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Perturbation theory for particle in a box

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Abstract

Recently developed strong-coupling theory opens up the possibility of treating quantum-mechanical systems with hard-wall potentials via perturbation theory. To test the power of this theory we study here the exactly solvable quantum mechanics of a point particle in a one-dimensional box. Introducing an auxiliary harmonic frequency term ω, the ground-state energy $E^{(0)}$ can be expanded perturbatively in powers of $\pi^2/\omega d^2$, where d is the box size. The removal of the infrared cutoff ω requires the resummation of the series at an infinitely strong coupling. We show that strong-coupling theory yields a fast-convergent sequence of approximations to the well-known quantum-mechanical energy $E^{(0)} = \pi^2/2d^2$.

1. Variational perturbation theory [1] permits us to convert divergent weak-coupling expansions into convergent strong-coupling expansions. In particular, a constant strong-coupling limit of a function can be evaluated from its weak-coupling expansion with any desired accuracy. As an important application, this has led to a novel way of calculating critical exponents without using the renormalization group [2].

Given this theory, new classes of physical systems become accessible to perturbation theory. For instance, the important problem a the pressure exerted by a stack of membranes upon the enclosing walls [3] has now become calculable analytically with the help of perturbation theory. For a single membrane, this has already be done successfully [4,5]. Realistic physical problems have usually the disadvantage that the maximally accessible order of perturbation theory is quite limited. If we want to gain a better understanding of the convergence of the successive approximations as the order goes to infinity it is useful to study a system where the result is known exactly. This will be done in the present note for a quantum-mechanical point particle in a one-dimensional box. The ground state energy of this system is known exactly, $E^{(0)} = \pi^2/2d^2$ (in natural units), where d is the size of the box. We shall demonstrate how this result is found via strong-coupling theory from a perturbation expansion, thus illustrating the reliability of the earlier membrane calculations [4,5].

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2. The partition function of a particle in a box is given by the Euclidean path integral (always in natural units)

$$Z = \int \mathscr{D} u(t) \mathrm{e}^{1/2 \int dt (\partial u)^2} \tag{1}$$

where the particle coordinate $u(t)$ is restricted to the interval $-d/2 \leq u(t) \leq d/2$. Since such a hard-wall restriction is hard to treat analytically in the path integral Eq. (1), we make the hard-walls soft by adding to the Euclidean action E in the exponent of Eq. (1) a potential term diverging near the walls. Thus we consider the auxiliary Euclidean action

$$E = \frac{1}{2} \int dt \left\{ \left[\partial u(t) \right]^2 + V(u(t)) \right\}, \tag{2}$$

where $V(u)$ is given by

$$V(u) = \frac{\omega^2}{2} \left(\frac{d}{\pi} \tan \frac{\pi u}{d} \right)^2 = \frac{\omega^2}{2} \left(u^2 + \frac{2}{3} g u^4 + \dots \right). \tag{3}$$

On the right-hand side we have introduced a parameter $g \equiv \pi^2/d^2$.

3. The expansion of the potential in powers of g can now be treated perturbatively, leading to an expansion of Z around the harmonic part of the partition function, in which the integrations over $u(t)$ run over the entire u-axis and yield

$$Z_\omega = \mathrm{e}^{-(1/2) \mathrm{Tr} \log (\partial^2 + \omega^2)}. \tag{4}$$

For $L \to \infty$, the exponent gives a free energy density $f = -L^{-1} \log Z$ equal to the ground state energy of the harmonic oscillator

$$f_0 = \frac{\omega}{2}. \tag{5}$$

The treatment of the interaction terms can be organized in powers of g, and give rise to an expansion of the free energy with the generic form

$$f = f_0 + \omega \sum_{k=1}^{\infty} a_k \left(\frac{g}{\omega} \right)^k. \tag{6}$$

The calculation of the coefficients a_k in this expansion proceeds as follows. First we expand the potential in Eq. (2) to identify the power series for the interaction energy

$$E^{\mathrm{int}} = \frac{\omega^2}{2} \int dt \left\{ g \varepsilon_4 u^4 + g^2 \varepsilon_6 u^6 + g^3 \varepsilon_8 u^8 + \dots \right\} = \frac{\omega^2}{2} \sum_{k=1}^{\infty} \int dt \, g^k \varepsilon_{2k+2} \left[u^2(t) \right]^{k+1}, \tag{7}$$

with coefficients

$$\begin{aligned}
&\varepsilon_4 = \frac{2}{3}, \quad \varepsilon_6 = \frac{17}{45}, \quad \varepsilon_8 = \frac{62}{315}, \quad \varepsilon_{10} = \frac{1382}{14175}, \quad \varepsilon_{12} = \frac{21844}{467775}, \quad \varepsilon_{14} = \frac{929569}{42567525}, \\
&\varepsilon_{16} = \frac{6404582}{638512875}, \quad \varepsilon_{18} = \frac{443861162}{97692469875}, \quad \varepsilon_{20} = \frac{18888466084}{9280784638125}, \quad \varepsilon_{22} = \frac{113927491862}{126109485376875}, \\
&\varepsilon_{24} = \frac{58870668456604}{147926426347074375}, \quad \varepsilon_{26} = \frac{8374643517010684}{48076088562799171875}, \quad \varepsilon_{28} = \frac{689005380505609448}{9086380738369043484375}, \\
&\varepsilon_{30} = \frac{129848163681107301953}{3952575621190533915703125}, \quad \varepsilon_{32} = \frac{173664079220990164722 2}{12252984425690655138679687 5}, \\
&\varepsilon_{34} = \frac{418781231495293038913922}{68739242628124575327993046875}, \dots .
\end{aligned} \tag{8}$$

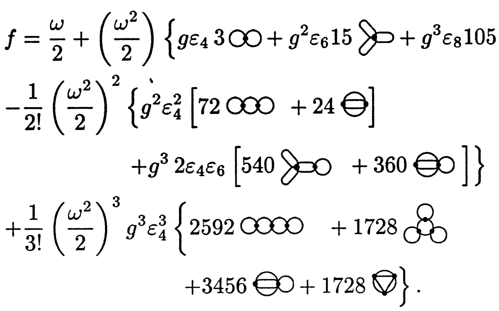
The interaction terms $\int dt\,[u^2(t)]^{k+1}$ and their products are expanded according to Wick's rule into sums of products of Wick contractions representing harmonic two-point correlation functions

$$\langle u(t_1)u(t_2)\rangle = \int \frac{dk}{2\pi}\frac{\mathrm{e}^{ik(t_1-t_2)}}{k^2+\omega^2} = \frac{\mathrm{e}^{-\omega|t_1-t_2|}}{2\omega}. \tag{9}$$

Associated local expectation values are $\langle u^2\rangle = 1/2\omega$, and

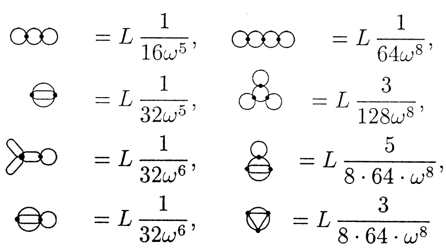
$$\langle u\partial u\rangle = \int \frac{dk}{2\pi}\frac{k}{k^2+\omega^2} = 0$$
$$\langle \partial u\partial u\rangle = \int \frac{dk}{2\pi}\frac{k^2}{k^2+\omega^2} = -\frac{\omega}{2}, \tag{10}$$

where the last integral is calculated using dimensional regularization in which $\int dk\,k^{\alpha}=0$ for all α. The Wick contractions are organized with the help of Feynman diagrams. Only the connected diagrams contribute to the free energy density. The graphical expansion of free energy up to four loops is



(11)

Note different numbers of loops contribute to the terms of order g^n. The calculation of the diagrams in Eq. (11) is simplified by the factorization property: If a diagram consists of two subdiagrams touching each other at a single vertex, the associated Feynman integral factorizes into those of the subdiagrams. In each diagram, the last t-integral yields an overall factor L, due to translational invariance along the t-axis, the others produce a factor $1/\omega$. Using the explicit expression Eq. (10) for the lines in the diagrams, we find the following values for the Feynman integrals:



(12)

Adding all contributions in reftextEq. (Eq. (11)), we obtain up to the order g^3:

$$f_3 = \omega\left\{\frac{1}{2} + \frac{3}{8}\varepsilon_4\left(\frac{g}{\omega}\right) + \left[\frac{15}{16}\varepsilon_6 - \frac{21}{32}\varepsilon_4^2\right]\left(\frac{g}{\omega}\right)^2 + \left[\frac{105}{32}\varepsilon_8 - \frac{45}{8}\varepsilon_4\varepsilon_6 + \frac{333}{128}\varepsilon_4^3\right]\left(\frac{g}{\omega}\right)^3\right\}, \tag{13}$$

which has the generic form (6). We can go to higher orders by extending the Bender–Wu recursion relation for the ground-state energy of the quartic anharmonic oscillator as follows:

$$2jC_{n,j}=(j+1)(2j+1)C_{n,j}-\frac{1}{2}\sum_{k=1}^{n}(-1)^{k}\varepsilon_{2k+2}C_{n-k},j-k-1-\sum_{k=1}^{n-1}C_{k,1}C_{n-k},j,\quad 1\le j\le 2n,$$
$$C_{0,0}=1,\quad C_{n,j}=0 \qquad (n\ge 1,j<1). \tag{14}$$

After solving these recursion relations, the coefficients a_k in Eq. (6) are given by $a_k=(-1)^{k+1}C_{k,1}$. For brevity, we list here the first sixteen expansion coefficients for f, calculated with the help of the algebra program REDUCE:

$$a_0=\frac{1}{2},\quad a_1=\frac{1}{4},\quad a_2=\frac{1}{16},\quad a_3=0,\quad a_4=-\frac{1}{256},\quad a_5=0,\quad a_6=\frac{1}{2048},\quad a_7=0,$$
$$a_8=-\frac{5}{65536},\quad a_9=0,\quad a_{10}=\frac{7}{524288},\quad a_{11}=0,\quad a_{12}=-\frac{21}{8388608},\quad a_{13}=0,$$
$$a_{14}=\frac{33}{67108864},\quad a_{15}=0,\quad a_{16}=-\frac{429}{4294967296},\ldots. \tag{15}$$

4. We are now ready to calculate successive strong-coupling approximations to the function $f(g)$. It will be convenient to remove the expected correct d dependence π^2/d^2 from $f(g)$, and study the function $\tilde{f}(\bar{g})\equiv f(g)/g$ which depemds only on the dimensionless reduced coupling constant $\bar{g}=g/\omega$. The limit $\omega\to 0$ corresponds to a strong-coupling limit in the reduced coupling constant $\bar{g}$. According to the general theory in Refs. [2,1], the Nth order approximation to the strong-coupling limit of $\tilde{f}(\bar{g})$, to be denoted by $\tilde{f}^*$, is found by replacing, in the series truncated after the Nth term, $\tilde{f}_N(g/\omega)$, the frequency ω by the identical expression $\sqrt{\Omega^2-rg}$, where $r\equiv(\Omega^2-\omega^2)/g$. For a moment, this is treated as an independent variable, whereas Ω is a dummy parameter. Then the square root is expanded binomially in powers of g, and $\tilde{f}_N(g)$ is re-expanded up to order g^N. After that, r is replaced by its proper value. In this way we obtain a function $\tilde{f}_N(g,\Omega)$ which depends on Ω, which thus becomes a variational parameter. The best approximation is obtained by extremizing $\tilde{f}_N(g,\Omega)$ with respect to ω. Setting $\omega=0$, we go to the strong-coupling limit $\bar{\to}\infty$. There the optimal Ω grows proportionally to g, so that $g/\Omega=1/c$ is finite, and the variational expression $\tilde{f}_N(g,\Omega)$ becomes a function of $\tilde{f}_N(1/c)$. In this limit, the above reexpansion amounts simply to replacing each power ω^n in each expansion terms of $\tilde{f}_N(\bar{g})$ by the binomial expansion of $(1-1)^{-n/2}$ truncated after the $(N-n)$th term, and replacing $\bar{g}$ by $1/c$. The first nine variational functions $\tilde{f}_N(1/c)$ are listed in Table 1. The functions $\tilde{f}_N(1/c)$ are minimized

Table 1
First eight variational functions $\tilde{f}_N(1/c)$

$\tilde{f}_2(1/c)=\frac{1}{4}+\frac{1}{16c}+\frac{3c}{16}$
$\tilde{f}_3(1/c)=\frac{1}{4}+\frac{3}{32c}+\frac{5c}{32}$
$\tilde{f}_4(1/c)=\frac{1}{4}-\frac{1}{256c^3}+\frac{15}{128c}+\frac{35c}{256}$
$\tilde{f}_5(1/c)=\frac{1}{4}-\frac{5}{512c^3}+\frac{35}{256c}+\frac{63c}{512}$
$\tilde{f}_6(1/c)=\frac{1}{4}+\frac{1}{2048c^5}-\frac{35}{2048c^3}+\frac{315}{2048c}+\frac{231c}{2048}$
$\tilde{f}_7(1/c)=\frac{1}{4}+\frac{7}{4096c^5}-\frac{105}{4096c^3}+\frac{693}{4096c}+\frac{429c}{4096}$
$\tilde{f}_8(1/c)=\frac{1}{4}-\frac{5}{65536c^7}+\frac{63}{16384c^5}-\frac{1155}{32768c^3}+\frac{3003}{16384c}+\frac{6435c}{65536}$
$\tilde{f}_9(1/c)=\frac{1}{4}-\frac{45}{131072c^7}+\frac{231}{32768c^5}-\frac{3003}{65536c^3}+\frac{6435}{32768c}+\frac{12155c}{131072}$

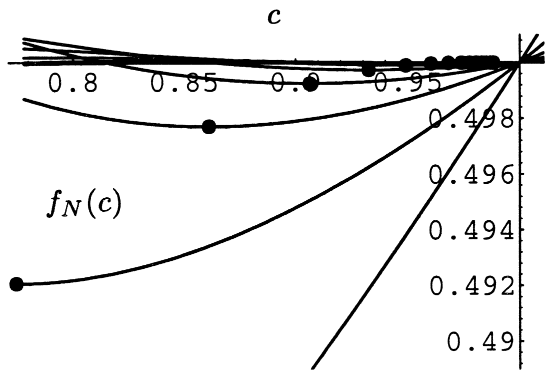


Fig. 1. Variational functions $\tilde{f}_N(1/c)$ up to $N=16$ are shown together with their minima whose y-coordinates approach rapidly the correct limiting value $1/2$.

starting from $\tilde{f}_2(1/c)$ and searching the minimum of each successive $\tilde{f}_3(1/c)$, $\tilde{f}_3(1/c),\dots$ nearest to the previous one. The functions $\tilde{f}_N(1/c)$ together with their minima are plotted in Fig. 1. The minima lie at

$$\begin{aligned}\left(N,\tilde{f}_N^{\min}\right) &= (2,0.466506),(3,0.492061),(4,0.497701),(5,0.499253),(6,0.499738),(7,0.499903),\\ &(8,0.499963),(9,0.499985),(10,0.499994),(11,0.499998),(12,0.499999),\\ &(13,0.5000),(14,0.50000),(15,0.50000),(16,0.5000). \end{aligned} \tag{16}$$

They converge exponentially fast against the known result $1/2$, as shown in Fig. 2.

5. The alert reader will have noted that the expansion coefficients (15) possesses two special properties: First, they lack the factorial growth at large orders which would be found for a single power $[u^2(t)]^{k+1}$ of the interaction potential [6]. The factorial growth is canceled by the specific combination of the different powers in the interaction (7), making the series (6) convergent inside a certain circle. Still, since this circle is has a finite radius (the ratio test shows that it is unity), this convergent series cannot be evaluated in the limit of large g which we want to do, so that variational strong-coupling theory is not superfluous. However, there is a second remarkable property of the coefficients (15): They contain an infinite number of zeros in the sequence of

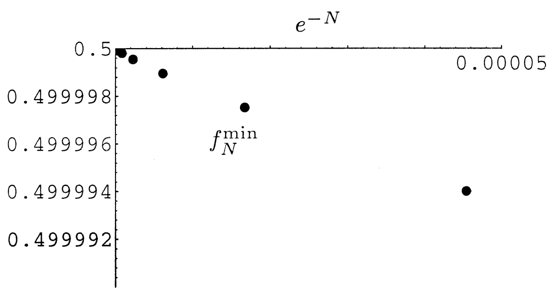


Fig. 2. Exponentially fast convergence of the strong-coupling approximations towards the exact value.

coefficients for each odd number, except for the first one. We may take advantage of this property by separating off the irregular term $a_1 g = g/4 = \pi^2/4d^2$, setting $\alpha = g^2/4\omega^2$, and rewriting $\tilde{f}(\bar{g})$ as

$$\tilde{f}(\alpha) = \frac{1}{4}\left[1 + \frac{1}{\sqrt{\alpha}} h(\alpha)\right], \quad h(\alpha) \equiv \sum_{n=0}^{N} 2^{2n+1} a_{2n} \alpha^n. \tag{17}$$

Inserting the numbers (Eq. (15)), the expansion of $h(\alpha)$ reads

$$h(\alpha) = 1 + \frac{\alpha}{2} - \frac{\alpha^2}{8} + \frac{\alpha^3}{16} - \frac{5}{128}\alpha^4 + \frac{7}{256}\alpha^5 - - \frac{21}{1024}\alpha^6 + \frac{33}{2048}\alpha^7 - \frac{429}{32768}\alpha^8 + \dots . \tag{18}$$

We now realize that this is the binomial power series expansion of $\sqrt{1+\alpha}$. Substituting this into Eq. (17), we find the exact ground state energy for the Euclidean action (Eq. (2))

$$E^{(0)} = \frac{\pi^2}{4d^2}\left(1 + \sqrt{1 + \frac{1}{\alpha}}\right) = \frac{\pi^2}{4d^2}\left(1 + \sqrt{1 + 4\omega^2 \frac{d^4}{\pi^4}}\right). \tag{19}$$

Here we can go directly to the strong-coupling limit $\alpha \to \infty$ to recover the exact ground-state energy $E^{(0)} = \pi^2/2d^2$.

6. The energy (9) can of course be obtained directly by solving the Schrödinger equation associated with the potential (7)

$$\frac{1}{2}\left\{-\frac{\partial^2}{\partial x^2} + \left[\frac{\lambda(1-\lambda)}{\cos^2 x} - 1\right]\right\}\psi(x) = \frac{d^2}{\pi^2} E\psi(x), \tag{20}$$

where we have replaced $u \to dx/\pi$ and set $\omega^2 d^4/\pi^4 \equiv \lambda(\lambda - 1)$, so that

$$\lambda = \frac{1}{2}\left(1 + \sqrt{1 + 4\omega^2 \frac{d^4}{\pi^4}}\right). \tag{21}$$

Eq. (20) is of the Pöschl–Teller type and has the ground state wave function [7]

$$\psi_0(x) = \text{const} \cdot \cos^{\lambda} x, \tag{22}$$

with the eigenvalue $\pi^2 E^{(0)}/d^2 = (\lambda^2 - 1)/2$, which agrees of course with Eq. (19).

If we were to apply the variational procedure to the series $h(\alpha)/\sqrt{\alpha}$ in f of Eq. (19), by replacing the factor $1/\omega^{2n}$ contained in each power α^n by $\Omega = \sqrt{\Omega^2 - r\alpha}$ and reexpanding now in powers of α rather than g, we would find that all approximation $h_N(1/c)$ would posses a minimum with unit value, such that the corresponding extremal functions $\tilde{f}_N(1/c)$ yield the correct final energy in *each* order N.

7. With the exact result being known, let us calculate the exponential approach of the variational approximations obeserved in Fig. 2. Let us write the exact energy (19) as

$$E^{(0)} = \frac{1}{4}\left(g + \sqrt{g^2 + 4\omega^2}\right), \tag{23}$$

After the replacement $\omega \to \sqrt{\Omega^2 - rg}$, this becomes

$$E^{(0)} = \frac{\Omega}{4}\left(\hat{g} + \sqrt{\hat{g}^2 - 4r\hat{g} + 4}\right). \tag{24}$$

where $\hat{g} \equiv g/\Omega^2$. The Nth-order approximant $f_N(g)$ of $E^{(0)}$ is obtained by expanding (Eq. (24)) in powers of $\hat{g}$ up to order N,

$$f_N(g) = \Omega \sum_0^N h_k(r)\,\hat{g}^k, \tag{25}$$

and substituting r by $(1-\hat{\omega}^2)/\hat{g}$, with $\hat{\omega}^2 \equiv \omega^2/\Omega^2$. The resulting function of $\hat{g}$ is then optimized.

It is straightforward to find an integral representation for $f_N((g)$. Setting $r\hat{g} \equiv z$, we have

$$f_N = \frac{1}{2\pi i}\oint_{C_0} \frac{dz}{z^{N+1}} \frac{1-z^{N+1}}{1-z} f(z), \tag{26}$$

where the contour C_0 refers to small circle around the origin and

$$f(z) = \frac{\Omega}{4}\left(\frac{z}{r} + \sqrt{\frac{z^2}{r^2} - 4z + 4} \right) = \frac{1}{4r}\left(z + \sqrt{(z-z_1)(z-z_2)} \right), \tag{27}$$

with branch points at $z_{1,2} = 2r^2\left(1 \pm \sqrt{1-1/r^2}\right)$. For $z<1$, we rewrite

$$1 - z^{N+1} = (1-z)(1+z+\ldots+z^N) = (1-z)(N+1) - (1-z)^2\left[N + (N-1)z + \ldots + z^{N-1}\right] \tag{28}$$

and estimate this for $z \approx 1$ as

$$1 - z^{N+1} = (1-z)(N+1) + \mathscr{O}\left(|1-z|^2 N^2\right). \tag{29}$$

With (28), divided the approximant (26) divided by Ω, indicated by a hat, becomes the sum of the discontinuities across each branch cut

$$\hat{f}_N = \frac{(N+1)}{2\pi i}\oint_{C_0} \frac{dz\hat{f}(z)}{z^{N+1}} \hat{f}(z) = \frac{(N+1)}{N!}\hat{f}^{(N)}(0) = (N+1)\sum_{i=1}^{2}\int_{z_i}^{\infty} \frac{dz}{z^{N+1}} \hat{f}(z) \tag{30}$$

The integral over the cuts in $f(z)$ yields a constant plus a product

$$\Delta \hat{f}_N \approx \frac{(N+1)(N-3/2)!}{N!} \frac{1}{(r^2)^N} \frac{1}{(1+r^2)^N}, \tag{31}$$

which for large N can be approximated by

$$\Delta \hat{f}_N \approx \frac{A}{(r^2)^N \sqrt{N}} \mathrm{e}^{-r^2 N}. \tag{32}$$

In the strong-coupling limit of interest here, $\hat{\omega}^2 = 0$, and $r = 1/\hat{g} = \Omega/g = c$. In Fig. 1 we see that the optimal c-values tend to unity for $N \to \infty$, so that $\Delta \hat{f}_N$ goes to zero like e^{-N}, as observed in Fig. 2.

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