A correspondence from renormalized frequency to heat capacity for particles in an anharmonic potential

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For particles in an anharmonic potential, classical mechanics asserts that there is a renormalization of the bare frequency of the oscillatory motion, and statistical mechanics claims that the anharmonicity causes a correction to the heat capacity of an ideal gas composed of particles in the anharmonic potential. When the frequency and the heat capacity are expressed in perturbative series, respective, in terms of the characteristic lengths in mechanics and statistical physics, the expansion coefficients have an order-by-order correspondence. This correspondence is in contrast to our intuition that the renormalized frequency enters the statistical mechanics as a single quantity.

Keywords: renormalization, anharmonicity, heat capacity, Poincare–Lindstedt method.

I. INTRODUCTION

The anharmonicity plays crucial roles in modern physics, for instance, the classical $\phi^4$ model in quantum field theory [1] and various anharmonic effects in condensed matter physics. [2–10] These anharmonicities in distant areas are usually treated in separation. It is well-known that once the anharmonicity presents, the bare frequency needs to be renormalized to remove the superficial divergence, i.e., to eliminate the secular term in the bare solution. [11–13] During the past decade, a novel relationship between the renormalization in quantum field theory and removal of the secular term in perturbation expansion has been uncovered, and many advances have been made. [14–21] We note a curious fact that, on one hand, in classical mechanics the anharmonicity usually leads to a renormalization of the bare frequency, and on the other, in statistical mechanics the simplest situation is that the anharmonicity causes a correction to the heat capacity of an ideal gas composed of particles in the anharmonic potential. An immediate problem arises how the renormalization of the bare frequency enters the heat capacity with the same anharmonicity in the potential. The renormalization and the thermal effects must be mutually correlated, and there is a relation in which is nevertheless unknown. The relation is not superficial for the renormalized frequency depends on the oscillation amplitude determined by the amount of energy input into the oscillator, while the partition function takes account of all possible microstates accessible to the system and the energy levels of the system with the anharmonicity.

In present paper, we study a one-dimensional system. Assume that there is a particle of mass $m$ moving in a potential field $U(r)$ given by,

$$U(r) = U(0) + \frac{1}{2}m\omega_0^2\left(r^2 - \alpha r^3 + \gamma r^4\right),$$

where $\omega_0$ is the bare spring constant of the unperturbed potential $m\omega_0^2r^2/2$, and $\alpha$ and $\gamma$ are two small constants accounting for the anharmonicity. The origin of the coordinate is $r = 0$, and usually, we set $U(0) = 0$. The Hamilton of the system is,

$$H = \frac{p^2}{2m} + U(r).$$

This system appears in two areas: One is in mechanics dealing with the periodic motion of a single particle around the central point $r = 0$, and another is in statistical mechanics dealing with thermal effect of the ideal gas composed by many such particles. Since the renormalized frequency is a single quantity, and it would enter the heat capacity as an integrated quantity. In fact, it is not the case as we demonstrate in the present paper. The renormalized frequency influences the heat capacity, order by order.

In section II, we utilize the Poincare–Lindstedt method to solve the equation of motion of position $r$ in terms of time $t$, from which we see in detail how the bare frequency is renormalized. In section III, the anharmonicity induced...
correction of the heat capacity is calculated and an order-by-order correspondence from the renormalized frequency to the heat capacity is then identified. In section IV, a model containing higher order anharmonicities is studied, and the correspondence is demonstrated to be true. In final section V, a brief conclusion is given.

II. RENORMALIZED FREQUENCIES FOR ANHARMONIC OSCILLATOR

The equation of motion for one particle in one-dimensional potential $U(r)$ is,

$$\frac{d^2r}{dt^2} = -\frac{dU(r)}{dr} = -\omega_0^2 \left( r - \frac{3}{2} \alpha r^2 + 2\gamma r^3 \right). \quad (3)$$

To this equation, no exact solution is possible due to the nonlinearity in $r$, and even worse, the regular perturbation approaches fail for they lead to the secular term in the solutions of $r = r(t)$. Instead, the Poincare–Lindstedt method offers a standard technique for uniformly approximate periodic solutions to ordinary differential equations. \(11\) \(12\)

By the method, we mean that both the time parameter $t$ and the dependence of $r(t)$ on $t$ must be simultaneously transformed into,

$$t \to \tau = \frac{\omega_0}{\omega_0 + \omega_1 + \omega_2 + \ldots} t, \quad r(t) \to \xi(\tau). \quad (4)$$

The bare frequency $\omega_0$ in the equation (3) is modified, and $\omega_1 \sim O(\alpha)$ and $\omega_2 \sim O(\alpha^2) \sim O(\gamma)$ are the first and second order renormalization of the frequency, and so forth. In the same time, we have,

$$\xi(\tau) \approx \xi_0(\tau) + \xi_1(\tau) + \xi_2(\tau) + \ldots \quad (5)$$

in which $\xi_0(\tau)$ satisfies the equation of motion for the unperturbed oscillator, and $\xi_1 \sim O(\alpha)$ and $\xi_2 \sim O(\alpha^2)$ are the first and second order correction of the position $r(t)$, and so forth.

The correct equation of motion takes the following form, accurate up to $O(\gamma)$ or $O(\alpha^2)$,

$$\frac{d^2\xi}{d\tau^2} \approx -(\omega_0 + \omega_1 + \omega_2 + \ldots)^2 \left( \xi - \frac{3}{2} \alpha \xi^2 + 2\gamma \xi^3 \right), \quad (6)$$

The zeroth order equation of motion of Eq. (3) is,

$$\frac{d^2\xi_0}{d\tau^2} + \omega_0^2 \xi_0 = 0, \quad \xi_0(0) = A, \quad \frac{d\xi_0(0)}{d\tau} = 0, \quad (7)$$

where $A$ is the amplitude of the unperturbed oscillator. The first order equation of motion of Eq. (3) is,

$$\xi_1'' + \left( \omega_0^2 (2\xi_1 - 3\alpha \xi_0^2) + 4\omega_1 \omega_0 \xi_0 \right) = 0, \quad (8)$$

together with the initial conditions $\xi_1(0) = 0, d\xi_1(0)/d\tau = 0$. The second order equation of motion of Eq. (3) is,

$$\xi_2'' + \omega_0^2 \xi_2 + (2\omega_1 \omega_0 - 3\alpha \xi_0 \omega_0^2) \xi_1 + 2\omega_0^2 \gamma \xi_0^3 - 3\alpha \omega_1 \omega_0 \xi_0^2 + (2\omega_2 \omega_0 + \omega_1^2) \xi_0 = 0, \quad (9)$$

together with the initial conditions $\xi_2(0) = 0, d\xi_2(0)/d\tau = 0$.

The zeroth order equation of motion gives the usual harmonic oscillatory solution,

$$\xi_0(\tau) = A \cos(\omega_0 \tau). \quad (10)$$

The "bare" solution of the first order equation of motion is then,

$$\xi_1(\tau) = -\omega_1 \tau A \sin(\omega_0 \tau) + \alpha A^2 \left( 1 - \frac{1}{2} \cos(\omega_0 \tau) - \frac{1}{2} \cos^2(\omega_0 \tau) \right). \quad (11)$$

The first term gives the divergent oscillatory amplitude $\omega_1 \tau A$ as time $\tau \to \infty$ with $\omega_1 \neq 0$. To remove the divergence, we have to choose,

$$\omega_1 = 0. \quad (12)$$
The correct first order solution of equation of motion becomes,

$$\xi_1(\tau) = \frac{1}{4} \alpha A^2 (3 - 2 \cos (\omega_0 \tau) - \cos (2\omega_0 \tau)),$$

(13)

The "bare" solution of the second order equation of motion is,

$$\xi_2(\tau) = \frac{A\tau}{16} (3A^2 (5\alpha^2 - 4\gamma) \omega_0 - 16\omega_2) \sin(\omega_0 \tau)$$

$$- \frac{A^3}{16} \left( 12\alpha^2 + \left( \gamma - \frac{29}{4} \alpha^2 \right) \cos (\omega_0 \tau) - 4\alpha^2 \cos (2\omega_0 \tau) - \left( \gamma + \frac{3}{4} \alpha^2 \right) \cos (3\omega_0 \tau) \right).$$

(14)

The first term gives also the divergent oscillatory amplitude as time \( \tau \to \infty \), but this divergence can simply be removed with \( \omega_2 \) being selected to satisfy,

$$3 \frac{A^2}{\tau_0^2} (5\alpha^2 - 4\gamma) \omega_0 - 16\omega_2 = 0.$$  

(15)

It amounts to the second order correction of the frequency \( \omega_2 \) to be,

$$\omega_2 = \frac{A^2}{2} \left( \frac{15}{8} \alpha^2 - \frac{3}{2} \gamma \right) \omega_0.$$  

(16)

Therefore, the correct second order solution of equation of motion is,

$$\xi_2(\tau) = - \frac{A^3}{16} \left( 12\alpha^2 + \left( \gamma - \frac{29}{4} \alpha^2 \right) \cos (\omega_0 \tau) - 4\alpha^2 \cos (2\omega_0 \tau) - \left( \gamma + \frac{3}{4} \alpha^2 \right) \cos (3\omega_0 \tau) \right).$$

(17)

The important result is then the bare frequency \( \omega_0 \) is renormalized to be, up to accuracy of second order anharmonicity \( O(\alpha^2) \sim O(\gamma) \),

$$\omega = \omega_0 + \frac{A^2}{2} \left( \frac{15}{8} \alpha^2 - \frac{3}{2} \gamma \right) \omega_0 = \omega_0 \left( 1 + \frac{A^2}{2} \left( \frac{15}{8} \alpha^2 - \frac{3}{2} \gamma \right) \right),$$

(18)

where the modified part of \( \omega_2 \) is related to the external parameter \( A \). The renormalization introduces a complicated combination of the intrinsic parameters \( \alpha \) and \( \gamma \) in the following,

$$\chi^{(2)} = \frac{3}{16} (5\alpha^2 - 4\gamma),$$

(19)

from which we have,

$$\omega_2 = A^2 \chi^{(2)} \omega_0,$$

(20)

in which \( A \) is an extrinsic mechanical parameter. The factor \( \chi^{(2)} \) can be considered essential in \( \omega_2 \) for it is only definable via the intrinsic parameters \( \alpha \) and \( \gamma \).

It is interesting to explore the energy of oscillation in the presence of the anharmonicity. The oscillation is composed of a single prime frequency \( \omega_0 \) and its higher order harmonics,

$$\xi(\tau) \approx A \cos (\omega_0 \tau) + \frac{1}{4} \alpha A^2 (3 - 2 \cos (\omega_0 \tau) - \cos (2\omega_0 \tau))$$

$$- \frac{A^3}{16} \left( 12\alpha^2 + \left( \gamma - \frac{29}{4} \alpha^2 \right) \cos (\omega_0 \tau) - 4\alpha^2 \cos (2\omega_0 \tau) - \left( \gamma + \frac{3}{4} \alpha^2 \right) \cos (3\omega_0 \tau) \right),$$

(21)

and the energy is, with setting \( U (r_0) = 0 \),

$$E = \frac{1}{2} m \left( \frac{dr}{dt} \right)^2 + U (r).$$

(22)

Explicitly it is, accurate up to \( O(\gamma) \) or \( O(\alpha^2) \),

$$E \approx \frac{1}{2} m (\omega_0 A)^2 \left( 1 - \alpha A + \left( \frac{15}{8} \alpha^2 - \frac{3}{2} \gamma \right) A^2 \right).$$

(23)
It amounts to that the frequency and the amplitude of the oscillation are both modified so that $E$ can also be expressible in the following way,

$$E \approx \frac{1}{2} m (\omega A')^2,$$

(24)

with,

$$A' = A \left(1 - \frac{\alpha}{2} A - \frac{(\alpha^2 - 4\gamma)}{8} A^2 \right).$$

(25)

The amount of energy shift is,

$$\Delta E \equiv E - \frac{1}{2} m (\omega_0 A)^2 = -\frac{1}{2} m (\omega_0 A)^2 \left(\alpha A - \chi^{(2)} A^2 \right).$$

(26)

which depends not only on material parameters $m$, $\omega_0$, $\alpha$, and $\chi$, but also on the external parameter $A$. Requiring that the energy shift is small,

$$\left|\frac{\Delta E}{\frac{1}{2} m (\omega_0 A)^2}\right| = \left|\alpha A - \chi^{(2)} A^2 \right| < 1,$$

(27)

we have thus simultaneously,

$$|\alpha| < \frac{1}{A}, \text{ and } |\gamma| < \frac{1}{A^2}.$$  

(28)

This is what small constants $\alpha$ and $\gamma$ mean in mechanics: Once these conditions break, the perturbation method does not apply.

### III. ANHARMONICITY INDUCED CORRECTION OF THE HEAT CAPACITY

For considering the thermal effect of the ideal gas composed by many particles in potential $U(r)$, we need to compute the partition function in Boltzmann statistical mechanics,

$$Z = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp(-\beta H) \frac{dr dp}{h} = \left(\int_{-\infty}^{\infty} \exp(-\beta \frac{p^2}{2m}) \frac{dp}{h}\right) Z_U$$

(29)

where $h$ is the Planck’s constant, and $Z_U$ is the configurational factor of the partition function, with setting $U(r_0) = 0$,

$$Z_U = \int_{-\infty}^{\infty} \exp(-\beta U(r)) dr$$

$$= \int_{-\infty}^{\infty} \exp \left(-\beta \frac{1}{2} m \omega_0^2 \left(r^2 - \alpha r^3 + \gamma r^4\right)\right) dr$$

$$\approx \int_{-\infty}^{\infty} \exp \left(-\frac{r^2}{\rho^2}\right) \left(1 + \frac{\alpha r^3 - \gamma r^4}{\rho^2} + \frac{1}{2} \left(\frac{\alpha r^3}{\rho^2}\right)^2\right) dr,$$  

(30)

where $\rho$ is the thermodynamic characteristic length, defined via,

$$\rho^2 = \frac{1}{\beta m \omega_0^2 / 2} = \frac{2k_B T}{m \omega_0^2},$$

(31)

The anharmonicity gives rise to the correction to the unperturbed partition function via $Z_U$, and thus we are interested in $Z_U$ only, which is, accurate up to $O(\gamma)$ or $O(\alpha^2)$,

$$Z_U = \sqrt{\pi} \rho + \sqrt{\pi} \rho^3 \frac{3}{16} \left(5\alpha^2 - 4\gamma\right),$$

(32)
which is in terms of $\chi^{(2)}$,

$$Z_U \approx \sqrt{\pi} \rho \left(1 + \chi^{(2)} \rho^2 \right).$$

(33)

The first term, unity, in round bracket () comes from the unperturbed oscillator. Requiring that the correction to the unperturbed partition function is small,

$$\left| \chi^{(2)} \right| \rho^2 < 1$$

(34)

we have simultaneously,

$$|\alpha| < \frac{1}{\rho}, \text{ and } |\gamma| < \frac{1}{\rho^2}.$$  

(35)

or,

$$k_B T < \frac{m\omega_0^2}{2 |\alpha|}, \text{ and } k_B T < \frac{m\omega_0^2}{2 |\gamma|}.$$  

(36)

This is what small constants $\alpha$ and $\gamma$ mean in statistical physics: Once these conditions break, the small parameter expansion in (30) does not apply.

The configurational part of the free energy $F_U$ is, with $N$ being the total number of the particles,

$$F_U \approx -Nk_B T \ln Z_U \approx -Nk_B T \ln \left(\sqrt{\pi} \rho \right) - Nk_B T \chi^{(2)} \rho^2,$$

(37)

where the lowest correction is second order $O(\gamma) \sim O(\alpha^2)$, induced by the anharmonicity to the oscillatory free energy is,

$$\Delta F^{(2)}_U \approx -Nk_B T \chi^{(2)} \rho^2.$$ 

(38)

It is clearly that the correction to the oscillatory free energy is closely related to renormalization of the frequency, but irrespective of the external parameter $A$. The resultant correction to the internal energy is then,

$$\Delta U^{(2)}_U \approx -\chi^{(2)} N \frac{\partial}{\partial \beta} \rho^2 = Nk_B T \chi^{(2)} \rho^2.$$ 

(39)

The corresponding correction to heat capacity is,

$$\Delta C^{(2)} = \frac{\partial \Delta U}{\partial T} = 2Nk_B \chi^{(2)} \rho^2.$$ 

(40)

Evidently, in view of statistical mechanics, $\Delta C^{(2)}$ is the second order quantity for it depends on $O(\chi^{(2)})$. The correspondence from the renormalized frequency to the heat capacity is, explicitly, with $\omega_1 = 0$ and $\Delta C^{(1)} = 0$,

$$\left(\omega_1, \omega_2\right) \rightarrow \left(\Delta C^{(1)}, \Delta C^{(2)}\right).$$ 

(41)

It suggests an order-by-order correspondence from mechanics to statistical physics, rather than the renormalized frequency enter the heat capacity as a single quantity. One may wonder whether the order-by-order correspondence in equations (35) and (36) is a mere coincidence between the renormalization and the heat capacity for the anharmonicity. In next section, we show how the correspondence persists for high order anharmonicities.

IV. HIGH ORDER ANHARMONICITIES: HEAT CAPACITY CORRECTION AND RENORMALIZATION OF THE BARE FREQUENCY

For our purpose, we examine a theoretical model of the anharmonic oscillation, and the potential assumes the following form,

$$U(r) = \frac{1}{2}m\omega_0^2 \left( r^2 - \alpha r^3 + \gamma r^4 + \mu r^5 + vr^6 \right),$$ 

(42)
which involves the fourth order anharmonicities $O(v) \sim O(\alpha^4)$. Utilization of the Poincare–Lindstedt method to solve the equation of motion of position $r$ in terms of time $t$ gives results for each order in the following. The first three solutions $(\xi_0(\tau), \xi_1(\tau), \xi_2(\tau))$ are already given in (21), and the third order solution $\xi_3(\tau)$ is,

$$
\xi_3(\tau) = \frac{1}{96} A^4 (\Lambda_0 + \Lambda_1 \cos(\tau) + \Lambda_2 \cos(2\tau) + \Lambda_3 \cos(3\tau) + \Lambda_4 \cos(4\tau)),
$$

where,

$$
\Lambda_0 = \frac{675\alpha^3}{4} - 189\alpha\gamma - 90\mu,
\Lambda_1 = -\frac{357\alpha^3}{4} + 105\alpha\gamma + 48\mu,
\Lambda_2 = -72\alpha^3 + 96\alpha\gamma + 40\mu,
\Lambda_3 = -\frac{27\alpha^3}{4} - 9\alpha\gamma,
\Lambda_4 = -\frac{3\alpha^3}{4} - 3\alpha\gamma + 2\mu.
$$

The fourth order solution $\xi_4(\tau)$ is,

$$
\xi_4(\tau) = -\frac{1}{3072} A^5 (\Omega_0 + \Omega_1 \cos(\tau) + \Omega_2 \cos(2\tau) + \Omega_3 \cos(3\tau) + \Omega_4 \cos(4\tau) + \Omega_5 \cos(5\tau)),
$$

where,

$$
\Omega_0 = 144\alpha (75\alpha^3 - 116\alpha\gamma - 56\mu),
\Omega_1 = \frac{-21213\alpha^4}{4} + 8850\alpha^2\gamma + 4672\alpha\mu - 276\gamma^2 + 384\nu,
\Omega_2 = 256\alpha (-18\alpha^3 + 30\alpha\gamma + 13\mu),
\Omega_3 = -9(93\alpha^4 - 44\alpha^2\gamma + 12\alpha\mu - 32\gamma^2 + 40\nu),
\Omega_4 = -16\alpha (3\alpha^3 + 12\alpha\gamma - 8\mu),
\Omega_5 = -\frac{15\alpha^4}{4} - 30\alpha^2\gamma + 44\alpha\mu - 12(\gamma^2 + 2\nu).
$$

The third order and fourth order normalized frequencies are, respectively,

$$
\omega_3 = -A^3 \alpha \chi^{(2)} \omega_0,
$$

and

$$
\omega_4 = \frac{3A^4}{1024} (1155\alpha^4 - 2200\alpha^2\gamma - 1120\alpha\mu + 304\gamma^2 - 320\nu) \omega_0.
$$

Similarly, we have $\omega_3 = \chi^{(3)} A^3$ and $\omega_4 = \chi^{(4)} A^4$ with $\chi^{(3)}$ and $\chi^{(4)}$ being introduced, respectively, via,

$$
\chi^{(3)} \equiv -\alpha \chi^{(2)}, \text{ and } \chi^{(4)} \equiv \frac{3}{1024} (1155\alpha^4 - 2200\alpha^2\gamma - 1120\alpha\mu + 304\gamma^2 - 320\nu).
$$

The expression of $\omega_4$ in terms of fourth order combinations of the intrinsic mechanical parameters $O(v) \sim O(\alpha^4) \sim O(\alpha^2\gamma) \sim O(\gamma^2) \sim O(\alpha\mu)$, and the combinations are quite complicated, and we anticipate that $\chi^{(3)}$ and $\chi^{(4)}$ are going to show off in the heat capacity.

To see how two quantities $\chi^{(3)}$ and $\chi^{(4)}$ appear in the higher order corrections to heat capacity, let us examine the corrections to the partition function due to the higher order approximations $\mu \xi^5 + \nu \xi^6$ in the potential [12]. The result is, with calculations similar to (30–33),

$$
\Delta Z_U = \frac{15}{512} \left( 231\alpha^4 - 504\alpha^2\gamma - 224\alpha\mu + 112\gamma^2 - 64\nu \right) \rho^4 = 2\rho^4 \left( \frac{\gamma}{\alpha} \chi^{(3)} + \chi^{(4)} \right).
$$

(48)
It causes following third order and fourth order energy shift,

\[
\left( \Delta U_U^{(3)}, \Delta U_U^{(4)} \right) = -2N \left( \frac{\gamma}{\alpha} \chi^{(3)}, \chi^{(4)} \right) \frac{\partial}{\partial \beta} \rho^4 = 4Nk_BT \left( \frac{\gamma}{\alpha} \chi^{(3)}, \chi^{(4)} \right) \rho^4
\]

(49)

The corresponding corrections to the heat capacity is, respectively,

\[
\left( \Delta C^{(3)}, \Delta C^{(4)} \right) = \frac{\partial}{\partial T} \left( \Delta U_U^{(3)}, \Delta U_U^{(4)} \right) = 12Nk_B \left( \frac{\gamma}{\alpha} \chi^{(3)}, \chi^{(4)} \right) \rho^4.
\]

(50)

We thus show that the correspondence similar to (41) holds,

\[
(\omega_3, \omega_4) \rightarrow \left( \Delta C^{(3)}, \Delta C^{(4)} \right).
\]

(51)

V. CONCLUSIONS AND DISCUSSIONS

Collecting together the results on normalized frequencies \(\Delta \omega\) and heat capacity corrections \(\Delta C\), we have, respectively,

\[
\Delta \omega \approx \left( \chi^{(2)} A^2 + \chi^{(3)} A^3 + \chi^{(4)} A^4 \right) \omega_0,
\]

(52)

and

\[
\Delta C = Nk_B \left( 2\chi^{(2)} \rho^2 + 12 \left( \frac{\gamma}{\alpha} \chi^{(3)} + \chi^{(4)} \right) \rho^4 \right).
\]

(53)

Since the dimensions of \(\alpha\) and \(\gamma\) are of \(1/\text{length}\) and \((1/\text{length})^2\), the quantity \(\gamma \rho / \alpha\) is dimensionless. It is evident that the renormalized frequency \(\omega\) is an expansion in terms of \(\chi^{(j)}\),

\[
\Delta \omega = \omega_0 \sum_{j=1}^{4} \alpha_j \chi^{(j)} A^j
\]

(54)

and total correction to the heat capacity \(\Delta C\) is also an expansion in terms of \(\chi^{(j)}\),

\[
\Delta C = Nk_B \sum_{j=1}^{4} \beta_j \chi^{(j)} \rho^j,
\]

(55)

where \(\alpha_j = (0, 1, 1, 1)\) but \(\beta_j = (0, 2, 12 \rho \gamma / \alpha, 12)\) \((j = 1, 2, 3, 4)\) are numerals and anharmonic constants in \(U \left( r \right)\). On one hand, it is easily understandable for either \(\Delta \omega\) or \(\Delta C\) can be expanded in the powers of mechanical and thermal physical characteristic length, \(A\) and \(\rho\), respectively. On the other hand, the expansion coefficients are complicated combinations of the the expansion coefficients of the anharmonic oscillations. The normalized frequency \(\omega\) does not enter the heat capacity as a single quantity. Instead, we have an order-by-order correspondence,

\[
\alpha_j \rightarrow \beta_j.
\]

(56)

To sum up, the present work reports a novel order-by-order correspondence from normalized frequencies to the heat capacity corrections. This correspondence illustrates the fundamental difference between Poincare–Lindstedt renormalization and the renormalization in quantum field theory; and for the latter, the normalized value of a physical quantity is always used to define an intrinsic attribute of the quantity.

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[1] Claude Itzykson, Jean-Bernard Zuber, Quantum Field Theory, (New York: Dover, 2006)
[2] R. Mankowsky, A. Subedi, M. Först, et al. Nonlinear lattice dynamics as a basis for enhanced superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$. Nature 516(2014)71–73.

[3] Yue Chen, Xinyuan Ai, and C. A. Marianetti, First-Principles Approach to Nonlinear Lattice Dynamics: Anomalous Spectra in PbTe. Phys. Rev. Lett. 113(2014)105501.

[4] C. W. Li, J. Ma, H. B. Cao, A. F. May, D. L. Abernathy, G. Ehlers, C. Hoffmann, X. Wang, T. Hong, A. Huq, O. Gourdon, and O. Delaire, Anharmonicity and atomic distribution of SnTe and PbTe thermoelectrics. Phys. Rev. B 90(2014)214303.

[5] Yao Tian, Shuang Jia, R. J. Cava, Ruidian Zhong, John Schneeloch, Genda Gu, and Kenneth S. Burch, Understanding the evolution of anomalous anharmonicity in Bi$_2$Te$_3$−$x$Se$_x$. Phys. Rev. B 95(2017)094104.

[6] R. Bianco, I. Errea, L. Paulatto, M. Calandra, and F. Maur, Second-order structural phase transitions, free energy curvature, and temperature-dependent anharmonic phonons in the self-consistent harmonic approximation: Theory and stochastic implementation, Phys. Rev. B 96(2017)014111.

[7] A. S. T. Nguetcho, G. M. Nkeumaleu, and J M Bilbault, Behavior of gap solitons in anharmonic lattices, Phys. Rev. E, 96(2017)022207.

[8] Yi Xia, Revisiting lattice thermal transport in PbTe: The crucial role of quartic anharmonicity, Appl. Phys. Lett., 113(2018)073901.

[9] Qiya Liu, Ruihui Shao, Ning Li, Weizheng Liang, Xinsheng Yang, S. N. Luo, and Yong Zhao, Anharmonicity of Bi$_2$Se$_3$ revealed by fs transient optical spectroscopy, Appl. Phys. Lett. 115(2019)201902.

[10] E. Manley, O. Hellman, N. Shulumba, A. F. May, P. J. Stonaha, J. W. Lynn, V. O. Garlea, A. Alatas, R. P. Hermann, J. D. Budai, H. Wang, B. C. Sales, and A. J. Minnich, Intrinsic anharmonic localization in thermoelectric PbSe, Nat. Commun. 10(2019)1928.

[11] Carl M. Bender, Steven A. Orszag, Advanced Mathematical Methods for Scientists and Engineers: Asymptotic Methods and Perturbation Theory, (New York: Springer, 1999). Chapter 11.

[12] L.-Y. Chen, N. Goldenfeld and Y. Oono, The renormalization group and singular perturbations: multiple scales, boundary layers and reductive perturbation theory, Phys. Rev. E 54(1996)376.

[13] Q. H. Liu, Z. Li, M. N. Zhang, Q. Li, B .J. Chen, Exponential functions of perturbative series and elimination of secular divergences in time-dependent perturbation theory in quantum mechanics, Results in Physics, 7(2017)890.

[14] B. Craps, O. Evnin, and J. Vanhoof, Renormalization group, secular term resummation and AdS (in)stability. J. High Energ. Phys. 2014(2014)48.

[15] O. J. C. Dias, G. T. Horowitz and J. E. Santos, Gravitational turbulent instability of anti-de Sitter space, Class. Quant. Grav. 29(2012)194002.

[16] O. J. C. Dias, G. T. Horowitz, D. Marolf and J. E. Santos, On the nonlinear stability of asymptotically anti-de Sitter solutions, Class. Quant. Grav. 29(2012)235019.

[17] M. Maliborski and A. Rostworowski, Time-periodic solutions in an Einstein AdS-massless-scalar-field system, Phys. Rev. Lett. 111(2013)051102.

[18] A. Buchel, S.L. Liebling and L. Lehner, Boson stars in AdS spacetime, Phys. Rev. D 87(2013)123006.

[19] J. Abajo-Arrastia, E. da Silva, E. Lopez, J. Mas and A. Serantes, Holographic relaxation of finite size isolated quantum systems, J. High Energ. Phys. 05(2014)126.

[20] M. Maliborski and A. Rostworowski, What drives AdS unstable?, Phys. Rev. D 89(2014)124006.

[21] V. Balasubramanian, A. Buchel, S.R. Green, L. Lehner and S.L. Liebling, Holographic thermalization, stability of AdS and the Fermi-Pasta-Ulam-Tsingou paradox, Phys. Rev. Lett. 113(2014)071601.