\right)\times(e^{-2i\Omega_M t}-1) \tag{51}$$

For the first order cluster cumulant, ${}^{(1)}S_{2,2}^{0,0,0}(t)$, is given by

$$i\frac{\partial\,{}^{(1)}S_{2,2}^{0,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{2,2}^{0,0,0}=\Lambda \tag{52}$$

Integrating eq. (52), we have

$${}^{(1)}S_{2,2}^{0,0,0}(t)=-i\,\Lambda\times t \tag{53}$$

For the first order cumulant, ${}^{(1)}S_{1,0}^{0,0,1}(t)$, we have

$$i\frac{\partial\,{}^{(1)}S_{1,0}^{0,0,1}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{1,0}^{0,0,1}$$

$$=\left[\left(\frac{\boldsymbol{g'_s}}{\sqrt{\alpha_1}}\right)\times e^{\lambda t}\times\theta_+(t)\right]\cdot e^{i\Omega_M t} \tag{54}$$

where $\theta_+(t)$ is defined in eq. (43) and generalised **Novikov's Theorem**[18] has been applied.

Integrating eq. (54), we have

$${}^{(1)}S_{1,0}^{0,0,1}(t)=-\left(\frac{\boldsymbol{g'_s}}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1-\alpha_1)}{(\omega_0+\Omega_M-i\lambda)}\right]$$
$$\times(e^{i(\omega_0+\Omega_M-i\lambda)t}-1.0)+$$
$$+\left(\frac{\boldsymbol{g'_s}}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1+\alpha_1)}{(\omega_0-\Omega_M+i\lambda)}\right]$$
$$\times(e^{i(\omega_0-\Omega_M+i\lambda)t}-1.0) \tag{55}$$

Similarly, for the first order cumulant, ${}^{(1)}S_{0,1}^{0,0,1}(t)$, we have

$$i\frac{\partial\,{}^{(1)}S_{0,1}^{0,0,1}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{0,1}^{0,0,1}$$

$$=\left[\left(\frac{\boldsymbol{g'_s}}{\sqrt{\alpha_1}}\right)\times e^{\lambda t}\times\theta_-(t)\right]\cdot e^{-i\Omega_M t} \tag{56}$$

where $\theta_-(t)$ is defined in eq. (43) and generalised **Novikov's Theorem**[18] has been applied.

Integrating eq. (56), we have

$${}^{(1)}S_{0,1}^{0,0,1}(t)=\left(\frac{\boldsymbol{g'_s}}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1-\alpha_1)}{(\omega_0+\Omega_M+i\lambda)}\right]$$
$$\times(e^{-i(\omega_0+\Omega_M+i\lambda)t}-1.0)+$$
$$-\left(\frac{\boldsymbol{g'_s}}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1+\alpha_1)}{(\omega_0-\Omega_M-i\lambda)}\right]$$
$$\times(e^{i(\omega_0-\Omega_M-i\lambda)t}-1.0) \tag{57}$$

For the cumulant, ${}^{(1)}S_{1,0}^{0,k,0}(t)$, we have

$$i\frac{\partial\,^{(1)}S_{1,0}^{0,k,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{1,0}^{0,k,0}$$

$$=+\Sigma_k\left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}}\cdot\gamma'_k\right]\times e^{i(\Omega_M-\omega_k)t} \tag{58}$$

This leads to

$$^{(1)}S_{1,0}^{0,k,0}(t)=-\Sigma_k\left(\frac{\gamma'_k}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1+\alpha_1)}{(\Omega_M-\omega_k)}\right]$$

$$\times(e^{i(\Omega_M-\omega_k)t}-1.0) \tag{59}$$

Similarly, for the cumulant, $^{(1)}S_{0,1}^{0,k,0}$ (t), we have

$$i\frac{\partial\,^{(1)}S_{0,1}^{0,k,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{0,1}^{0,k,0}$$

$$=+\Sigma_k\left[\frac{(1-\alpha_1)}{2\sqrt{\alpha_1}}\cdot\gamma'_k\right]\times e^{-i(\Omega_M+\omega_k)t} \tag{58}$$

This leads to

$$^{(1)}S_{0,1}^{0,k,0}(t)=\Sigma_k\left(\frac{\gamma'_k}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1-\alpha_1)}{(\Omega_M+\omega_k)}\right]$$

$$\times(e^{-i(\Omega_M+\omega_k)t}-1.0) \tag{59}$$

For the cumulant, $^{(1)}S_{1,0}^{k,0,0}$ (t), we have

$$i\frac{\partial\,^{(1)}S_{1,0}^{k,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{1,0}^{k,0,0}$$

$$=+\Sigma_k\left[\frac{(1-\alpha_1)}{2\sqrt{\alpha_1}}\cdot\gamma'_k\right]\times e^{i(\Omega_M+\omega_k)t} \tag{60}$$

This leads to

$$^{(1)}S_{1,0}^{k,0,0}(t)=-\Sigma_k\left(\frac{\gamma'_k}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1-\alpha_1)}{(\Omega_M+\omega_k)}\right]$$

$$\times(e^{i(\Omega_M+\omega_k)t}-1.0) \tag{61}$$

Similarly, for the cumulant, $^{(1)}S_{0,1}^{k,0,0}$ (t), we have

$$i\frac{\partial\,^{(1)}S_{0,1}^{k,0,0}}{\partial t}=\left[\left\{\{[V_I(t)]\}_\beta\right\}_f\right]_{0,1}^{k,0,0}$$

$$=+\Sigma_k\left[\frac{(1+\alpha_1)}{2\sqrt{\alpha_1}}\cdot\gamma'_k\right]\times e^{-i(\Omega_M-\omega_k)t} \tag{62}$$

This leads to

$$^{(1)}S_{0,1}^{k,0,0}(t)=\Sigma_k\left(\frac{\gamma'_k}{2\sqrt{\alpha_1}}\right)\times\left[\frac{(1+\alpha_1)}{(\Omega_M-\omega_k)}\right]$$

$$\times(e^{-i(\Omega_M-\omega_k)t}-1.0) \tag{63}$$

The time-dependent equation for the first order cluster cumulant, $^{(1)}X_{0,0}(t)$, is given by

$$i\frac{\partial^{(1)}X_{0,0}}{\partial t}=\langle \boldsymbol{H}\rangle \tag{64}$$

where < ***H*** > is purely a number. The solution of eq. (53) is simply

$$^{(1)}X_{0,0}(t)=-i\langle \boldsymbol{H}\rangle t \tag{65}$$

where < ***H*** > is given by eq. (43).

Similarly, the time-dependent equation for the second order cluster cumulant, $^{(2)}X_{0,0}(t)$, is given by

$$i\frac{\partial^{(2)}X_{0,0}}{\partial t}=\left[\{[V_I(t)]\}_\beta\right]_{0,0} \tag{66}$$

where

$$\left[\{[V_I(t)]\}_\beta\right]_{0,0}=\frac{1}{4!}\cdot\Lambda_{4,0}\cdot n^4\cdot{}^{(1)}S_{0,4}^{0,0,0}+$$

$$+\frac{1}{4!}\cdot\Lambda_{0,4}\cdot(n+1)^4\cdot{}^{(1)}S_{4,0}^{0,0,0}+$$

$$+\frac{1}{3!}\cdot\Lambda_{3,1}\cdot n^3\cdot(n+1)\cdot{}^{(1)}S_{1,3}^{0,0,0}+$$

$$+\frac{1}{3!}\cdot\Lambda_{1,3}\cdot n\cdot(n+1)^3\cdot{}^{(1)}S_{3,1}^{0,0,0}+$$

$$+\frac{1}{2!2!}\cdot\Lambda_{2,2}\cdot n^2\cdot(n+1)^2\cdot{}^{(1)}S_{2,2}^{0,0,0}+$$

$$+G_{0,1}^{0,0,1}\cdot\left(\frac{\lambda}{2}\right)\cdot e^{-\lambda t}\cdot(n+1)\cdot{}^{(1)}S_{1,0}^{0,0,1}+$$

$$+ G_{1,0}^{0,0,1} \cdot \left(\frac{\lambda}{2}\right) \cdot e^{-\lambda t} \cdot n \cdot {}^{(1)}S_{0,1}^{0,0,1} +$$

$$+ \sum_{k=1}^{N_B} G_{0,1}^{k,0,0} \cdot n_k \cdot (n+1) \cdot {}^{(1)}S_{1,0}^{0,k,0} +$$

$$+ \sum_{k=1}^{N_B} G_{1,0}^{k,0,0} \cdot n_k \cdot n \cdot {}^{(1)}S_{0,1}^{0,k,0}$$

$$+ \sum_{k=1}^{N_B} G_{0,1}^{0,k,0} \cdot (n_k+1) \cdot (n+1) \cdot {}^{(1)}S_{1,0}^{k,0,0} +$$

$$+ \sum_{k=1}^{N_B} G_{1,0}^{0,k,0} \cdot (n_k+1) \cdot n \cdot {}^{(1)}S_{0,1}^{k,0,0}$$

where $\boldsymbol{n}$ and $\boldsymbol{n_k}$ are given by eqs. (35) and (40) respectively and $\Lambda_{4,0} = \Lambda_{0,4} = \Lambda_{3,1} = \Lambda_{1,3} = \Lambda_{2,2} = \Lambda$.

Substituting the value of ${}^{(1)}S_{0,4}^{0,0,0}$, ${}^{(1)}S_{4,0}^{0,0,0}$, ${}^{(1)}S_{1,3}^{0,0,0}$, ${}^{(1)}S_{3,1}^{0,0,0}$, ${}^{(1)}S_{2,2}^{0,0,0}$, ${}^{(1)}S_{1,0}^{0,0,1}$, ${}^{(1)}S_{0,1}^{0,0,1}$, ${}^{(1)}S_{1,0}^{0,k,0}$, ${}^{(1)}S_{0,1}^{0,k,0}$, ${}^{(1)}S_{1,0}^{k,0,0}$ and ${}^{(1)}S_{0,1}^{k,0,0}$, from the above eqs. (45)-(63) into eq. (67) and integrating eq. (66), the explicit expression of ${}^{(2)}X_{0,0}(t)$ is derived as

$${}^{(2)}X_{0,0}(t) = \left(\frac{1}{24}\right) \times \Lambda^2 \times \left(\frac{1}{4\Omega_M}\right)^2 \cdot n^4 \left\{\left(e^{i4\Omega_M t} - 1\right) + i4\Omega_M t\right\} +$$

$$+\left(\frac{1}{24}\right) \times \Lambda^2 \times \left(\frac{1}{4\Omega_M}\right)^2 \cdot (n+1)^4 \left\{\left(e^{-i4\Omega_M t} - 1\right) - i4\Omega_M t\right\} +$$

$$+\left(\frac{1}{6}\right) \times \Lambda^2 \times \left(\frac{1}{2\Omega_M}\right)^2 \cdot n^3 (n+1) \left\{\left(e^{-i2\Omega_M t} - 1\right) + i2\Omega_M t\right\} +$$

$$+\left(\frac{1}{6}\right) \times \Lambda^2 \times \left(\frac{1}{2\Omega_M}\right)^2 \cdot n (n+1)^3 \left\{\left(e^{i2\Omega_M t} - 1\right) - i2\Omega_M t\right\} -$$

$$-\left(\frac{1}{4}\right) \times \Lambda^2 \cdot n^2 (n+1)^2 \cdot \left(\frac{t^2}{2}\right) +$$

$$+ G_{0,1}^{0,0,1} \cdot G_s \cdot \left(\frac{\lambda}{2}\right) \cdot (n+1) \cdot \frac{(1-\alpha_1)}{\Omega_1} \cdot \left[\frac{(e^{i(\Omega_1 + i\lambda)t} - 1)}{(\Omega_1 + i\lambda)} - \frac{(e^{-\lambda t} - 1)}{(i\lambda)}\right] -$$

$$- G_{0,1}^{0,0,1} \cdot G_s \cdot \left(\frac{\lambda}{2}\right) \cdot (n+1) \cdot \frac{(1+\alpha_1)}{\Omega_2} \cdot \left[\frac{(e^{i(\Omega_2 + i\lambda)t} - 1)}{(\Omega_2 + i\lambda)} - \frac{(e^{-\lambda t} - 1)}{(i\lambda)}\right] +$$

$$+ G_{1,0}^{0,0,1} \cdot G_s \cdot \left(\frac{\lambda}{2}\right) \cdot n \cdot \frac{(1-\alpha_1)}{\Omega_3} \cdot \left[\frac{(e^{-i(\Omega_3 - i\lambda)t} - 1)}{(\Omega_3 - i\lambda)} - \frac{(e^{-\lambda t} - 1)}{(i\lambda)}\right] +$$

$$+ G_{1,0}^{0,0,1} \cdot G_s \cdot \left(\frac{\lambda}{2}\right) \cdot n \cdot \frac{(1+\alpha_1)}{\Omega_4} \cdot \left[\frac{(e^{i(\Omega_4 + i\lambda)t} - 1)}{(\Omega_4 + i\lambda)} - \frac{(e^{-\lambda t} - 1)}{(i\lambda)}\right] +$$

$$+ \sum_{k=1}^{N_B} G_{0,1}^{k,0,0} \cdot \Gamma_k \cdot \left(\frac{1+\alpha_1}{\Omega_5^2}\right) \cdot n_k \cdot (n+1) \cdot \left\{\left(e^{i\Omega_5 t} - 1\right) - i\Omega_5 t\right\} +$$

$$+ \sum_{k=1}^{N_B} G_{1,0}^{k,0,0} \cdot \Gamma_k \cdot \left(\frac{1-\alpha_1}{\Omega_6^2}\right) \cdot n_k \cdot n \cdot \left\{\left(e^{-i\Omega_6 t} - 1\right) + i\Omega_6 t\right\} +$$

$$+ \sum_{k=1}^{N_B} G_{0,1}^{0,k,0} \cdot \Gamma_k \cdot \left(\frac{1-\alpha_1}{\Omega_6^2}\right) \cdot (n_k+1) \cdot (n+1) \cdot \left\{\left(e^{i\Omega_6 t} - 1\right) - i\Omega_6 t\right\} +$$

$$+ \sum_{k=1}^{N_B} G_{1,0}^{0,k,0} \cdot \Gamma_k \cdot \left(\frac{1+\alpha_1}{\Omega_5^2}\right) \cdot (n_k+1) \cdot n \cdot \left\{\left(e^{-i\Omega_5 t} - 1\right) + i\Omega_5 t\right\}.$$

where $\boldsymbol{G_s} = \left(\frac{g'_s}{2\sqrt{\alpha_1}}\right)$, $\boldsymbol{\Gamma_k} = \left(\frac{\gamma'_k}{2\sqrt{\alpha_1}}\right)$,

$\boldsymbol{\Omega}_1 = \omega_0 + \boldsymbol{\Omega}_M - i\lambda$, $\boldsymbol{\Omega}_2 = \omega_0 - \boldsymbol{\Omega}_M + i\lambda$,
$\boldsymbol{\Omega}_3 = \omega_0 + \boldsymbol{\Omega}_M + i\lambda$, $\boldsymbol{\Omega}_4 = \omega_0 - \boldsymbol{\Omega}_M - i\lambda$,
$\boldsymbol{\Omega}_5 = \boldsymbol{\Omega}_M - \omega_k$, and $\boldsymbol{\Omega}_6 = \boldsymbol{\Omega}_M + \omega_k$.

It is worthy to note that the n-th order perturbative cluster cumulants ${}^{(n)}S_{m,n}^{p,q,f}(t)$ and ${}^{(n)}X_{k,k}(t)$ can be obtained by using the value of cluster cumulant of lower orders and subsequent time-integration.

Thus, the value of $X_{0,0}(t)$ up to second order is given by

$$ {}^{(2)}\overline{X}_{0,0}(t) = {}^{(1)}X_{0,0}(t) + {}^{(2)}X_{0,0}(t) \tag{69} $$

Finally, having obtained the value of $\overline{X}_{0,0}(t)$, the ground state Survival Probability, $P_{0,0}(t)$ is given by

$$ P_{0,0}(t) = |< 0|U_I(t)|0 >|^2 = |\exp[{}^{(2)}\overline{\boldsymbol{X}}_{0,0}(t)]|^2 \tag{70} $$

The power spectrum can be obtained from the expression given by

$$ I(\omega) \propto \int_0^\infty \exp\left[{}^{(2)}\overline{X}_{0,0}(t) \right] \times e^{i\omega t} dt \tag{71} $$

From the power spectrum we can predict the effect of anharmonicity, system-bath coupling strength, colored noise strength, temperature of both the system and the bath degrees of freedom on the spectral line shape and peak position.

6. The concluding remarks

In this paper, a time-dependant multireference unified cluster cumulant (TDMRUCC) method has been introduced for computing the effect of bath or the surrounding degrees of freedom on a quantum particle trapped in a 1-dimensional anharmonic oscillator potential that is coupled to both the stochastic and the thermal bath. This formalism uses the key features of the time-dependent multi-reference cluster cumulant (TDMRCC) method and the thermal cluster cumulant (TCC) method developed by Mukherjee and his coworkers guarantying its size-consistency. As an initial venture, the explicit analytical expression of the amplitude of the model space cumulant, $X_{0,0}(t)$ up to second order is derived in order to get the dynamics of the quantum particle in presence of both the thermal and the stochastic bath and their mutual interplay. The nonperturbative cluster cumulant equations under a suitable truncation scheme with respect to the power of the cluster amplitudes of exponential ansatz will be presented in the forthcoming paper.

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