Smearing formula for higher-order effective classical potentials

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Abstract. In the variational approach to quantum statistics, a smearing formula efficiently describes the consequences of quantum fluctuations upon an interaction potential. The result is an effective classical potential from which the partition function can be obtained by a simple integral. In this work, the smearing formula is extended to higher orders in the variational perturbation theory. An application to the singular Coulomb potential exhibits the same fast convergence with increasing orders that has been observed in previous variational perturbation expansions of the anharmonic oscillator with quartic potential.

1. Introduction

The variational approach to quantum statistics, initially based on the Jensen–Peierls inequality for imaginary-time path integrals [1, 2], yields upper bounds for the free energy of many quantum mechanical systems at all temperatures and coupling strengths, which are often quite close to the exact results. By abandoning the inequality, the approach has been extended to a systematic variational perturbation theory [3], in which the original approach is just a first-order approximation. Detailed calculations [4–6] and extensions [7–9], showed an exponentially fast convergence of this systematic theory, which was recently explained [10]. Thermodynamic and some local quantities can now be evaluated to any desired accuracy, starting out from an ordinary perturbation expansion of arbitrary order.

A particularly attractive feature of the original variational approach was the existence of a smearing formula in the form of a Gaussian convolution integral which compactly accounts for the effect of quantum fluctuations upon the interaction potential and other local quantities [2, 9]. This formula was applicable to some classes of singular potentials such as the Coulomb potential [9, 11]. There is a definite need for such a formula in higher orders of variational perturbation theory, which so far has been based on Feynman diagrams, thus being limited to polynomial interactions. The purpose of this paper is to derive the desired higher-order smearing formula. This will be done in section 3 after a brief review of variational perturbation theory in section 2. An application to the Coulomb potential is given in section 4, where the effective classical potential is calculated to second order in the variational perturbation theory. Its zero-temperature limit yields in section 5 a variational perturbation expansion for the ground-state energy up to second order. Section 6 reproduces this result by a direct variational treatment of the Rayleigh–Schrödinger perturbation expansion, and carries it to third order to demonstrate the fast convergence of the variational perturbation expansion.

2. Review of variational perturbation theory

Consider a quantum mechanical point particle of mass M moving in a one-dimensional time-independent potential $V(x)$. Its thermodynamic partition function is given by the imaginary-time path integral [9]

$$Z = \oint \mathcal{D}x(\tau) \exp\left\{-\frac{1}{\hbar}\mathcal{A}[x(\tau)]\right\} \tag{1}$$

with the Euclidean action

$$\mathcal{A}[x(\tau)] = \int_0^{\hbar\beta} d\tau \left[\frac{M}{2}\dot{x}(\tau)^2 + V(x(\tau))\right] \tag{2}$$

and the abbreviation $\beta \equiv 1/k_B T$. The paths $x(\tau)$ satisfy the periodic boundary condition $x(0) = x(\hbar\beta)$. Following Feynman [1], we decompose the path integral for the partition function (1) into an ordinary integral over the time-averaged position

$$x_0 = \bar{x} \equiv \frac{1}{\hbar\beta}\int_0^{\hbar\beta} d\tau\, x(\tau) \tag{3}$$

and a remaining path integral over the fluctuations

$$\delta x(\tau) = x(\tau) - x_0 \tag{4}$$

around x_0. Thus we rewrite (1) as an integral

$$Z = \int_{-\infty}^{+\infty} \tilde{d}x_0\, Z^{x_0} \tag{5}$$

over a *local partition function* Z^{x_0} which is defined by the restricted path integral

$$Z^{x_0} \equiv \oint \mathcal{D}x(\tau)\tilde{\delta}(\bar{x} - x_0) \exp\left\{-\frac{1}{\hbar}\mathcal{A}[x(\tau)]\right\} \tag{6}$$

with the notation

$$\tilde{d}x_0 \equiv \sqrt{\frac{M}{2\pi\hbar^2\beta}}\, dx_0 \qquad \tilde{\delta}(\bar{x} - x_0) \equiv \sqrt{\frac{2\pi\hbar^2\beta}{M}}\delta(\bar{x} - x_0). \tag{7}$$

The free energy associated with the local partition function (6) is defined as the *effective classical potential* [9]

$$V^{\mathrm{eff,cl}}(x_0) = -\frac{1}{\beta}\log Z^{x_0} \tag{8}$$

which accounts for the effects of all quantum fluctuations.

In order to calculate $V^{\mathrm{eff,cl}}(x_0)$, we decompose the Euclidean action (2) into a sum

$$\mathcal{A}[x(\tau)] = \mathcal{A}_\Omega^{x_0}[x(\tau)] + \mathcal{A}_{\mathrm{int}}^{x_0}[x(\tau)] \tag{9}$$

where the first term is the action of a harmonic oscillator centred around x_0 with an undetermined local *trial frequency* $\Omega(x_0)$,

$$\mathcal{A}_\Omega^{x_0}[x(\tau)] = \int_0^{\hbar\beta} d\tau \left\{\frac{M}{2}\dot{x}(\tau)^2 + \frac{M}{2}\Omega^2(x_0)[x(\tau) - x_0]^2\right\} \tag{10}$$

and the second term is the remaining interaction

$$\mathcal{A}_{\mathrm{int}}^{x_0}[x(\tau)] = \int_0^{\hbar\beta} d\tau\, V_{\mathrm{int}}^{x_0}(x(\tau)) \tag{11}$$

of the potential difference

$$V_{\text{int}}^{x_0}(x) = V(x) - \frac{M}{2}\Omega^2(x_0)(x - x_0)^2. \tag{12}$$

With this decomposition, the local partition function (6) may be expanded in powers of the interaction potential (12) around the local harmonic partition function

$$Z_{\Omega}^{x_0} = \oint \mathcal{D}x(\tau)\,\tilde{\delta}(\bar{x} - x_0)\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\Omega}^{x_0}[x(\tau)]\right\}. \tag{13}$$

The expansion reads

$$Z^{x_0} = Z_{\Omega}^{x_0}\left\{1 - \frac{1}{\hbar}\int_0^{\hbar\beta}d\tau_1\,\langle V_{\text{int}}^{x_0}(x(\tau_1))\rangle_{\Omega}^{x_0} + \frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\,\langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))\rangle_{\Omega}^{x_0}\right.$$
$$\left. -\frac{1}{6\hbar^3}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\int_0^{\hbar\beta}d\tau_3\,\langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))V_{\text{int}}^{x_0}(x(\tau_3))\rangle_{\Omega}^{x_0} + \cdots\right\} \tag{14}$$

where the x_0-dependent expectation values $\langle F_1(x(\tau_1))\ldots F_n(x(\tau_n))\rangle_{\Omega}^{x_0}$ are correlation functions of the local harmonic trial system:

$$\langle F_1(x(\tau_1))\ldots F_n(x(\tau_n))\rangle_{\Omega}^{x_0} = \frac{1}{Z_{\Omega}^{x_0}}\oint \mathcal{D}x(\tau)\,F_1(x(\tau_1))\ldots F_n(x(\tau_n))\tilde{\delta}(\bar{x} - x_0)$$
$$\times \exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\Omega}^{x_0}[x(\tau)]\right\}. \tag{15}$$

The correlation functions can be decomposed into connected ones via the standard cumulant expansion [9, 12], yielding for the effective classical potential $V^{\text{eff,cl}}(x_0)$ the following perturbation expansion [9]

$$V^{\text{eff,cl}}(x_0) = F_{\Omega}^{x_0} + \frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau_1\,\langle V_{\text{int}}^{x_0}(x(\tau_1))\rangle_{\Omega}^{x_0}$$
$$-\frac{1}{2\hbar^2\beta}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\,\langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))\rangle_{\Omega,c}^{x_0}$$
$$+\frac{1}{6\hbar^3\beta}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2\int_0^{\hbar\beta}d\tau_3\,\langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))V_{\text{int}}^{x_0}(x(\tau_3))\rangle_{\Omega,c}^{x_0}$$
$$+\cdots. \tag{16}$$

The first term on the right-hand side is the free energy of the local harmonic partition function

$$F_{\Omega}^{x_0} \equiv -\frac{1}{\beta}\log Z_{\Omega}^{x_0} = \frac{1}{\beta}\log\frac{\sinh\hbar\beta\Omega(x_0)/2}{\hbar\beta\Omega(x_0)/2}. \tag{17}$$

The second term contains the local harmonic expectation value of the potential for which there exists the above mentioned smearing formula which we want to extend in this work. The cumulant in the third term is given by the following combination of expectation values:

$$\langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))\rangle_{\Omega,c}^{x_0} = \langle V_{\text{int}}^{x_0}(x(\tau_1))V_{\text{int}}^{x_0}(x(\tau_2))\rangle_{\Omega}^{x_0} - \langle V_{\text{int}}^{x_0}(x(\tau_1))\rangle_{\Omega}^{x_0}\langle V_{\text{int}}^{x_0}(x(\tau_2))\rangle_{\Omega}^{x_0}. \tag{18}$$

By construction, the effective classical potential $V^{\text{eff,cl}}(x_0)$ in (16) does not depend on the choice of the frequency $\Omega(x_0)$ in the trial action (10). However, when truncating the infinite sum (16) after the Nth order, we obtain an approximation $W_N^{\Omega}(x_0)$ for the effective classical potential $V^{\text{eff,cl}}(x_0)$ with an $\Omega(x_0)$-dependence, which decreases with

increasing order N of the expansion. With the expectation that the optimal truncated sum $W_N^\Omega(x_0)$ depends minimally on the frequency $\Omega(x_0)$, we therefore determine $\Omega(x_0)$ from the extremality condition

$$\frac{\partial W_N^\Omega(x_0)}{\partial \Omega(x_0)} = 0. \tag{19}$$

If this has no solution, we demand as the next-best condition of minimal dependence on $\Omega(x_0)$ [3, 5, 8, 9]

$$\frac{\partial^2 W_N^\Omega(x_0)}{\partial \Omega^2(x_0)} = 0. \tag{20}$$

The result is called the *optimal frequency* $\Omega_N(x_0)$ of order N. It yields the truncated sum $W_N(x_0) \equiv W_N^{\Omega_N(x_0)}(x_0)$ which represents the desired Nth-order approximation to the effective classical potential $V^{\text{eff,cl}}(x_0)$. The first-order approximation $W_1(x_0)$ coincides with the original variational result of Feynman and Kleinert [2] which satisfies the Jensen–Peierls inequality and guarantees the existence of an extremum (19).

The accuracy of the approximate effective classical potential $W_N(x_0)$ can be assessed by the following considerations [9]. In the limit of high temperatures where $\beta \to 0$, the approximation $W_N(x_0)$ becomes exact for any N:

$$\lim_{\beta \to 0} W_N(x_0) = V(x_0). \tag{21}$$

At low temperatures, where $\beta \to \infty$, we obtain from (5) and (8) an approximation to the free energy in form of an integral over the time-averaged position x_0

$$F_N = -\frac{1}{\beta} \log \left\{ \int_{-\infty}^{+\infty} \tilde{\mathrm{d}}x_0 \, \exp[-\beta W_N(x_0)] \right\} \tag{22}$$

whose integrand is centred sharply around the minimum $x_N^{\min}$ of $W_N(x_0)$. Performing this integral in the saddle-point approximation yields an Nth-order approximation $E_N^{(0)}$ for the ground-state energy $E^{(0)}$ of the quantum system.

$$E_N^{(0)} = \min_{x_0} \lim_{\beta \to \infty} W_N(x_0). \tag{23}$$

The same approximation to the ground-state energy can also be obtained by a variational resummation [9] of the Rayleigh–Schrödinger perturbation series for $E^{(0)}$. This will be shown in section 6 for the ground-state energy of the Coulomb potential up to the order $N = 2$.

3. Evaluation of path integrals

In order to calculate the different terms in the variational perturbation expansion (16), we must find efficient formulae for evaluating local correlation functions of type (15). For this we observe that, by fixing the temporal average at $\bar{x} = x_0$ in the path integral, the zero Matsubara frequency $\omega_0 = 0$ is removed from the Fourier decomposition of the periodic paths

$$x(\tau) = x_0 + \sum_{m=1}^{\infty} (x_m \mathrm{e}^{\mathrm{i}\omega_m \tau} + x_m^* \mathrm{e}^{-\mathrm{i}\omega_m \tau}) \qquad \omega_m = 2\pi m / \hbar \beta. \tag{24}$$

In fact, the restricted integration measure $\oint \mathcal{D}x(\tau)\tilde{\delta}(\bar{x} - x_0)$ in (15) may be decomposed into a product of ordinary integrals over real and imaginary parts x_m^{re} and x_m^{im} of the Fourier components x_m according to [9]:

$$\oint \mathcal{D}x(\tau)\tilde{\delta}(\bar{x} - x_0) = \prod_{m=1}^{\infty} \left(\int_{-\infty}^{+\infty} dx_m^{\text{re}} \int_{-\infty}^{+\infty} dx_m^{\text{im}} \frac{\beta M \omega_m^2}{\pi} \right). \tag{25}$$

The zero-frequency component x_0 remains unintegrated. With this decomposition, the basic local pair correlation function of the fluctuations $\delta x(\tau)$ in (4) can immediately be calculated from (15) as a Matsubara sum without the zero mode:

$$G_\Omega^{x_0}(\tau, \tau') \equiv \langle \delta x(\tau)\delta x(\tau')\rangle_\Omega^{x_0} = \frac{2}{M\beta} \sum_{m=1}^{\infty} \frac{\cos \omega_m(\tau - \tau')}{\omega_m^2 + \Omega^2(x_0)}. \tag{26}$$

Performing the sum yields the explicit result

$$G_\Omega^{x_0}(\tau, \tau') = \frac{\hbar}{2M\Omega(x_0)} \left\{ \frac{\cosh[\Omega(x_0)|\tau - \tau'| - \hbar\beta\Omega(x_0)/2]}{\sinh[\hbar\beta\Omega(x_0)/2]} - \frac{2}{\hbar\beta\Omega(x_0)} \right\}. \tag{27}$$

The first term is the ordinary oscillator correlation function of frequency Ω

$$G_\Omega(\tau, \tau') \equiv \langle x(\tau)x(\tau')\rangle_\Omega = \frac{1}{M\beta} \sum_{m=-\infty}^{\infty} \frac{\cos \omega_m(\tau - \tau')}{\omega_m^2 + \Omega^2(x_0)} \tag{28}$$

while the last term subtracts the zero mode which is absent in (26). This absence has the important consequence that

$$\int_0^{\hbar\beta} d\tau \, G_\Omega^{x_0}(\tau, \tau') = 0. \tag{29}$$

Using (27), the expectation values in (15) can easily be calculated for a polynomial potential using Wick's contraction rules, by which the expectation values can be reduced to sums over products of pair correlation functions $G_\Omega^{x_0}(\tau, \tau')$. In order to abbreviate the notation and to emphasize the dimension (length)^2 of these quantities, we shall denote the local Green functions in (27) from now on by $a_{\tau\tau'}^2(x_0)$. The harmonic expectation value of any odd power n in the fluctuation variable $\delta x(\tau)$ is zero. For even n, the Wick expansion reads

$$\left\langle \prod_{k=1}^{n} \delta x(\tau_k) \right\rangle_\Omega^{x_0} = \sum_P a_{\tau_{P(1)}\tau_{P(2)}}^2(x_0) \dots a_{\tau_{P(n-1)}\tau_{P(n)}}^2(x_0) \tag{30}$$

where the sum runs over all $(n-1)!!$ pair contractions. For an exponential, Wick's rule implies

$$\left\langle \exp\left[i \int_0^{\hbar\beta} d\tau \, j(\tau)\delta x(\tau) \right] \right\rangle_\Omega^{x_0} = \exp\left[-\frac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \, j(\tau)a_{\tau\tau'}^2(x_0)j(\tau') \right]. \tag{31}$$

In the special case $j(\tau) = \sum_{k=1}^{n} u_k\delta(\tau - \tau_k)$, we obtain the important formula for the expectation value of a product of exponentials

$$\left\langle \prod_{k=1}^{n} e^{iu_k\delta x(\tau_k)} \right\rangle_\Omega^{x_0} = \exp\left[-\frac{1}{2} \sum_{k=1}^{n} \sum_{k'=1}^{n} u_k a_{\tau_k\tau_{k'}}^2(x_0)u_{k'} \right]. \tag{32}$$

After Fourier-decomposing the functions $F_1(x), \ldots, F_n(x)$ in (15), formula (32) yields directly the desired smearing formula [13]

$$\langle F_1(x(\tau_1)) \ldots F_n(x(\tau_n)) \rangle_\Omega^{x_0} = \left[\prod_{k=1}^{n} \int_{-\infty}^{+\infty} dx_k \, F_k(x_k) \right] \frac{1}{\sqrt{(2\pi)^n \mathrm{Det}[a^2_{\tau_k \tau_{k'}}(x_0)]}}$$

$$\times \exp\left[-\frac{1}{2} \sum_{k=1}^{n} \sum_{k'=1}^{n} \delta x_k \, a^{-2}_{\tau_k \tau_{k'}}(x_0) \delta x_{k'} \right] \tag{33}$$

where $a^{-2}_{\tau_k \tau_{k'}}(x_0)$ denotes the inverse of the symmetric $n \times n$ matrix $a^2_{\tau_k \tau_{k'}}(x_0)$. This smearing formula determines the different harmonic expectation values in the variational perturbation expansion (16) as convolutions with Gaussian functions.

For $n = 1$, the smearing formula (33) reduces to the previous one [2, 9]

$$\langle F_1(x(\tau_1)) \rangle_\Omega^{x_0} = \int_{-\infty}^{+\infty} dx_1 \, F_1(x_1) \frac{1}{\sqrt{2\pi a^2(x_0)}} \exp\left[-\frac{(x_1 - x_0)^2}{2a^2(x_0)} \right] \tag{34}$$

where $a^2(x_0)$ denotes the τ-independent diagonal matrix element $a^2_{\tau\tau}(x_0)$. For polynomials $F_1(x)$, the smearing formula (33) reproduces Wick's rule: odd powers in $\delta x(\tau)$ have vanishing local correlation functions, whereas even powers result in (30), which for coinciding times τ_k reduces to

$$\langle [\delta x(\tau_k)]^n \rangle_\Omega^{x_0} = (n-1)!! a^n(x_0). \tag{35}$$

For two functions $F_1(x)$ and $F_2(x)$, our smearing formula (33) reads, more explicitly,

$$\langle F_1(x(\tau_1)) F_2(x(\tau_2)) \rangle_\Omega^{x_0} = \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 \, F_1(x_1) F_2(x_2) \frac{1}{\sqrt{(2\pi)^2 [a^4(x_0) - a^4_{\tau_1\tau_2}(x_0)]}}$$

$$\times \exp\left\{ -\frac{a^2(x_0)(x_1 - x_0)^2 - 2a^2_{\tau_1\tau_2}(x_0)(x_1 - x_0)(x_2 - x_0) + a^2(x_0)(x_2 - x_0)^2}{2[a^4(x_0) - a^4_{\tau_1\tau_2}(x_0)]} \right\}. \tag{36}$$

Specializing $F_2(x)$ to the square of the function δx, we obtain the useful rule

$$\langle F_1(x(\tau_1))[\delta x(\tau_2)]^2 \rangle_\Omega^{x_0} = a^2(x_0) \left[1 - \frac{a^4_{\tau_1\tau_2}(x_0)}{a^4(x_0)} \right] \langle F_1(x(\tau_1)) \rangle_\Omega^{x_0}$$

$$+ \frac{a^4_{\tau_1\tau_2}(x_0)}{a^4(x_0)} \langle F_1(x(\tau_1))[\delta x(\tau_1)]^2 \rangle_\Omega^{x_0} \tag{37}$$

which reduces the smearing procedure for different times τ_1 and τ_2 to corresponding ones at equal times $\tau_1 = \tau_2$. With this we immediately yield, for instance,

$$\langle [\delta x(\tau_1)]^2 [\delta x(\tau_2)]^2 \rangle_\Omega^{x_0} = a^4(x_0) + 2a^4_{\tau_1\tau_2}(x_0). \tag{38}$$

In three dimensions, the trial potential contains a 3×3 frequency matrix Ω_{ij} depending on the time-averaged position $\boldsymbol{x}_0$ and reads

$$\frac{M}{2} \sum_{i,j=1}^{3} \Omega^2_{ij}(\boldsymbol{x}_0)(x_i - x_{0i})(x_j - x_{0j}) \tag{39}$$

while the interaction potential (12) becomes

$$V_{\mathrm{int}}^{\boldsymbol{x}_0}(\boldsymbol{x}) = V(\boldsymbol{x}) - \frac{M}{2} \sum_{i,j=1}^{3} \Omega^2_{ij}(\boldsymbol{x}_0)(x_i - x_{0i})(x_j - x_{0j}). \tag{40}$$

Assuming the potential to depend only on $r = |\boldsymbol{x}|$, i.e. $V(\boldsymbol{x}) = v(r)$, the frequency matrix possesses only two invariant matrix elements, a longitudinal one $\Omega_L(r_0)$ and a transversal one $\Omega_T(r_0)$ [9, 11]. The interaction potential (40) can then be decomposed into a longitudinal and a transversal part according to

$$\Omega_{ij}^2(\boldsymbol{x}_0) = \Omega_L^2(r_0)\frac{x_{0i}x_{0j}}{r_0^2} + \Omega_T^2(r_0)\left(\delta_{ij} - \frac{x_{0i}x_{0j}}{r_0^2}\right) \tag{41}$$

so that (40) may be rewritten as

$$V_{\text{int}}^{\boldsymbol{x}_0}(\boldsymbol{x}) = v(r) - \frac{M}{2}\{\Omega_L^2(r_0)[\delta\boldsymbol{x}]_L^2 + \Omega_T^2(r_0)[\delta\boldsymbol{x}]_T^2\} \tag{42}$$

with obvious definitions of the longitudinal and transverse projections $\delta\boldsymbol{x}_L$ and $\delta\boldsymbol{x}_T$ of the fluctuations $\delta\boldsymbol{x}$.

To first order, the anisotropic generalization of the smearing formula (34) reads [9, 11]

$$\langle F_1(\boldsymbol{x}(\tau_1))\rangle_{\Omega_T,\Omega_L}^{r_0} = \int_{-\infty}^{+\infty} d^3x_1\, F_1(\boldsymbol{x}_1)\frac{1}{\sqrt{(2\pi)^3 a_T^4 a_L^2}}\exp\left\{-\frac{\boldsymbol{x}_{1T}^2}{2a_T^2} - \frac{(x_{1L}-r_0)^2}{2a_L^2}\right\}. \tag{43}$$

For the squares of transverse and longitudinal fluctuations, this generalizes (35) with $n = 2$ to

$$\langle[\delta\boldsymbol{x}(\tau_1)]_T^2\rangle_{\Omega_T,\Omega_L}^{r_0} = 2a_T^2 \qquad \langle[\delta\boldsymbol{x}(\tau_1)]_L^2\rangle_{\Omega_T,\Omega_L}^{r_0} = a_L^2. \tag{44}$$

The second-order smearing formula (36) becomes in three dimensions

$$\langle F_1(\boldsymbol{x}(\tau_1))F_2(\boldsymbol{x}(\tau_2))\rangle_{\Omega_T,\Omega_L}^{r_0} = \int_{-\infty}^{+\infty} d^3x_1 \int_{-\infty}^{+\infty} d^3x_2\, F_1(\boldsymbol{x}_1)F_2(\boldsymbol{x}_2)$$

$$\times \frac{1}{(2\pi)^3(a_T^4 - a_{T\tau_1\tau_2}^4)\sqrt{a_L^4 - a_{L\tau_1\tau_2}^4}}$$

$$\times \exp\left\{-\frac{a_T^2\boldsymbol{x}_{1T}^2 - 2a_{T\tau_1\tau_2}^2\boldsymbol{x}_{1T}\boldsymbol{x}_{2T} + a_T^2\boldsymbol{x}_{2T}^2}{2(a_T^4 - a_{T\tau_1\tau_2}^4)}\right\}$$

$$\times \exp\left\{-\frac{a_L^2(x_{1L}-r_0)^2 - 2a_{L\tau_1\tau_2}^2(x_{1L}-r_0)(x_{2L}-r_0) + a_L^2(x_{2L}-r_0)^2}{2(a_L^4 - a_{L\tau_1\tau_2}^4)}\right\} \tag{45}$$

so that the rule (37) for expectation values is generalized to

$$\langle F_1(\boldsymbol{x}(\tau_1)[\delta\boldsymbol{x}(\tau_2)]_T^2\rangle_{\Omega_T,\Omega_L}^{r_0} = 2a_T^2\left[1 - \frac{a_{T\tau_1\tau_2}^4}{a_T^4}\right]\langle F_1(\boldsymbol{x}(\tau_1))\rangle_{\Omega_T,\Omega_L}^{r_0}$$

$$+ \frac{a_{T\tau_1\tau_2}^4}{a_T^4}\langle F_1(\boldsymbol{x}(\tau_1))[\delta\boldsymbol{x}(\tau_1)]_T^2\rangle_{\Omega_T,\Omega_L}^{r_0} \tag{46}$$

$$\langle F_1(\boldsymbol{x}(\tau_1)[\delta\boldsymbol{x}(\tau_2)]_L^2\rangle_{\Omega_T,\Omega_L}^{r_0} = a_L^2\left[1 - \frac{a_{L\tau_1\tau_2}^4}{a_L^4}\right]\langle F_1(\boldsymbol{x}(\tau_1))\rangle_{\Omega_T,\Omega_L}^{r_0}$$

$$+ \frac{a_{L\tau_1\tau_2}^4}{a_L^4}\langle F_1(\boldsymbol{x}(\tau_1)[\delta\boldsymbol{x}(\tau_1)]_L^2\rangle_{\Omega_T,\Omega_L}^{r_0}. \tag{47}$$

Specializing $F_1(x)$ to a quadratic function, we obtain the corresponding generalizations of (38)

$$\langle [\delta \boldsymbol{x}(\tau_1)]_T^2 [\delta \boldsymbol{x}(\tau_2)]_T^2 \rangle_{\Omega_T,\Omega_L}^{r_0} = 4a_T^4 + 4a_{T\tau_1\tau_2}^4 \tag{48}$$

$$\langle [\delta \boldsymbol{x}(\tau_1)]_T^2 [\delta \boldsymbol{x}(\tau_2)]_L^2 \rangle_{\Omega_T,\Omega_L}^{r_0} = 2a_T^2 a_L^2 \tag{49}$$

$$\langle [\delta \boldsymbol{x}(\tau_1)]_L^2 [\delta \boldsymbol{x}(\tau_2)]_L^2 \rangle_{\Omega_T,\Omega_L}^{r_0} = a_L^4 + 2a_{L\tau_1\tau_2}^4. \tag{50}$$

4. Application to Coulomb potential

Let us demonstrate the use of the new smearing formulae by calculating the effective classical potential of the three-dimensional Coulomb potential

$$v(r) = -\frac{e^2}{r} \tag{51}$$

up to the second order in the variational perturbation expansion, thus going beyond the known first-order results in [9, 11]. To this end we express the Coulomb potential (51) as a 'proper-time' integral

$$\frac{1}{r} = 4\pi \int_{-\infty}^{+\infty} \frac{d^3 k}{(2\pi)^3} \int_0^{+\infty} d\sigma \, e^{-\sigma k^2 - i k x} \tag{52}$$

where σ has the dimension (length)^2, and find the expectation value

$$\left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} \right\rangle_{\Omega_T,\Omega_L}^{r_0} = \sqrt{\frac{2a_L^2}{\pi}} \int_0^1 d\lambda \, \frac{1}{(a_T^2 - a_L^2)\lambda^2 + a_L^2} \exp\left\{ -\frac{r_0^2}{2a_L^2} \lambda^2 \right\}. \tag{53}$$

From a straight-forward three-dimensional extension of (16), the first-order variational approximation to the effective classical potential is then [9, 11]

$$W_1^{\Omega_T,\Omega_L}(r_0) = \frac{2}{\beta} \log \frac{\sinh[\hbar\beta\Omega_T/2]}{\hbar\beta\Omega_T/2} + \frac{1}{\beta} \log \frac{\sinh[\hbar\beta\Omega_L/2]}{\hbar\beta\Omega_L/2} - \frac{M}{2}\{2\Omega_T^2 a_T^2 + \Omega_L^2 a_L^2\}$$

$$- e^2 \sqrt{\frac{2a_L^2}{\pi}} \int_0^1 d\lambda \, \frac{1}{(a_T^2 - a_L^2)\lambda^2 + a_L^2} \exp\left\{ -\frac{r_0^2}{2a_L^2} \lambda^2 \right\} \tag{54}$$

where we have omitted the argument r_0 from all functions on the right-hand side. A similar expression was derived in the isotropic approximation $\Omega_L = \Omega_T$ with the help of Gaussian wavepackets in the context of plasma physics for the purpose of faster simulations of molecular dynamics [14–16].

By inserting the 'proper-time' integral for the Coulomb potential (52) into the rules (46) and (47), we find

$$\left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} [\delta \boldsymbol{x}(\tau_2)]_T^2 \right\rangle_{\Omega_T,\Omega_L}^{r_0} = \sqrt{\frac{2a_L^2}{\pi}} \int_0^1 d\lambda \, \exp\left\{ -\frac{r_0^2}{2a_L^2} \lambda^2 \right\}$$

$$\times \left\{ \frac{2a_T^2}{(a_T^2 - a_L^2)\lambda^2 + a_L^2} - \frac{2a_{T\tau_1\tau_2}^4 \lambda^2}{[(a_T^2 - a_L^2)\lambda^2 + a_L^2]^2} \right\} \tag{55}$$

$$\left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} [\delta \boldsymbol{x}(\tau_2)]_L^2 \right\rangle_{\Omega_T,\Omega_L}^{r_0} = \sqrt{\frac{2a_L^2}{\pi}} \int_0^1 d\lambda \, \exp\left\{ -\frac{r_0^2}{2a_L^2} \lambda^2 \right\} \frac{a_L^6 + a_{L\tau_1\tau_2}^4 [r_0^2\lambda^4 - a_L^2\lambda^2]}{a_L^4[(a_T^2 - a_L^2)\lambda^2 + a_L^2]}. \tag{56}$$

Note that these results are also special cases of the general expectation value

$$
\left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} F(\boldsymbol{x}(\tau_2)) \right\rangle_{\Omega_T, \Omega_L}^{r_0} = \frac{1}{2\pi^2} \int_0^{+\infty} d\sigma \; \frac{\exp\left\{ -\dfrac{a_L^2 r_0^2}{2[a_L^4 - a_{L\tau_1\tau_2}^4 + 2a_L^2\sigma]} \right\}}{[a_T^4 - a_{T\tau_1\tau_2}^4 + 2a_T^2\sigma]\sqrt{a_L^4 - a_{L\tau_1\tau_2}^4 + 2a_L^2\sigma}}
$$

$$
\times \int_{-\infty}^{+\infty} d^3x \; F(\boldsymbol{x}) \exp\left\{ -\frac{(a_T^2 + 2\sigma)\boldsymbol{x}_T^2}{2[a_T^4 - a_{T\tau_1\tau_2}^4 + 2a_T^2\sigma]} \right.
$$

$$
\left. -\frac{(a_L^2 + 2\sigma)(x_L - r_0)^2 + 2a_{L\tau_1\tau_2}^2 r_0(x_L - r_0)}{2[a_L^4 - a_{L\tau_1\tau_2}^4 + 2a_L^2\sigma]} \right\}
\tag{57}
$$

which gives us the additional local expectation value

$$
\left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} \frac{1}{|\boldsymbol{x}(\tau_2)|} \right\rangle_{\Omega_T, \Omega_L}^{r_0} = \frac{2}{\pi} \int_0^{+\infty} d\sigma_1 \int_0^{+\infty} d\sigma_2 \; \frac{1}{[a_T^2 + 2\sigma_1][a_T^2 + 2\sigma_2] - a_{T\tau_1\tau_2}^4}
$$

$$
\times \frac{1}{\sqrt{[a_L^2 + 2\sigma_1][a_L^2 + 2\sigma_2] - a_{L\tau_1\tau_2}^4}} \exp\left\{ -\frac{r_0^2[a_L^2 + \sigma_1 + \sigma_2 - a_{L\tau_1\tau_2}^2]}{[a_L^2 + 2\sigma_1][a_L^2 + 2\sigma_2] - a_{L\tau_1\tau_2}^4} \right\}.
\tag{58}
$$

From these smearing results we calculate the connected correlation functions of the interaction potential (40) according to the cumulant law (18), and insert these into (16) to obtain the second-order effective classical potential

$$
W_2^{\Omega_T, \Omega_L}(r_0) = W_1^{\Omega_T, \Omega_L}(r_0) + \frac{e^2 M}{2\hbar} \sqrt{\frac{2a_L^2}{\pi}}
$$

$$
\times \int_0^1 d\lambda \left\{ \frac{2\Omega_T l_T^4 \lambda^2}{[(a_T^2 - a_L^2)\lambda^2 + a_L^2]^2} - \frac{\Omega_L l_L^4 [r_0^2 \lambda^4 - a_L^2 \lambda^2]}{a_L^4 [(a_T^2 - a_L^2)\lambda^2 + a_L^2]} \right\} \exp\left\{ -\frac{r_0^2}{2a_L^2} \lambda^2 \right\}
$$

$$
-\frac{M^2 [2\Omega_T^3 l_T^4 + \Omega_L^3 l_L^4]}{4\hbar} - \frac{e^4}{2\hbar^2 \beta} \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} \frac{1}{|\boldsymbol{x}(\tau_2)|} \right\rangle_{\Omega_T, \Omega_L, c}^{r_0}
\tag{59}
$$

with the abbreviation

$$
l_{T,L}^4 = \frac{\hbar[4 + \hbar^2 \beta^2 \Omega_{T,L}^2 - 4\cosh\hbar\beta\Omega_{T,L} + \hbar\beta\Omega_{T,L}\sinh\hbar\beta\Omega_{T,L}]}{8\beta M^2 \Omega_{T,L}^3 \sinh^2[\hbar\beta\Omega_{T,L}/2]}
\tag{60}
$$

which is a function of r_0 of dimension (length)^4. After extremizing (54) and (59) with respect to the trial frequencies Ω_T, Ω_L according to (19), which has to be done numerically we obtain the first- and second-order approximations for the effective classical potential of the Coulomb system. The isotropic approximations $\Omega_T = \Omega_L$ in the first and second order are plotted in figure 1 for various temperatures. The second-order curves lie all below the first-order ones, and the difference between the two decreases with increasing temperature and increasing distance from the origin. Figure 2 shows exemplarily that the anisotropic approximation slightly deviates from the isotropic one. The difference between both is only visible for intermediate distances from the origin.
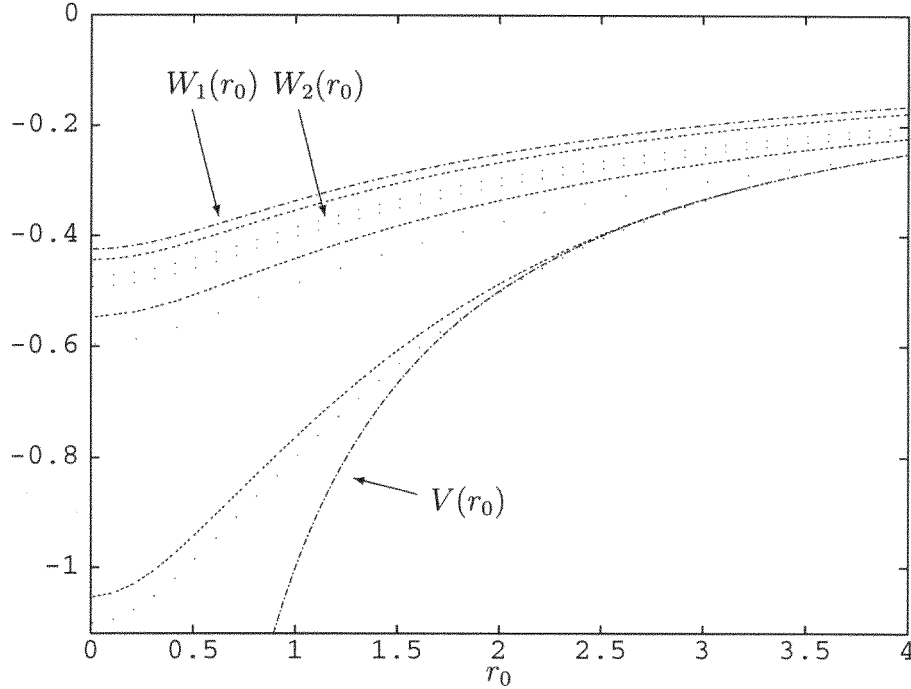
Figure 1. Isotropic approximations to the effective classical potential of the Coulomb system in the first (lines) and second order (dots). The temperatures are 0.0001, 0.001, 0.01, 0.1 and ∞ from the top to the bottom in atomic units. The high temperature limit is the same for all approximations $W_N(r_0)$.

5. Zero-temperature limit

In order to check our results we take (54) and (59) to the limit $T \to 0$, where $W_1^\Omega(r_0)$ and $W_2^\Omega(r_0)$ reduce at $r_0 = 0$, according to (23), to the ground-state energy of the Coulomb system. At $r_0 = 0$, the frequencies are isotropic $\Omega_L = \Omega_T = \Omega$ for symmetry reasons, thus simplifying the evaluation (54) and (59). Taking into account the low temperature limit of the two-point correlations (27)

$$\lim_{\beta \to \infty} a^2_{\tau_k \tau_{k'}}(x_0) = \frac{\hbar}{2M\Omega(x_0)} e^{-\Omega(x_0)|\tau_k - \tau_{k'}|} \tag{61}$$

we immediately deduce for the first-order approximation (54) at $x_0 = 0$ with $\Omega = \Omega(0)$ the limit

$$E_1^{(0)}(\Omega) = \lim_{\beta \to \infty} W_1^\Omega(0) = \frac{3}{4}\hbar\Omega - \frac{2}{\sqrt{\pi}}\sqrt{\frac{M\Omega}{\hbar}} e^2. \tag{62}$$

To second order, the limit is more involved. Performing the integrals over σ_1 and σ_2 in (58), we obtain with (18) the connected correlation function

$$\left\langle \frac{1}{|x(\tau_1)|} \frac{1}{|x(\tau_2)|} \right\rangle_{\Omega,c}^{0} = \frac{1}{a^4_{\tau_1 \tau_2}(0)} - \frac{2}{\pi a^4_{\tau_1 \tau_2}(0)} \arctan \sqrt{\frac{a^2_{\tau_1 \tau_2}(0)}{a_{\tau_1 \tau_2}(0)} - 1} - \frac{2}{\pi a^2_{\tau_1 \tau_2}(0)}. \tag{63}$$

Inserting here the zero-temperature limit (61), we can integrate these expressions over the
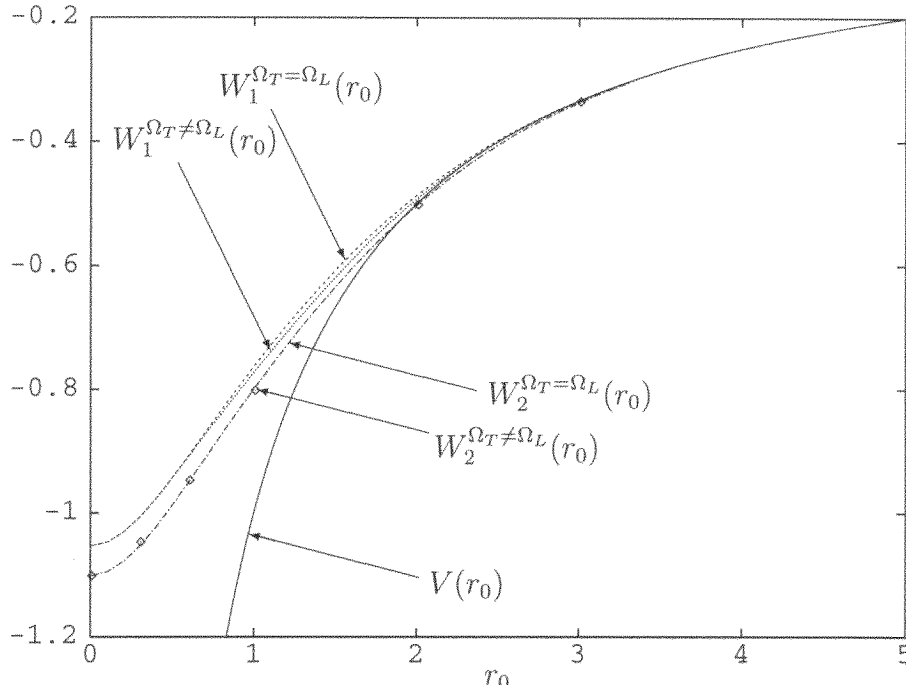
Figure 2. Isotropic and anisotropic approximations to the effective classical potential of the Coulomb system in the first and second order at the temperature 0.1 in atomic units. The lowest line represents the high temperature limit in which all isotropic and anisotropic approximations coincide.

imaginary times $\tau_1, \tau_2 \in [0, \hbar\beta]$, and find for large β

$$
\int_0^{\hbar\beta} \mathrm{d}\tau_1 \int_0^{\hbar\beta} \mathrm{d}\tau_2 \left\langle \frac{1}{|\boldsymbol{x}(\tau_1)|} \frac{1}{|\boldsymbol{x}(\tau_2)|} \right\rangle_{\Omega,c}^0 = \frac{4M}{\hbar\Omega} \left\{ \mathrm{e}^{\hbar\beta\Omega} - 1 - \hbar\beta\Omega - \frac{\hbar^2\beta^2\Omega^2}{\pi} - \frac{2}{\pi} \right.
$$
$$
\times \left[\mathrm{e}^{\hbar\beta\Omega} \arcsin\sqrt{1 - \mathrm{e}^{-2\hbar\beta\Omega}} + \frac{1}{2}\log\alpha(\beta) \right.
$$
$$
\left. \left. - \frac{1}{8}[\log\alpha(\beta)]^2 - \frac{1}{2}\int_{\alpha(\beta)}^1 \mathrm{d}u \frac{\log u}{1+u} \right] \right\} \tag{64}
$$

with the abbreviation

$$
\alpha(\beta) = \frac{1 - \sqrt{1 - \mathrm{e}^{-2\hbar\beta\Omega}}}{1 + \sqrt{1 - \mathrm{e}^{-2\hbar\beta\Omega}}}. \tag{65}
$$

Inserting this into (59) and going to the limit $\beta \to \infty$, we find the ground-state energy

$$
E_2^{(0)}(\Omega) = \lim_{\beta\to\infty} W_2^\Omega(\boldsymbol{0}) = \frac{9}{16}\hbar\Omega - \frac{3}{2\sqrt{\pi}}\sqrt{\frac{M\Omega}{\hbar}}e^2 - \frac{4}{\pi}\left(1 + \log 2 - \frac{\pi}{2}\right)\frac{M}{\hbar^2}e^4. \tag{66}
$$

Postponing for a moment the extremization of (62) and (66) with respect to the trial frequency Ω, let us first rederive this result from a variational treatment of the ordinary Rayleigh–Schrödinger perturbation expansion for the ground-state energy.

6. Variational treatment of Rayleigh–Schrödinger perturbation expansion

According to the rules laid out in [9], we must first calculate the ground-state energy for the Coulomb potential in the presence of a harmonic potential of frequency ω:

$$V_{\text{aux}}(\boldsymbol{x}) = \frac{M}{2}\omega^2\boldsymbol{x}^2 - \frac{e^2}{|\boldsymbol{x}|}. \tag{67}$$

After this, we make the trivial replacement $\omega \to \sqrt{\Omega^2 + \omega^2 - \Omega^2}$, and re-expand the energy in powers of the difference $\omega^2 - \Omega^2$, considering this quantity as being of the order e^2 and truncating the re-expansion accordingly. At the end we set $\omega = 0$, since the original Coulomb system contains no oscillator potential. Note that this limit is equivalent to a strong-coupling limit of (67) with respect to e^2. The result of this treatment will coincide precisely with the expansions (62) and (66), respectively.

The Rayleigh–Schrödinger perturbation expansion of the ground-state energy $E_N^{\text{aux}}(\omega)$ for the potential (67) requires knowledge of the matrix elements of the Coulomb potential (51) with respect to the eigenfunctions $\psi_{n,l,m}(r, \vartheta, \varphi)$ of the harmonic oscillator with the frequency ω [9]:

$$V_{n,l,m;n',l',m'} = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \mathrm{d}\vartheta \, \sin\vartheta \int_0^{\infty} \mathrm{d}r \, r^2 \psi_{n,l,m}^*(r, \vartheta, \varphi) \frac{-e^2}{r} \psi_{n',l',m'}(r, \vartheta, \varphi) \tag{68}$$

$$\psi_{n,l,m}(r, \vartheta, \varphi) = \sqrt{\frac{2n!}{\Gamma(n+l+3/2)}} \sqrt[4]{\frac{M\omega}{\hbar}} \left(\frac{M\omega}{\hbar}r^2\right)^{(l+1)/2}$$

$$\times L_n^{l+1/2}\left(\frac{M\omega}{\hbar}r^2\right) \exp\left\{-\frac{M\omega}{2\hbar}r^2\right\} Y_{l,m}(\vartheta, \varphi). \tag{69}$$

Here n denotes the radial quantum number, $L_n^{\alpha}(x)$ the Laguerre polynomials [17], and $Y_{l,m}(\vartheta, \varphi)$ the spherical harmonics obeying the orthonormality relation

$$\int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \mathrm{d}\vartheta \, \sin\vartheta \, Y_{l,m}^*(\vartheta, \varphi) Y_{l',m'}(\vartheta, \varphi) = \delta_{l,l'}\delta_{m,m'}. \tag{70}$$

Inserting (69) into (68), and evaluating the integrals with equation (2.19.14.15) in [18], we find

$$V_{n,l,m;n',l',m'} = -e^2 \sqrt{\frac{M\omega}{\pi\hbar}} \frac{\Gamma(l+1)\Gamma(n+1/2)}{\Gamma(l+\frac{3}{2})} \sqrt{\frac{\Gamma(n'+l+3/2)}{n!n'!\Gamma(n+l+\frac{3}{2})}}$$

$$\times {}_3F_2(-n', l+1, \tfrac{1}{2}; l+\tfrac{3}{2}, \tfrac{1}{2}-n; 1)\delta_{l,l'}\delta_{m,m'} \tag{71}$$

with the generalized hypergeometric series [17]

$${}_3F_2(\alpha_1, \alpha_2, \alpha_3; \beta_1, \beta_2; x) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k(\alpha_2)_k(\alpha_3)_k}{(\beta_1)_k(\beta_2)_k} \frac{x^k}{k!} \tag{72}$$

and the Pochhammer symbol $(\alpha)_k = \Gamma(\alpha+k)/\Gamma(\alpha)$.

These matrix elements are now inserted into the Rayleigh–Schrödinger perturbation expansion for the ground-state energy

$$E_{\text{aux}}(\omega) = E_{0,0,0} + V_{0,0,0;0,0,0} + \sideset{}{'}\sum_{n,l,m} \frac{V_{0,0,0;n,l,m}V_{n,l,m;0,0,0}}{E_{0,0,0} - E_{n,l,m}}$$

$$- \sideset{}{'}\sum_{n,l,m} V_{0,0,0;0,0,0} \frac{V_{0,0,0;n,l,m}V_{n,l,m;0,0,0}}{[E_{0,0,0} - E_{n,l,m}]^2}$$

$$+ \sum_{n,l,m}' \sum_{n',l',m'}' \frac{V_{0,0,0;n,l,m} V_{n,l,m;n',l',m'} V_{n',l',m';0,0,0}}{[E_{0,0,0} - E_{n,l,m}][E_{0,0,0} - E_{n',l',m'}]} + \cdots \tag{73}$$

the denominators containing the energy eigenvalues of the harmonic oscillator

$$E_{n,l,m} = \hbar\omega(2n + l + \tfrac{3}{2}). \tag{74}$$

The primed summations in (73) run over all values of the quantum numbers n, $l = -\infty, \ldots, +\infty$ and $m = -l, \ldots, +l$, excluding those for which the denominators vanish. For the first three orders we obtain from (71)–(74)

$$E_{\text{aux}}(\omega) = \frac{3}{2}\hbar\omega - \frac{2}{\sqrt{\pi}} \sqrt{\frac{M\omega}{\hbar}} e^2 - \frac{4}{\pi}\left(1 + \log 2 - \frac{\pi}{2}\right) \frac{M}{\hbar^2} e^4 - c\sqrt{\frac{M^3}{\hbar^7 \omega}} e^6 + \cdots \tag{75}$$

with the constant

$$c = \frac{1}{\pi^{3/2}} \left\{ \sum_{n=1}^{\infty} \frac{1 \cdot 3 \cdot \ldots \cdot (2n-1)}{2 \cdot 4 \cdot \ldots \cdot 2n} \frac{1}{n^2(n + \frac{1}{2})} - \sum_{n=1}^{\infty}\sum_{n'=1}^{\infty} \frac{1 \cdot 3 \cdot \ldots \cdot (2n-1)}{2 \cdot 4 \cdot \ldots \cdot 2n} \right.$$
$$\left. \times \frac{1 \cdot 3 \cdot \ldots \cdot (2n'-1)}{2 \cdot 4 \cdot \ldots \cdot 2n'} \frac{{}_3F_2(-n', l+1, \frac{1}{2}; l+\frac{3}{2}, \frac{1}{2} - n; 1)}{nn'(n + \frac{1}{2})} \right\} \approx 0.0318. \tag{76}$$

The variational re-expansion procedure described after equation (67) replaces ω in the first term by $\Omega(1-1)^{1/2}$, to be expanded in the second one up to third order as $1 - \frac{1}{2} - \frac{1}{8} - \frac{1}{16} = \frac{5}{16}$. Correspondingly the term $3\omega/2$ becomes $\frac{15}{32}\omega$. The factor $\omega^{1/2}$ goes over into $\Omega^{1/2}(1-1)^{1/4}$, to be expanded to second order in the second one, yielding $\Omega^{1/4}(1 - \frac{1}{4} - \frac{3}{32}) = \frac{21}{32}$. The next term in (75) happens to be independent of ω and needs no re-expansion, whereas the last term remains unchanged since it is of highest order. In this way we obtain from (75) the third-order variational expression

$$E_3^{(0)}(\Omega) = \frac{15}{32}\hbar\Omega - \frac{21}{16\sqrt{\pi}} \sqrt{\frac{M\Omega}{\hbar}} e^2 - \frac{4}{\pi}\left(1 + \log 2 - \frac{\pi}{2}\right)\frac{M}{\hbar^2}e^4 - c\sqrt{\frac{M^3}{\hbar^7\Omega}}e^6. \tag{77}$$

We are now ready to optimize successively the expansions of first, second, and third order (62), (66) and (77) with respect to the trial frequency Ω. From the extrema we find the frequencies

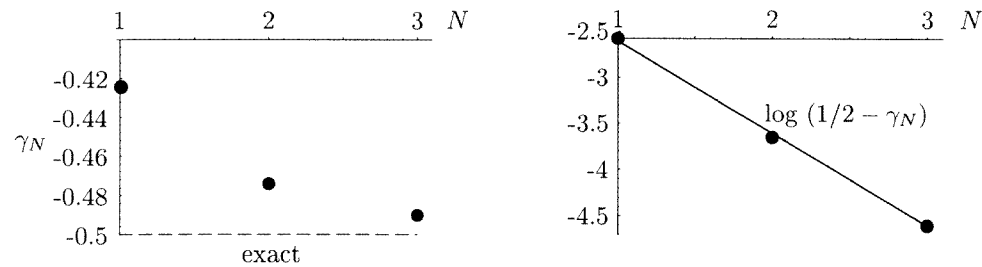$$\Omega_1 = \Omega_2 = \frac{16}{9\pi}\frac{Me^4}{\hbar^3} \qquad \Omega_3 = c'^2 \frac{Me^4}{\hbar^3} \tag{78}$$

where $c' \approx 0.7254$ is the largest of the three solutions of the cubic equation $15c'^3 - 21c'^2/\pi + 16c$. The corresponding approximations to the ground-state energy are

$$E_N^{(0)}(\Omega_N) = -\gamma_N \frac{Me^4}{\hbar^2} \tag{79}$$

with the constants

$$\gamma_1 = \frac{4}{3\pi} \approx 0.424 \qquad \gamma_2 = \frac{5 + 4\log 2}{\pi} - 2 \approx 0.474 \qquad \gamma_3 \approx 0.490 \tag{80}$$

which quickly approaching the exact value $\gamma_{\text{ex}} = 0.5$, as shown in figure 3.

Figure 3. Rapid approach of the variational approximations to the ground-state energy $E_N^{(0)}(\Omega_N)$ to the correct ground-state energy -0.5 (in natural energy units $Me^4/\hbar^2$). The right-hand logarithmic plot shows a slope -1.

7. Summary and outlook

In this work we have extended the rules for calculating higher orders in variational perturbation theory from polynomial to non-polynomial interactions. The effective classical potential of a quantum mechanical system is obtained from an extension of the known first-order smearing formula, and involves certain convolutions with Gaussian functions. As an example, we have applied the higher-order smearing formula to the Coulomb system. We have illustrated the fast convergence of the variational perturbation expansion even for such a singular potential. The new smearing formula will help improving the existing first-order variational results for partition function and density matrix, also in dissipative quantum systems [19, 20]. It will also be of use in treating field theories with nonpolynomial interactions such as sine-Gordon and Liouville theories.

Acknowledgments

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