Path-integral approach to the Wigner-Kirkwood expansion

Petr Jizba[1,2,*] and Václav Zatloukal[1,3,†]
[1]*FNSPE, Czech Technical University in Prague, Břehová 7, 115 19 Praha 1, Czech Republic*
[2]*ITP, Freie Universität in Berlin, Arnimallee 14, D-14195 Berlin, Germany*
[3]*Max Planck Institute for the History of Science, Boltzmannstrasse 22, 14195 Berlin, Germany*
(Received 22 September 2013; published 23 January 2014)

We study the high-temperature behavior of quantum-mechanical path integrals. Starting from the Feynman-Kac formula, we derive a functional representation of the Wigner-Kirkwood perturbation expansion for quantum Boltzmann densities. As shown by its applications to different potentials, the presented expansion turns out to be quite efficient in generating analytic form of the higher-order expansion coefficients. To put some flesh on the bare bones, we apply the expansion to obtain basic thermodynamic functions of the one-dimensional anharmonic oscillator. Further salient issues, such as generalization to the Bloch density matrix and comparison with the more customary world-line formulation, are discussed.

DOI: 10.1103/PhysRevE.89.012135 PACS number(s): 05.30.−d, 02.70.Rr, 02.30.Mv, 31.15.−p

I. INTRODUCTION

The Wigner-Kirkwood (WK) expansion was originally presented in two seminal papers [1,2], and since its very inception it has had two important implications. On the one hand, it has been used for studying the equilibrium statistical mechanics of a nearly classical system of particles obeying Maxwell-Boltzmann statistics. WK expansion is in its essence an expansion of the quantum Boltzmann density in powers of Planck's constant $\hbar$, or equivalently of the thermal de Broglie wavelength $\lambda = \hbar\sqrt{\beta/M}$, where β is the inverse temperature and M is the mass of a particle. On the other hand, it has paved a way for new alternative mathematical techniques and practical calculational schemes that are pertinent to the high-temperature regime in quantum systems.

In this paper, we pursue the study of the WK perturbation method by means of the path-integral (PI) calculus. The relevance of the PI treatment in a high-temperature context is due to several reasons: PI's allow us to connect evolutionary equations (Bloch equation or Fokker-Planck equation) with the underlying stochastic analysis [3,4], they are tailor-made for obtaining quasiclassical asymptotics [5,6], they allow us to utilize some powerful transformation techniques to simplify the original stochastic process [5,7], etc. Besides, PI's also provide an excellent tool for direct numerical simulations of the underlying stochastic dynamics including many-body systems [8,9]. One of the key advantages of the PI approach is, however, the fact that the techniques and methodologies used can efficiently bypass the explicit knowledge of the exact energy spectrum, the point that hindered earlier attempts to go beyond few leading orders in the expansion (see, e.g., Refs. [10–14]). In particular, one can progress without relying on the explicit use of approximate expressions or interpolation formulas for the energy eigenvalues which are often difficult to judge due to lack of reliability in their error estimates.

The idea to use PI's as a means of producing various WK-type expansions and related thermodynamic functions is clearly not new. Indeed, the first systematic discussions and analyses of these issues emerged already during the early 1970s. Among these belong the early attempts of PI treatments of the high-temperature behavior of partition functions for anharmonic oscillators [15–17] and gradient expansions of free energy [5]. These approaches belong in the class of the so-called *analytic perturbation schemes* which account for explicit analytic expressions of the coefficient functions. For many practical purposes it is desirable to have explicit analytical expressions for coefficients in the WK perturbation expansion. This is so, for instance, when the symmetry (Lorentz, gauge, global) is supposed to be broken by quantum or thermal fluctuations. Although these issues are more pressing in quantum field theories, they have in the recent two decades entered also in the realm of a few-body finite-temperature quantum mechanics. The catalyst has been theoretical investigations and ensuing state-of-the-art experiments in condensed Bose gases, degenerate Fermi gases, quantum clusters, or strongly coupled Coulomb systems. It is not only the zero-temperature regime that is of interest in these systems. Many issues revolve also around finite-temperature or "high"-temperature questions. These include thermal and thermoelectric transport of ultracold atomic gases [18,19], hydrogen, helium, and hydrogen and helium mixtures and their astrophysical implications [20,21], Lennard-Jones ^{3}He and ^{4}He gases [22], etc.

Apart from the aforementioned group of PI methods, there are also various nonanalytic methods among which the most prominent are computational methods, such as PI Monte Carlo and molecular dynamics simulations [23,24], accompanied by a host of PI reweighted techniques [25]. Another important type of nonanalytic method are the approximative schemes, to which belong variational approaches [5,26,27] and ergodic approximations [28]. Nice summaries of both analytic and nonanalytic PI approaches can be found, e.g., in Refs. [5,9].

A serious weakness of existent analytic WK expansions and their various disguises (be they based on PI's or not) resides in their inability to progress very far with the expansion order. This makes it difficult to address thermodynamically relevant intermediate-temperature regions that are particularly pertinent in molecular and condensed matter chemistry (binding energies, self-dissociation phenomena, order-disorder transitions, etc.). The best analytic expansions are presently available within the framework of the world-line path-integral

*p.jizba@fjfi.cvut.cz
†v.zatloukal@fu-berlin.de

method (known also as the string inspired method) [29]. In this approach, the expansion coefficients are available up to order $O(\beta^{12})$, subject to the actual interaction potential (cf. Refs. [29–31]). Other more conventional approaches, such as the recursive or nonrecursive heat-kernel calculations [32,33] or higher derivative expansions by Feynman diagrams [34–36], achieve at best the order $O(\beta^7)$. The key problem is a rapid escalation in the complexity of higher-order terms which is difficult to handle without some type of resummation. In this paper, we derive a resummation formula that provides a rather simple and systematic way of deriving the coefficient functions. Its main advantages rely on both an analytic control of the high-temperature behavior and on an accurate description over a wide temperature range via numerical calculations that can be simply carried out at the level of an undergraduate exercise.

The structure of the paper is as follows. To set the stage, we recall in the next section some fundamentals of PI formulations of the Bloch density matrix and the ensuing partition function and Boltzmann density. With the help of the space-time transformation that transforms the Wiener-process sample paths to the Brownian-bridge sample paths we obtain the PI that represents a useful alternative to the original Feynman-Kac representation. Consequently, we arrive at a functional representation of the Boltzmann density which is more suitable for tackling the high-temperature regime than the genuine Wigner-Kirkwood formulation (see Secs. II A, II B, and III). While the method resembles in principle the Wentzel-Kramers-Brillouin (WKB) solution for the transition amplitude, its details are quite different. In two associated sections, we examine some salient technical issues related to the low-order high-temperature expansion in one dimension. To illustrate the potency of our approach, we consider in Sec. III the high-temperature expansion of the one-dimensional anharmonic oscillator. In particular, we perform the Boltzmann density and ensuing partition function expansions and compute the related thermodynamic quantities. The expansions obtained improve over the classic results of Schwarz [14] and Padé-approximation-based expansion of Gibson [37]. In Sec. IV, we proceed by extending our expansion to the whole Bloch density matrix. The expansion thus obtained is compared with the more conventional Wick's theorem based perturbation expansion based on the Onofri-Zuk Green's functions. There we show that our prescription comprises substantially less (in fact, exponentially less) terms contributing to higher perturbation orders. Also, the algebraic complexity of the coefficient functions involved is substantially lower in our approach. Various remarks and generalizations are proposed in the concluding section. For the reader's convenience, the paper is supplemented with two appendices which clarify some finer technical details. The paper is also accompanied by MATHEMATICA code that generates the higher-order expansion terms for arbitrary smooth local potentials up to 18th order in β.

Let us add a final note. Most of the presented mathematical derivations are of a heuristic nature, as it should be expected from the mathematical analysis based on the path-integral calculus. For example, it is assumed throughout that the expansions such as (7) or (14) have meaning and represent, at least asymptotically, convergent series. Further, in a number of places, we assume that integration and summation may be interchanged. The basic purpose of this paper is to find explicit formulas for the coefficient functions $Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$, and in doing so to reveal the elaborate algebraic and combinatorial structure present in these functions. A more rigorous treatment of the aforementioned mathematical aspects is possible, but would involve different language and techniques than are employed in this paper.

II. WIGNER-KIRKWOOD EXPANSION

In this section, we derive the Wigner-Kirkwood expansion by means of path-integral techniques. To this end, we consider a D-dimensional nonrelativistic quantum-mechanical system described with the Hamiltonian

$$\hat{H} = \sum_{j=1}^{D} \frac{\hat{p}_j^2}{2M_j} + V(\hat{\boldsymbol{x}}), \tag{1}$$

where $V(\boldsymbol{x})$ is a generic smooth potential, and $\hat{p}_j = -i\hbar\frac{\partial}{\partial x_j}$. We define the Gibbs operator $e^{-\beta\hat{H}}$, where $\beta = 1/(k_B T)$ is the inverse temperature and k_B the Boltzmann constant. The partition function $Z(\beta)$ is defined as the trace of the Bloch (or canonical) density matrix, i.e., in the position representation we have the formula

$$Z(\beta) = \int_{\mathbb{R}^D} d\boldsymbol{x}\langle \boldsymbol{x}|e^{-\beta\hat{H}}|\boldsymbol{x}\rangle = \int_{\mathbb{R}^D} d\boldsymbol{x}\,\varrho(\boldsymbol{x},\beta). \tag{2}$$

For brevity, we use here and throughout the convention $d\boldsymbol{x} \equiv d^D x$. The un-normalized probability density $\varrho(\boldsymbol{x},\beta)$ is also known as the Boltzmann density.

Matrix elements of the Bloch density matrix can be represented by the path integral as [5,38]

$$\begin{aligned}\langle \boldsymbol{x}_b|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle &= \int_{\boldsymbol{x}(0)=\boldsymbol{x}_a}^{\boldsymbol{x}(\beta\hbar)=\boldsymbol{x}_b} \mathcal{D}\boldsymbol{x}(\tau) \\ &\quad\times \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\sum_{j=1}^{D}\frac{M_j}{2}\dot{x}_j^2(\tau) + V[\boldsymbol{x}(\tau)]\right]\right\},\end{aligned} \tag{3}$$

which can be viewed as the Wick-rotated quantum-mechanical transition amplitude. Indeed, if one changes the time τ in $i\tau$, one recovers the usual transition amplitude $\langle \boldsymbol{x}_b,\tau_b|\boldsymbol{x}_a,\tau_a\rangle$ satisfying the Schödinger equation with the Hamiltonian $\hat{H}$ (cf., e.g., Refs. [5,6]). In the literature on stochastic processes is the path-integral representation of the Bloch density matrix also known as the Feynman-Kac formula [39].

For the purpose of the density matrix computation, we shall primarily consider here only diagonal matrix elements, i.e., the case when $\boldsymbol{x}_b = \boldsymbol{x}_a$. We shall briefly return to the off-diagonal matrix elements in Sec. IV. To proceed, we perform a change of space and time variables $\boldsymbol{x} \to \boldsymbol{x}_a + \Lambda\boldsymbol{\xi}$, $\tau \to \beta\hbar s$, where Λ is a diagonal matrix $\mathrm{diag}(\lambda_1,\ldots,\lambda_D)$ with entries $\lambda_j = \sqrt{\beta\hbar^2/M_j}$ (corresponding to the thermal de Broglie wavelength of the jth degree of freedom). The

ensuing path integral

$$\langle \boldsymbol{x}_a|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle = \frac{1}{\det\Lambda}\int_{\boldsymbol{\xi}(0)=\boldsymbol{0}}^{\boldsymbol{\xi}(1)=\boldsymbol{0}}\mathcal{D}\boldsymbol{\xi}(s) \times \exp\left\{-\int_0^1 ds\left[\frac{1}{2}\dot{\boldsymbol{\xi}}^2(s)+\beta V[\boldsymbol{x}_a+\Lambda\boldsymbol{\xi}(s)]\right]\right\} \quad (4)$$

is formulated in terms of dimensionless time s and position $\boldsymbol{\xi}$. Note that the size of quantum fluctuations is now controlled by the parameters λ_j, i.e., the only place (apart from the overall PI normalization factor) where the measure of quantum fluctuations $\hbar$ is present. Since β and $\hbar^2$ appear in (4) on the same footing, the small regime allows us to treat in a unified manner both the semiclassical (small $\hbar$) and/or high-temperature (small β) approximations. By assuming small Λ, the potential term can be Taylor expanded as

$$V[\boldsymbol{x}_a+\Lambda\boldsymbol{\xi}(s)] = V(\boldsymbol{x}_a)+\sum_{\boldsymbol{m}\neq\boldsymbol{0}}\frac{V^{(\boldsymbol{m})}(\boldsymbol{x}_a)}{\boldsymbol{m}!}[\Lambda\boldsymbol{\xi}(s)]^{\boldsymbol{m}}, \quad (5)$$

where the D-dimensional index $\boldsymbol{m}=(m^1,\ldots,m^D)$ runs through all choices of m^j's $\in\{0,\ldots,\infty\}$ except for $(m^1,\ldots,m^D)=(0,\ldots,0)$. The multiderivative $(\boldsymbol{m})$ is defined through the identity

$$V^{(\boldsymbol{m})}(\boldsymbol{x}_a) = \left.\frac{\partial^{|\boldsymbol{m}|}V(\boldsymbol{x})}{\partial\boldsymbol{x}^{\boldsymbol{m}}}\right|_{\boldsymbol{x}=\boldsymbol{x}_a} \equiv \left.\frac{\partial^{m^1+\cdots+m^D}V(\boldsymbol{x})}{\partial x_1^{m^1}\ldots\partial x_D^{m^D}}\right|_{\boldsymbol{x}=\boldsymbol{x}_a}, \quad (6)$$

with $|\boldsymbol{m}|=m^1+\cdots+m^D$. Finally, the multifactorial $\boldsymbol{m}!\equiv m^1!\ldots m^D!$, and the multipower of a D-dimensional vector $\boldsymbol{v}$ is defined componentwise as $\boldsymbol{v}^{\boldsymbol{m}}\equiv v_1^{m^1}\ldots v_D^{m^D}$. Expanding the exponential, followed by some rearrangement, allows us to cast (4) in the form

$$\langle \boldsymbol{x}_a|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle = \frac{e^{-\beta V(\boldsymbol{x}_a)}}{\det\Lambda}\sum_{n=0}^{\infty}(-\beta)^n\sum_{\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n\neq\boldsymbol{0}} \times\prod_{j=1}^{D}\lambda_j^{m_1^j+\cdots+m_n^j}\frac{V^{(\boldsymbol{m}_1)}(\boldsymbol{x}_a)\ldots V^{(\boldsymbol{m}_n)}(\boldsymbol{x}_a)}{\boldsymbol{m}_1!\ldots\boldsymbol{m}_n!}\bar{Q}. \quad (7)$$

At this point, we have introduced the dimensionless quantity

$$\bar{Q}(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n) = \frac{1}{n!}\int_0^1 ds_1\ldots ds_n\int_{\boldsymbol{\xi}(0)=\boldsymbol{0}}^{\boldsymbol{\xi}(1)=\boldsymbol{0}}\mathcal{D}\boldsymbol{\xi}(s)\boldsymbol{\xi}^{\boldsymbol{m}_1}(s_1)\ldots\boldsymbol{\xi}^{\boldsymbol{m}_n}(s_n) \times\exp\left[-\int_0^1 ds\frac{1}{2}\dot{\boldsymbol{\xi}}^2(s)\right] = \frac{1}{n!}\int_0^1 ds_1\ldots ds_n\langle\boldsymbol{\xi}^{\boldsymbol{m}_1}(s_1)\ldots\boldsymbol{\xi}^{\boldsymbol{m}_n}(s_n)\rangle \quad (8)$$

that does not depend on physical constants or parameters of the system. $\bar{Q}$ is also manifestly symmetric under any permutation of its arguments. Let us stress that the $n=0$ term in the expansion (7) equals 1.

In (8) we have denoted with $\langle\cdots\rangle$ the $(|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|)$-point correlation function. It can be evaluated using a diagrammatic approach based on the so-called Onofri-Zuk (or "world-line") Green's function [6,29,40,41]

$$\Delta_{ij}(t,u) = -\tfrac{1}{2}\delta_{ij}\left[|t-u|-(t+u-2tu)\right]. \quad (9)$$

We shall briefly sketch this approach in Sec. IV in connection with the off-diagonal density matrix elements. At any rate, the procedure based on Green's function (9) proves rather impractical when higher-order terms are to be calculated. Inasmuch, we shall follow a different route. To this end, we rewrite expression (8) as a sum of $n!$ integrals over time-ordered sets $s_1<\cdots<s_n$, slice the path integral at corresponding time instances, and replace the free-particle path integrals by more compact bra-ket notation by virtue of (3). We obtain

$$\bar{Q}(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n) = \frac{1}{n!}\sum_{\sigma\in S_n}Q(\boldsymbol{m}_{\sigma(1)},\ldots,\boldsymbol{m}_{\sigma(n)}), \quad (10)$$

where the sum runs over all permutations of n indices, and

$$Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n) = \int_{0<s_1<\cdots<s_n<1}ds_1\ldots ds_n\int_{\mathbb{R}^D}d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \times\prod_{\nu=0}^{n}\langle\boldsymbol{y}_{\nu+1}|\exp\left[-(s_{\nu+1}-s_\nu)\frac{\hat{\boldsymbol{q}}^2}{2}\right]|\boldsymbol{y}_\nu\rangle\boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}. \quad (11)$$

In the preceding we have defined $\boldsymbol{m}_0=\boldsymbol{0}$, $s_0=0$, $s_{n+1}=1$, $\boldsymbol{y}_0=\boldsymbol{y}_{n+1}=\boldsymbol{0}$, and the momentum $\hat{\boldsymbol{q}}=(\hat{q}_1,\ldots,\hat{q}_D)$, conjugated to the (dimensionless) position operator $\hat{\boldsymbol{y}}=(\hat{y}_1,\ldots,\hat{y}_D)$. Here and throughout, we use the standard convention $\hat{q}_j=-i\frac{\partial}{\partial y_j}$ and $\langle\boldsymbol{y}|\boldsymbol{q}\rangle=e^{i\boldsymbol{q}\boldsymbol{y}}/(2\pi)^{D/2}$.

Combinatorial complexity can be reduced significantly by observing that for any function $F(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$, the following identity holds:

$$\sum_{\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n\neq\boldsymbol{0}}\frac{1}{n!}\sum_{\sigma\in S_n}F(\boldsymbol{m}_{\sigma(1)},\ldots,\boldsymbol{m}_{\sigma(n)}) = \sum_{\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n\neq\boldsymbol{0}}F(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n). \quad (12)$$

This statement is not trivial since F is not supposed to be invariant under permutations of the $\boldsymbol{m}$'s. When applied to (7) for

$$F(\boldsymbol{m}_{\sigma(1)},\ldots,\boldsymbol{m}_{\sigma(n)}) = \prod_{j=1}^{D}\lambda_j^{m_1^j+\cdots+m_n^j}\frac{V^{(\boldsymbol{m}_1)}(\boldsymbol{x}_a)\ldots V^{(\boldsymbol{m}_n)}(\boldsymbol{x}_a)}{\boldsymbol{m}_1!\ldots\boldsymbol{m}_n!} \times Q(\boldsymbol{m}_{\sigma(1)},\ldots,\boldsymbol{m}_{\sigma(n)}), \quad (13)$$

the expansion can be then reduced to

$$\langle \boldsymbol{x}_a|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle = \frac{e^{-\beta V(\boldsymbol{x}_a)}}{\det\Lambda}\sum_{n=0}^{\infty}(-\beta)^n\sum_{\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n\neq\boldsymbol{0}} \times\prod_{j=1}^{D}\lambda_j^{m_1^j+\cdots+m_n^j}\frac{V^{(\boldsymbol{m}_1)}(\boldsymbol{x}_a)\ldots V^{(\boldsymbol{m}_n)}(\boldsymbol{x}_a)}{\boldsymbol{m}_1!\ldots\boldsymbol{m}_n!}Q. \quad (14)$$

In addition, in the Appendix we derive an explicit expression for the coefficients Q which prove to be very useful in the

determination of the higher-order terms. In particular, there we show that

$$Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n) = K\int_{\mathbb{R}^D}\frac{d\boldsymbol{q}}{(2\pi)^D}\left(\frac{i^{|\boldsymbol{m}_n|}}{1+\frac{\boldsymbol{q}^2}{2}}\frac{\partial^{|\boldsymbol{m}_n|}}{\partial\boldsymbol{q}^{\boldsymbol{m}_n}}\right)\cdots \times\left(\frac{i^{|\boldsymbol{m}_1|}}{1+\frac{\boldsymbol{q}^2}{2}}\frac{\partial^{|\boldsymbol{m}_1|}}{\partial\boldsymbol{q}^{\boldsymbol{m}_1}}\right)\frac{1}{1+\frac{\boldsymbol{q}^2}{2}}, \tag{15}$$

where the multiplicative constant has the form

$$K = \frac{1}{\Gamma\left(n+1-\frac{D}{2}+\frac{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}{2}\right)}. \tag{16}$$

From Appendix B we can observe that the integral (15) suffers the infrared divergencies precisely in those instances when the Γ function in K has pole. Consequently, in practical applications, one should appropriately regularize (e.g., via dimensional regularization) both K and the integral in (15) in order to resolve the indeterminate form of the product.

In passing, we may note that because Q is real, it must be equal to zero when $|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|$ together with all partial sums $m_1^j+\cdots+m_n^j$ $(j=1,\ldots,D)$ is an even number (cf. also Sec. IV and Appendix B). So, the expansion of the density matrix (14) can be reorganized as an expansion in $\hbar^2$. This is emblematic of the Wigner-Kirkwood expansion [1] for systems with differentiable potentials. In the case of the nondifferentiable potentials (cavities, billiards, etc.), the generalized derivative of Schwartz must be used instead [42].

Result (14) might be used for calculating higher-order terms beyond the $\hbar^2$ correction (terms up to order $\hbar^6$ have been already determined in the literature [43]). Moreover, the structure of (14) clearly emphasizes that expansion is appropriate only when the involved thermal de Broglie wavelengths are much smaller than the typical length of variation of the potential.

A. Calculation of low-order terms in D dimensions

In order to get further insight into structure of (14), we will now calculate the first few terms in the expansion. To this end, we notice that a typical term in (15) has the generic structure

$$\begin{aligned}\int_{\mathbb{R}^D}\frac{d\boldsymbol{q}}{(2\pi)^D}\frac{q_1^{2r_1}\ldots q_D^{2r_D}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^s} &= \int_0^\infty d\sigma\,\frac{\sigma^{s-1}}{(s-1)!}e^{-\sigma}\\ &\quad\times\int_{\mathbb{R}^D}\frac{d\boldsymbol{q}}{(2\pi)^D}q_1^{2r_1}\ldots q_D^{2r_D}e^{-\sigma\frac{\boldsymbol{q}^2}{2}}\\ &= \frac{\Gamma\left(s-\frac{D}{2}-|\boldsymbol{r}|\right)}{(s-1)!(2\pi)^{D/2}2^{|\boldsymbol{r}|}}\prod_{j=1}^D\frac{(2r_j)!}{r_j!},\end{aligned} \tag{17}$$

where $r_1,\ldots,r_D,s\in\mathbb{N}$. If the power of any q_j is odd, the above integral obviously vanishes. For the sake of simplicity, the discussion here will be restricted to the orders in $O(\beta^3)$, but it can be naturally extended to higher orders (cf. next section). At this level, we need to know (15) for $n=1$ and 2.

Case $n=1$. Here, the lowest-order nontrivial contribution comes from $|\boldsymbol{m}_1|=2$, with $m_1^i=\delta_{ij}+\delta_{ik}$. After differentiating

$$\frac{\partial^2}{\partial q_j\partial q_k}\frac{1}{1+\frac{\boldsymbol{q}^2}{2}} = -\frac{\delta_{jk}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^2}+\frac{2q_jq_k}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^3}, \tag{18}$$

we can use the formulas (15) and (17) to find

$$Q(\boldsymbol{m}_1) = \frac{1}{(2\pi)^{D/2}}\frac{\delta_{jk}}{6}. \tag{19}$$

Case $n=2$. Here, the lowest-order nontrivial contribution comes from $|\boldsymbol{m}_1|=|\boldsymbol{m}_2|=1$, with $m_1^i=\delta_{ij}$, $m_2^i=\delta_{ik}$. Consequently, we need to estimate

$$\frac{\partial}{\partial q_k}\left(\frac{1}{1+\frac{\boldsymbol{q}^2}{2}}\frac{\partial}{\partial q_j}\frac{1}{1+\frac{\boldsymbol{q}^2}{2}}\right) = -\frac{\delta_{jk}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^3}+\frac{3q_jq_k}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^4}, \tag{20}$$

which gives

$$Q(\boldsymbol{m}_1,\boldsymbol{m}_2) = \frac{1}{(2\pi)^{D/2}}\frac{\delta_{jk}}{24}. \tag{21}$$

By gathering the results (19) and (21) together we can write the expansion (14) in the $n=2$ approximation as

$$\langle\boldsymbol{x}_a|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle \sim \frac{e^{-\beta V(\boldsymbol{x}_a)}}{(2\pi)^{D/2}\det\Lambda}\left(1-\frac{\beta}{12}\sum_{j=1}^D\lambda_j^2\frac{\partial^2V(\boldsymbol{x}_a)}{\partial x_j^2} +\frac{\beta^2}{24}\sum_{j,k=1}^D\lambda_j\lambda_k\frac{\partial V(\boldsymbol{x}_a)}{\partial x_j}\frac{\partial V(\boldsymbol{x}_a)}{\partial x_k}\right). \tag{22}$$

This agrees, for $\lambda_j=\lambda$ (i.e., for equal-mass particles), with the usual low-order Wigner-Kirkwood expansion (see, e.g., Refs. [5,44]).

B. Expansion for $D=1$

Here, we show that the form of the coefficients $Q(m_1,\ldots,m_n)$ can be substantially simplified in one dimension $(D=1)$. It is rather interesting that the simplification basically involves only arithmetic operations. To see what is involved, we denote

$$I(m_1,\ldots,m_n|r,s) = \int_{\mathbb{R}}\frac{dq}{2\pi}\left(\frac{i^{m_n}}{1+\frac{q^2}{2}}\frac{\partial^{m_n}}{\partial q^{m_n}}\right)\cdots\left(\frac{i^{m_1}}{1+\frac{q^2}{2}}\frac{\partial^{m_1}}{\partial q^{m_1}}\right)\left(\frac{1}{\left(1+\frac{i}{\sqrt{2}}q\right)^r}\frac{1}{\left(1-\frac{i}{\sqrt{2}}q\right)^s}\right), \tag{23}$$

so that [cf. Eq. (15)] $Q(m_1,\ldots,m_n)=K(m_1,\ldots,m_n)I(m_1,\ldots,m_n|1,1)$. By the m_1-fold differentiation of the last bracket, we obtain the recurrence relation

$$I(m_1,\ldots,m_n|r,s) = \frac{(-1)^{m_1}}{2^{m_1/2}}m_1!\sum_{k_1=0}^{m_1}(-1)^{k_1}\binom{r-1+k_1}{r-1}\binom{s-1+m_1-k_1}{s-1}I(m_2,\ldots,m_n|r+1+k_1,s+1+m_1-k_1), \tag{24}$$

with the initial condition

$$I(\emptyset|r,s) = \int_{\mathbb{R}} \frac{dq}{2\pi} \frac{1}{\left(1+\frac{i}{\sqrt{2}}q\right)^r} \frac{1}{\left(1-\frac{i}{\sqrt{2}}q\right)^s} = \frac{2^{3/2}}{2^{r+s}} \binom{r+s-2}{r-1}. \tag{25}$$

The latter identity is a straightforward consequence of Cauchy's integral theorem where the contour integration is taken at either the pole $i\sqrt{2}$ or $-i\sqrt{2}$. Repeated use of (24), with (25) as the last step, leads to an explicit form for $Q(m_1,\ldots,m_n)$, namely,

$$Q = \frac{(\frac{m_1+\cdots+m_n}{2}+n)!}{\sqrt{2\pi}2^{(m_1+\cdots+m_n)/2}} \sum_{\ell_1=0}^{m_1} \cdots \sum_{\ell_n=0}^{m_n} \prod_{k=1}^{n} \frac{(-1)^{\ell_k}\binom{m_k}{\ell_k}}{(\ell_1+\cdots+\ell_k+k)(m_1-\ell_1+\cdots+m_k-\ell_k+k)}. \tag{26}$$

In deriving we have used the duplication formula [45] $\sqrt{\pi}2^{1-2z}\Gamma(2z) = \Gamma(z)\Gamma(z+1/2)$. The resulting one-dimensional expansion takes the form

$$\langle x_a|e^{-\beta\hat{H}}|x_a\rangle = \frac{e^{-\beta V(x_a)}}{\lambda} \sum_{n=0}^{\infty}(-\beta)^n \sum_{m_1,\ldots,m_n=1}^{\infty} \lambda^{m_1+\cdots+m_n} \frac{V^{(m_1)}(x_a)\ldots V^{(m_n)}(x_a)}{m_1!\ldots m_n!} Q. \tag{27}$$

Apart from the initial constant term $\beta^0\hbar^0$, the latter expansion contains terms proportional to $\beta^i(\hbar^2)^j$, where $i,j \in \mathbb{N}$ and $i/3 \leqslant j \leqslant i-1$ (or, equivalently, $j+1 \leqslant i \leqslant 3j$).

For the first few orders, the coefficients of the expansion can be found rather straightforwardly. In Table I, we list the coefficients of the series $e^{\beta V(x)}\sqrt{2\pi}\lambda\langle x|e^{-\beta\hat{H}}|x\rangle$. To order β^8 these can be obtained without any excessive hardship (for further comments, see [46]). The higher orders in fixed β can now be simply obtained by grouping terms with equal order of β and performing a number of multidifferentiations for $V(x_a)$ which can be easily done with MAPLE or MATHEMATICA. To this end, we supplement the paper with MATHEMATICA code that allows us to generate the higher-order expansion terms (up to 18th order) for arbitrary smooth local potentials.

III. EXAMPLE: ANHARMONIC OSCILLATOR IN $D = 1$

In the previous section, we have seen in some detail how the coefficient functions in the Wigner-Kirkwood expansion can be resolved in an explicit form. The basic results there were the formulas (14)–(16). The expressions found are quite general, valid for any smooth potential and in $D = 1$ are analytically accessible up to order β^{18}. Nevertheless, for consistency reasons, it is useful to examine a problem possessing an exact solution in which it is possible to find closed expressions for the expansion coefficients. The $D = 1$ harmonic oscillator provides us with just such an exactly solvable example. Rather than starting directly with a simple harmonic oscillator, it is instructive to start with an *anharmonic* oscillator first and then regain the harmonic oscillator solution in the limit of vanishing coupling constant (i.e., zero anharmonicity limit). In addition, the anharmonic oscillator, which can be regarded as a field theory in one dimension, has long served as a testing ground for new ideas for solving field theories and hence is bolstered by a large body of literature. In this respect, it is a natural model which any new approximation scheme should address. For definiteness, we start with the anharmonic potential

$$V(x) = \frac{M}{2}\omega^2x^2 + \frac{g}{4!}x^4, \tag{28}$$

for which the high-temperature expansion (27) yields

$$\langle x|e^{-\beta\hat{H}}|x\rangle = \frac{\exp\left[-\beta\left(\frac{M}{2}\omega^2x^2+\frac{g}{4!}x^4\right)\right]}{\sqrt{2\pi}\lambda}\left[1-\frac{\beta^2\hbar^2(gx^2+2M\omega^2)}{24M}+\frac{\beta^3(5Mx^2\hbar^2(gx^2+6M\omega^2)^2-18g\hbar^4)}{4320M^2}\right.$$
$$\left.+\frac{\beta^4\hbar^4(17g^2x^4+84gMx^2\omega^2+36M^2\omega^4)}{5760M^2}+O(\beta^5)\right]. \tag{29}$$

The higher-order corrections can be explicitly obtained with the help of Table I (up to order β^8) or with the enclosed MATHEMATICA code quoted in [46] (up to order β^{18}).

In the case of zero anharmonicity ($g = 0$), we can check our results against the exact solution of the harmonic oscillator problem. The expansion (29) reduces to

$$\langle x|e^{-\beta\hat{H}}|x\rangle_{g=0} = \frac{\exp\left(-\beta\frac{M}{2}\omega^2x^2\right)}{\sqrt{2\pi}\lambda}\left[1-\frac{1}{12}\beta^2\omega^2\hbar^2+\frac{1}{24}\beta^3Mx^2\omega^4\hbar^2+\frac{1}{160}\beta^4\omega^4\hbar^4+O(\beta^5)\right], \tag{30}$$

which, indeed, coincides with the corresponding expansion of the well-known analytic form of the Bloch density matrix for harmonic oscillator (see, e.g., Refs. [5,6])

$$\langle x|e^{-\beta\hat{H}}|x\rangle_{g=0} = \frac{\exp\left(-\beta\frac{M}{2}\omega^2x^2\right)}{\sqrt{2\pi}\lambda}\sqrt{\frac{\beta\omega\hbar}{\sinh(\beta\omega\hbar)}}\exp\left[-\frac{Mx^2\omega}{\hbar}\left(\tanh\frac{\beta\omega\hbar}{2}-\frac{\beta\omega\hbar}{2}\right)\right]. \tag{31}$$

TABLE I. Coefficients of the series $e^{\beta V(x)}\sqrt{2\pi}\lambda\langle x|e^{-\beta\hat{H}}|x\rangle$, at terms $\beta^i(\hbar^2)^j$, calculated according to formulas (26) and (27). Here, $0 \leqslant i \leqslant 8$ and $0 \leqslant j \leqslant 7$, which allows us to determine the series up to the eighth order in β. Coefficients of terms $(\hbar^2)^j$, which are polynomials in β, can be read off completely only for $j \leqslant 2$. (For instance, the $\hbar^6$ term is lacking a contribution from β^9.)

	$\hbar^0$	$\hbar^2$	$\hbar^4$	$\hbar^6$	$\hbar^8$	$\hbar^{10}$
β^0	1	0	0	0	0	0
β^1	0	0	0	0	0	0
β^2	0	$-\frac{V''(x)}{12M}$	0	0	0	0
β^3	0	$\frac{V'(x)^2}{24M}$	$-\frac{V^{(4)}(x)}{240M^2}$	0	0	0
β^4	0	0	$\frac{V''(x)^2}{160M^2}$ $+\frac{V'(x)V^{(3)}(x)}{120M^2}$	$-\frac{V^{(6)}(x)}{6720M^3}$	0	0
β^5	0	0	$-\frac{11V'(x)^2V''(x)}{1440M^2}$	$\frac{23V^{(3)}(x)^2}{40320M^3}$ $+\frac{19V''(x)V^{(4)}(x)}{20160M^3}$ $+\frac{V'(x)V^{(5)}(x)}{2240M^3}$	$-\frac{V^{(8)}(x)}{241920M^4}$	0
β^6	0	0	$\frac{V'(x)^4}{1152M^2}$	$-\frac{61V''(x)^3}{120960M^3}$ $-\frac{43V'(x)V^{(3)}(x)V''(x)}{20160M^3}$ $-\frac{5V'(x)^2V^{(4)}(x)}{8064M^3}$	$\frac{23V^{(4)}(x)^2}{483840M^4}$ $+\frac{19V^{(3)}(x)V^{(5)}(x)}{241920M^4}$ $+\frac{11V''(x)V^{(6)}(x)}{241920M^4}$ $+\frac{V'(x)V^{(7)}(x)}{60480M^4}$	$-\frac{V^{(10)}(x)}{10644480M^5}$

	$\hbar^6$	$\hbar^8$	$\hbar^{10}$	$\hbar^{12}$	$\hbar^{14}$
β^7	$\frac{V^{(3)}(x)V'(x)^3}{2016M^3}$ $+\frac{83V''(x)^2V'(x)^2}{80640M^3}$	$-\frac{V^{(6)}(x)V'(x)^2}{32256M^4}$ $-\frac{V^{(3)}(x)V^{(4)}(x)V'(x)}{4480M^4}$ $-\frac{V''(x)V^{(5)}(x)V'(x)}{6720M^4}$ $-\frac{31V''(x)V^{(3)}(x)^2}{161280M^4}$ $-\frac{5V''(x)^2V^{(4)}(x)}{32256M^4}$	$\frac{71V^{(5)}(x)^2}{21288960M^5}$ $+\frac{61V^{(4)}(x)V^{(6)}(x)}{10644480M^5}$ $+\frac{19V^{(3)}(x)V^{(7)}(x)}{5322240M^5}$ $+\frac{17V''(x)V^{(8)}(x)}{10644480M^5}$ $+\frac{V'(x)V^{(9)}(x)}{2128896M^5}$	$-\frac{V^{(12)}(x)}{553512960M^6}$	0
β^8	$-\frac{17V'(x)^4V''(x)}{69120M^3}$	$\frac{1261V''(x)^4}{29030400M^4}$ $+\frac{227V'(x)V^{(3)}(x)V''(x)^2}{604800M^4}$ $+\frac{527V'(x)^2V^{(4)}(x)V''(x)}{2419200M^4}$ $+\frac{659V'(x)^2V^{(3)}(x)^2}{4838400M^4}$ $+\frac{17V'(x)^3V^{(5)}(x)}{483840M^4}$	$-\frac{71V^{(8)}(x)V'(x)^2}{63866880M^5}$ $-\frac{3067V^{(4)}(x)V^{(5)}(x)V'(x)}{159667200M^5}$ $-\frac{13V^{(3)}(x)V^{(6)}(x)V'(x)}{950400M^5}$ $-\frac{109V''(x)V^{(7)}(x)V'(x)}{15966720M^5}$ $-\frac{6353V''(x)V^{(4)}(x)^2}{319334400M^5}$ $-\frac{7939V^{(3)}(x)^2V^{(4)}(x)}{319334400M^5}$ $-\frac{13V''(x)V^{(3)}(x)V^{(5)}(x)}{394240M^5}$ $-\frac{3001V''(x)^2V^{(6)}(x)}{319334400M^5}$	$\frac{3433V^{(6)}(x)^2}{16605388800M^6}$ $+\frac{1501V^{(5)}(x)V^{(7)}(x)}{4151347200M^6}$ $+\frac{2003V^{(4)}(x)V^{(8)}(x)}{8302694400M^6}$ $+\frac{5V^{(3)}(x)V^{(9)}(x)}{41513472M^6}$ $+\frac{73V''(x)V^{(10)}(x)}{1660538880M^6}$ $+\frac{V'(x)V^{(11)}(x)}{92252160M^6}$	$-\frac{V^{(14)}(x)}{33210777600M^7}$

In passing, we may note that the expansion of the single-particle partition function $Z(\beta)$ associated with (29) can be phrased in terms of the *parabolic cylindric function* and its derivatives which, after reexpansion, give

$$Z(\beta) = \frac{1}{\sqrt{2\pi}\lambda}\sqrt[4]{\frac{3}{2\beta g}}\left[\Gamma\left(\frac{1}{4}\right) + \frac{\sqrt{\frac{3}{2}}\sqrt{\beta}M\omega^2\Gamma\left(-\frac{1}{4}\right)}{2\sqrt{g}} + \frac{3\beta M^2\omega^4\Gamma\left(\frac{5}{4}\right)}{g} - \frac{\beta^{3/2}\left[\Gamma\left(\frac{3}{4}\right)(g^2\hbar^2 + 18M^4\omega^6)\right]}{4(\sqrt{6}g^{3/2}M)}\right.$$
$$\left. - \frac{\beta^2\left[\Gamma\left(-\frac{3}{4}\right)(2g^2\omega^2\hbar^2 + 45M^4\omega^8)\right]}{128g^2} + O(\beta^{5/2})\right]. \tag{32}$$

This, when combined with appropriate thermodynamic formulas, yields the following expressions for entropy S, the heat capacity C_V, and internal energy U:

$$\begin{aligned}
\frac{S}{k_B} &= -\frac{1}{k_B}\left(\frac{\partial F}{\partial T}\right)_V = \ln Z(\beta) - \frac{\beta}{Z(\beta)}\left(\frac{\partial Z(\beta)}{\partial \beta}\right)_V \\
&= \frac{3}{4} + \ln\left(\frac{2\Gamma\left(\frac{5}{4}\right)}{\lambda}\sqrt[4]{\frac{6}{\pi^2\beta g}}\right) - \frac{\sqrt{\frac{3}{2}}\sqrt{\beta}M\omega^2\Gamma\left(\frac{3}{4}\right)}{\sqrt{g}\Gamma\left(\frac{1}{4}\right)} + \frac{\beta^{3/2}\left(\pi g^2\hbar^2\Gamma\left(\frac{5}{4}\right) + 3\sqrt{2}M^4\omega^6\Gamma\left(\frac{3}{4}\right)^3\right)}{\sqrt{3}g^{3/2}M\Gamma\left(\frac{1}{4}\right)^3} + O(\beta^2), \\
\frac{C_V}{k_B} &= \frac{T}{k_B}\left(\frac{\partial S}{\partial T}\right)_V = -\frac{\beta}{k_B}\left(\frac{\partial S}{\partial \beta}\right)_V = \frac{3}{4} + \frac{\sqrt{\frac{3}{2}}\sqrt{\beta}M\omega^2\Gamma\left(\frac{3}{4}\right)}{2\sqrt{g}\Gamma\left(\frac{1}{4}\right)} - \frac{\beta^{3/2}\left(\sqrt{3}\pi g^2\hbar^2\Gamma\left(\frac{5}{4}\right) + 3\sqrt{6}M^4\omega^6\Gamma\left(\frac{3}{4}\right)^3\right)}{2g^{3/2}M\Gamma\left(\frac{1}{4}\right)^3} + O(\beta^2), \\
U &= -T^2\left(\frac{\partial F/T}{\partial T}\right)_V = \left(\frac{\partial F\beta}{\partial \beta}\right)_V \\
&= \frac{3}{4\beta} + \frac{\sqrt{\frac{3}{2}}M\omega^2\Gamma\left(\frac{3}{4}\right)}{\sqrt{\beta}\sqrt{g}\Gamma\left(\frac{1}{4}\right)} - \frac{3M^2\omega^4\left(\Gamma\left(\frac{1}{4}\right)^2 - 4\Gamma\left(\frac{3}{4}\right)^2\right)}{4g\Gamma\left(\frac{1}{4}\right)^2} + \frac{\sqrt{\beta}\left(2\sqrt{3}\pi g^2\hbar^2\Gamma\left(\frac{9}{4}\right) + 15\sqrt{6}M^4\omega^6\Gamma\left(\frac{3}{4}\right)^3\right)}{320g^{3/2}M\Gamma\left(\frac{5}{4}\right)^3} + O(\beta). \qquad (33)
\end{aligned}$$

[$F = -k_B T \ln Z(\beta)$ is the Helmholtz free energy.] These expansions are not only in excellent agreement with the classic (spectral-theorem based) expansions of Schwarz [14] and Gibson [37], but they also go beyond these expansions by providing explicit forms for higher-order terms not present in Refs. [14,37].

Unfortunately, when M in (28) is negative (i.e., we would have a double-well potential) the WK approach would fail. Indeed, the WK expansion can not accommodate nonperturbation effects such as multi-instanton contribution and ensuing tunneling, as by its very construction it is basically a perturbation expansion around a free solution. From this point of view, a tunneling in a double-well potential seems to be beyond reach in our expansion. Of course, tunneling could be included by considering some sort of a hybrid approach in which the "phase part" of the transition probability would be calculated via WKB (possibly including multi-instanton contribution), while the fluctuating factor would be evaluated perturbatively via the WK method. One of the potential bonuses would be the fact that one could bypass the notorious problems with the Van Vleck determinant on caustics. Such a hybrid approach would, however, clearly go beyond the simple WK approach that is used in our paper. In our future investigation, we will touch more upon this issue.

IV. OFF-DIAGONAL BLOCH DENSITY MATRIX ELEMENTS

So far, we have almost exclusively been dealing with the diagonal elements of the Bloch density matrix: Boltzmann density. This was well justified by expected applications in statistical physics, where typically only the partition function is required and hence only diagonal elements of the density matrix are relevant (of course, only as long as the Maxwell-Boltzmann statistics is considered). This is also the linchpin of the original Wigner-Kirkwood work.

Expansion and the formula for the Bloch density matrix (14) can be straightforwardly generalized beyond the original Wigner-Kirkwood analysis by considering the off-diagonal form of the density matrix (also called the heat kernel or Euclidean Feynman amplitude). This would be particularly pertinent in cases when one would like to incorporate the exchange effects that are a consequence of fermion or boson statistics or when the linear response theory would be in question. By following the same train of thought as in Sec. II, we can phrase the path-integral representation of the full Bloch density matrix in terms of the sum over the Brownian bridge sample paths. The path transformation that transforms the Wiener process $\Omega_W = \{\boldsymbol{x}(\ldots)\}$ to the Brownian bridge process $\Omega_{BB} = \{\boldsymbol{\xi}(\ldots)\}$ is

$$\boldsymbol{x}(\tau) = \boldsymbol{x}_a(1-s) + \boldsymbol{x}_b s + \Lambda\boldsymbol{\xi}(s). \qquad (34)$$

Let us recall that the "Euclidean time" variable τ is connected with s via the relation $\tau = \beta\hbar s$.

The Brownian bridge sample paths fulfill the Dirichlet boundary conditions $\boldsymbol{\xi}(0) = \boldsymbol{\xi}(1) = \boldsymbol{0}$. With this, the Feynman-Kac formula for the Bloch density matrix (3) acquires the form

$$\langle \boldsymbol{x}_b|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle = \frac{\exp\left\{-\frac{1}{2}[\Lambda^{-1}(\boldsymbol{x}_b - \boldsymbol{x}_a)]^2\right\}}{\det\Lambda}\int_{\boldsymbol{\xi}(0)=\boldsymbol{0}}^{\boldsymbol{\xi}(1)=\boldsymbol{0}} \mathcal{D}\boldsymbol{\xi}(s)\exp\left\{-\int_0^1 ds\left[\frac{1}{2}\dot{\boldsymbol{\xi}}^2(s) + \beta V[\boldsymbol{x}_a(1-s) + \boldsymbol{x}_b s + \Lambda\boldsymbol{\xi}(s)]\right]\right\}, \qquad (35)$$

where the surface term in the action got canceled due to boundary conditions of the Brownian bridge. We can expand the potential $V(\ldots)$ around the free-particle classical solution as

$$V[\boldsymbol{x}_a(1-s) + \boldsymbol{x}_b s + \Lambda\boldsymbol{\xi}(s)] = V[\boldsymbol{x}_a(1-s) + \boldsymbol{x}_b s] + \sum_{\boldsymbol{m}\neq\boldsymbol{0}} \frac{V^{(\boldsymbol{m})}[\boldsymbol{x}_a(1-s) + \boldsymbol{x}_b s]}{\boldsymbol{m}!}[\Lambda\boldsymbol{\xi}(s)]^{\boldsymbol{m}}, \qquad (36)$$

and write the density matrix in the form

$$\langle \boldsymbol{x}_b|e^{-\beta\hat{H}}|\boldsymbol{x}_a\rangle = \frac{\exp\left\{-\frac{1}{2}[\Lambda^{-1}(\boldsymbol{x}_b-\boldsymbol{x}_a)]^2-\beta\tilde{V}(\boldsymbol{x}_b,\boldsymbol{x}_a)\right\}}{\det\Lambda} \times\sum_{n=0}^{\infty}(-\beta)^n\sum_{\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n\neq\boldsymbol{0}}\prod_{j=1}^{D}\lambda_j^{m_1^j+\cdots+m_n^j}\frac{\left[\tilde{V}_{s_1}^{(\boldsymbol{m}_1)}(\boldsymbol{x}_b,\boldsymbol{x}_a)\ldots\tilde{V}_{s_n}^{(\boldsymbol{m}_n)}(\boldsymbol{x}_b,\boldsymbol{x}_a)*\bar{Q}_{s_1\cdots s_n}\right](t=1)}{\boldsymbol{m}_1!\ldots\boldsymbol{m}_n!}. \tag{37}$$

In the preceding we have introduced the abbreviations

$$\tilde{V}(\boldsymbol{x}_b,\boldsymbol{x}_a)=\int_0^1 ds\,V[\boldsymbol{x}_a(1-s)+\boldsymbol{x}_b s],\quad \tilde{V}_{s_i}^{(\boldsymbol{m}_k)}(\boldsymbol{x}_b,\boldsymbol{x}_a)=V^{(\boldsymbol{m}_k)}[\boldsymbol{x}_b-s_i(\boldsymbol{x}_b-\boldsymbol{x}_a)]. \tag{38}$$

The multidimensional convolution appearing in (37) is a straightforward extension of the one-dimensional convolution

$$[X(s_i)*Y(s_i)](t)=[Y(s_i)*X(s_i)](t)=\int_0^t ds_i X(t-s_i)Y(s_i). \tag{39}$$

It is the above definition of the convolution which dictates the (seemingly strangely appearing) form of the right-hand side of (38). Subindices s_i appearing in $\bar{Q}$ in (37) just indicate the integration variables in the convolution. We see again that the key object is the coefficient function $\bar{Q}$ [cf. Eq. (8)] or better the ensuing $(|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|)$-point correlator $\bar{Q}_{s_1\ldots s_n}$:

$$\begin{aligned}\int_{\boldsymbol{\xi}(0)=\boldsymbol{0}}^{\boldsymbol{\xi}(1)=\boldsymbol{0}}\mathcal{D}\boldsymbol{\xi}(s)\boldsymbol{\xi}^{\boldsymbol{m}_1}(s_1)\ldots\boldsymbol{\xi}^{\boldsymbol{m}_n}(s_n)\exp\left[-\int_0^1 ds\frac{1}{2}\dot{\boldsymbol{\xi}}^2(s)\right]&=\frac{\delta^{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}}{\delta\boldsymbol{j}(s_1)^{\boldsymbol{m}_1}\ldots\delta\boldsymbol{j}(s_n)^{\boldsymbol{m}_n}}\\ &\times\int_{\boldsymbol{\xi}(0)=\boldsymbol{0}}^{\boldsymbol{\xi}(1)=\boldsymbol{0}}\mathcal{D}\boldsymbol{\xi}(s)\exp\left[-\int_0^1 ds\frac{1}{2}\dot{\boldsymbol{\xi}}^2(s)+\int_0^1 ds\,\boldsymbol{j}(s)\cdot\boldsymbol{\xi}(s)\right]\Bigg|_{j=0}\\ &=\mathcal{N}\frac{\delta^{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}}{\delta\boldsymbol{j}(s_1)^{\boldsymbol{m}_1}\ldots\delta\boldsymbol{j}(s_n)^{\boldsymbol{m}_n}}\exp\left[\frac{1}{2}\int_0^1 ds\,du\,j_i(s)\Delta_{ij}(s,u)j_j(u)\right]\Bigg|_{j=0}.\end{aligned} \tag{40}$$

The normalization constant $\mathcal{N}$ denotes the path integral for a simple Brownian bridge. The summation convention is automatically utilized in the argument of the exponent on the last line. The Green's function $\Delta_{ij}(s,u)$ is chosen so that it satisfies the equations

$$\begin{aligned}\frac{\partial^2}{\partial t^2}\Delta_{ij}(t,u)&=-\delta_{ij}\delta(t-u),\\ \Delta_{ij}(0,u)&=\Delta_{ij}(1,u)=0.\end{aligned} \tag{41}$$

The solution is the world-line Green's function of Onofri and Zuk [40,41]

$$\Delta_{ij}(s,u)=-\tfrac{1}{2}\delta_{ij}[|t-u|-(t+u-2tu)]. \tag{42}$$

As a result, we can write $\bar{Q}(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$ in the form

$$\bar{Q}=\frac{\mathcal{N}}{n!}\int_0^1 ds_1\ldots ds_n\frac{\delta^{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}}{\delta\boldsymbol{j}(s_1)^{\boldsymbol{m}_1}\ldots\delta\boldsymbol{j}(s_n)^{\boldsymbol{m}_n}} \times\exp\left[\frac{1}{2}\int_0^1 dt\,du\,j_i(t)\Delta_{ij}(t,u)j_j(u)\right]\Bigg|_{j=0}. \tag{43}$$

The former can be further simplified with the help of Coleman's identity:

$$F(-i\partial/\partial\boldsymbol{x})G(\boldsymbol{x})=G(-i\partial/\partial\boldsymbol{y})F(\boldsymbol{y})e^{i\boldsymbol{y}\cdot\boldsymbol{x}}|_{y=0}, \tag{44}$$

which is valid for any (sufficiently smooth) functions F and G. After some additional algebra, one verifies that

$$\bar{Q}=\frac{\mathcal{N}i^{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}}{n!} \times\exp\left[-\frac{1}{2}\int_0^1 dt\,du\frac{\delta}{\delta z_i(t)}\Delta_{ij}(t,u)\frac{\delta}{\delta z_j(u)}\right] \times\int_0^1 ds_1\ldots ds_n z(s_1)^{\boldsymbol{m}_1}\ldots z(s_n)^{\boldsymbol{m}_n}\Bigg|_{z=0}. \tag{45}$$

For similar reasons, as in ordinary quantum field theory, i.e., namely for the Wick theorem application, it might be convenient to formulate the $\bar{Q}$ function in the Fourier picture. In this case, the Fourier transform is discrete due to the Dirichlet boundary conditions for $\boldsymbol{\xi}$. In addition, when we periodically extend the shape of the potential V from the interval $s\in[0,1]$ to the whole $\mathbb{R}$ and take the Fourier transform, the calculations of (37) will substantially simplify due to the convolution theorem [42].

Form (45) indicates that Q can be calculated via Wick's theorem with world-line Green's functions (42) (cf. also Refs. [5,29,47,48]). In fact, it is not difficult to list the corresponding Feynman-type diagrammatic rules for $\bar{Q}(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$. On the other hand, the number of terms involved in evaluating $\bar{Q}$ via (45) grows as $(2\mathfrak{m}-1)!!=(2\mathfrak{m})!/2^{\mathfrak{m}}\mathfrak{m}!$ where $\mathfrak{m}=(|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|)$ (see, for instance, Ref. [49]). This should be contrasted with (15) where

the number of terms grows as (see Appendix B)

$$\prod_{j=1}^{D}\left[\left(m_1^j+\cdots+m_n^j\right)/2+1\right]. \tag{46}$$

Our prescription comprises substantially less terms and this is even more pronounced at high values of $\boldsymbol{m}_j$'s (i.e., at high derivative orders). In Appendix B, we prove that the inequality

$$(2\mathfrak{m}-1)!!\geqslant\prod_{j=1}^{D}\left[\left(m_1^j+\cdots+m_n^j\right)/2+1\right] \tag{47}$$

always holds whenever $\mathfrak{m}\geqslant 2$. There, we also show that the number of terms is in our case exponentially lower than in Wick's theorem based approaches.

Note also that the number of s integrations in (45) matches the perturbation order, i.e., n, while the number of integrations in our formula (15) equals to the dimension of particle configuration space. In this respect, the presented method is less complex with the increasing perturbation order than other methods in use. As a matter of fact, with the method based on the world-line Green's function, a complete calculation of all coefficients was achieved to order $O(\beta^{12})$ (see Ref. [50]). Closely related gradient expansion calculations (with the same order of precision) were performed in Ref. [51].

Finally, note that $\bar{Q}$ from (45) is nonzero only when $|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|$ together with all partial sums $m_1^j+\cdots+m_n^j$ $(j=1,\ldots,D)$ is even. In fact, also all partial sums $m_1^j+\cdots+m_n^j$ $(j=1,\ldots,D)$ must be zero. This fact was already pointed out in Sec. II in connection with the coefficient Q. Again, the evenness is true only for smooth potentials. In the general case, the space derivatives must be substituted with the generalized derivative of Schwartz [42] which can bring about also odd terms, i.e., odd powers of $\hbar$. Also, other nonanalytical behavior can emerge, e.g., it was shown in [52] that exchange contributions to the free energy of the jellium vanish exponentially fast with $\hbar$ as a consequence of the Coulomb repulsion between identical charges which diverge at zero separation.

V. CONCLUSIONS AND PERSPECTIVES

In this paper, we have presented a PI-based high-temperature expansion of the Boltzmann's density $\varrho(\boldsymbol{x},\beta)$ and partition function $Z(\beta)$. Ensuing generalizations to the full Bloch density matrix were also discussed and explicitly compared with the Onofri-Zuk world-line approach. It was found that our prescription comprises substantially less terms contributing to higher perturbation orders than the more conventional Wick's-theorem-based perturbation expansions. Also, the algebraic complexity of the coefficient functions involved is markedly lower in our approach.

The expansions obtained are valid for an arbitrary number of particles and provide an analytic control of the high-temperature behavior. In addition, the implementation is sufficiently general for any system described by smooth potential energy functions. Because of its analytic form, the presented high-temperature expansion can be further conveniently used, e.g., to analyze the breakdown of symmetry, generate a gradient expansion for the free energy for a wide class of potentials, calculate ground-state energies, set up the extended Thomas-Fermi approximations, or serve as the starting point for a numerical evaluation of various thermodynamical quantities (e.g., virial coefficients, specific heat, or entropy). As a demonstration, we have briefly discussed the high-temperature thermodynamics of the anharmonic oscillator.

We would like to remark that the compactness of our form for the coefficient function Q might be deceptive with regard to applications requiring the use of nonlocal potentials. In the genuine Wigner-Kirkwood method, the single-particle density is expressed as a functional of the one-body potential $V(\boldsymbol{x})$. Although our treatment can accommodate also few-body potentials, it is intrinsically formulated only for local potentials. Since nonlocal potentials are an integral part of statistical quantum theory, e.g., in cases when the exchange part of the Hartree-Fock self-consistent potential is considered, the corresponding generalization of Eqs. (15) and (37) to nonlocal potentials would be desirable. The situation is simple only for two-particle systems with potentials of the form $V(\boldsymbol{x}_1,\boldsymbol{x}_2)=V(\boldsymbol{x}_1-\boldsymbol{x}_2)$. There, the transformation to the center of mass frame allows us to reduce the problem to a single particle in an external potential $V(\boldsymbol{x})$. For other cases, the formula (15) for the coefficient functions Q could be derived in the same spirit as in Sec. II, but the appealing simplicity of Q would be clearly lost.

The versatility of the method developed in this paper together with a renewed interest in the study of the high-temperature asymptotic expansions of the Bloch density matrix suggest several extensions of this work. A pertinent extension could address spin-dependent potentials, such as the spin-orbit interaction whose interest in nuclear physics is well known. Also, the case of momentum dependent terms which are relevant in charged particle systems interacting with electromagnetic field or in Brueckner's theory used in nuclear physics would be desirable to include. Important limitation of our method lies in the fact that our discussion was confined only to cases where Hamiltonians did not include fermionic degrees of freedom. Similarly as the original WK method, also our approach is inherently formulated within the framework of Boltzmann statistics and so it does not incorporate the exchange effects (which are relevant, e.g., in a hot fermionic plasma). There exist various generalizations of the WK formalism to include the effects of magnetic field [53] or exchange corrections (see, e.g., Refs. [54,55]) and the corresponding extension of our approach in this direction would be also worth pursuing particularly in view of a naturalness with which PI's handle fermionic particle systems [5]. All these aforementioned issues are currently under active investigation.

It appears worthwhile to stress that the WK expansion is not the WKB expansion. For instance, the leading asymptotic behaviors are different; while the WK expansion starts with $\exp[-\beta V(x)]$, the WKB starts with $\exp(-\beta S[x_{\rm cl},x])$ [here the action functional S is evaluated along the classical solutions $x_{\rm cl}$ with the boundary conditions $x(0)=x(\hbar\beta)=x$]. Even starting points for both these expansions were historically different. WK started with the Wigner transform approach

to statistical physics [1,2], while WKB (in PI's) started with the expansion (in terms of moments of Gaussian fluctuations) around classical trajectory [5,6]. It is also clear that in the WK one does not organize the expansion in terms of orders of fluctuations around classical solution (as the WKB does). Naturally, both approaches share many common features and there is a bulk of the literature comparing both methods and their respective pros and cons. The interested reader can see, e.g., Refs. [56,57].

Let us finally make a few comments concerning the low-temperature regime. It is clear that when the temperature decreases, the de Broglie wavelength increases, and the Wigner-Kirkwood perturbation expansion becomes unwarranted. This happens whenever the involved thermal de Broglie wavelength is comparable with a typical length over which the potential varies. So, the low-temperature expansion is normally beyond reach of the WK method. Nevertheless, with the high-temperature expansion at one's disposal, one can tackle also the low-temperature expansion (at least numerically) provided the sufficient number of the coefficient functions in the high-temperature series is available. To this end, one is free to employ some of the existent duality approaches. Among these, a particularly powerful nonperturbative approximation scheme is called *variational* or *optimized perturbation theory* [5,58–60]. There, the basic idea is to combine the renormalization-group concept known as the *principle of minimal sensitivity* [60] with the techniques of perturbation theory and the variational principle to convert the divergent weak-coupling power series into a convergent strong-coupling power series (and vice versa).

Last but not least, recently Paulin *et al.* [28] employed the concept of the occupation time for Wiener processes to formulate the so-called *ergodic local-time approximation* to PI's. The ergodic approximation is particularly well suited for the low-temperature regime. In the high-temperature domain, it performs less satisfactorily since the nontrivial correlations between occupation times must be taken into account [28]. Finding the dictionary that would allow a simple passage between our approach and that of Paulin *et al.* in the high- and intermediate-temperature regimes would be particularly desirable in light of a similar mathematical structure [namely, Eq. (4)] that both approaches share. Work along these lines is presently in progress.

ACKNOWLEDGMENTS

We would like to acknowledge helpful feedback from J. Klauder, H. Kleinert, and C. Schubert. This work was supported by GAČR Grant No. P402/12/J077. V.Z. received support from the Grant Agency of the Czech Technical University in Prague, Grant No. SGS13/217/OHK4/3T/14.

APPENDIX A: SIMPLIFICATION OF COEFFICIENTS $Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$

Here, we employ a convenient trick that will allow us to carry out the s integrations in (11) explicitly. We first formally promote the upper limit of the s integrations (i.e., 1) to a new variable s_{n+1}, and Laplace transform Q with respect to s_{n+1}, i.e.,

$$\widetilde{Q}(E) = \int_0^\infty ds_{n+1} e^{-Es_{n+1}} \int_{0<s_1<\cdots<s_n<s_{n+1}} ds_1\ldots ds_n \times \int_{\mathbb{R}^D} d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \times \prod_{\nu=0}^{n} \langle \boldsymbol{y}_{\nu+1}| \exp\left[-(s_{\nu+1}-s_\nu)\frac{\hat{\boldsymbol{q}}^2}{2}\right] |\boldsymbol{y}_\nu\rangle \boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}. \quad \text{(A1)}$$

Change of variables $s'_\nu = s_{\nu+1} - s_\nu$, $\nu = 0,\ldots,n$, then leads to

$$\widetilde{Q}(E) = \int_0^\infty ds'_0\ldots ds'_n \int_{\mathbb{R}^D} d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \prod_{\nu=0}^{n} \langle \boldsymbol{y}_{\nu+1}| \times \exp\left[-s'_\nu\left(E+\frac{\hat{\boldsymbol{q}}^2}{2}\right)\right] |\boldsymbol{y}_\nu\rangle \boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}. \quad \text{(A2)}$$

The s integrations can now be done easily,

$$\widetilde{Q}(E) = \int_{\mathbb{R}^D} d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \prod_{\nu=0}^{n} \langle \boldsymbol{y}_{\nu+1}| \frac{1}{E+\frac{\hat{\boldsymbol{q}}^2}{2}} |\boldsymbol{y}_\nu\rangle \boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}. \quad \text{(A3)}$$

In order to further simplify (A3), we perform the rescaling $\boldsymbol{y}_\nu \to \boldsymbol{y}_\nu/\sqrt{E}$, and use the fact that

$$\left\langle \frac{\boldsymbol{y}_{\nu+1}}{\sqrt{E}}\middle| \frac{1}{E+\frac{\hat{\boldsymbol{q}}^2}{2}} \middle|\frac{\boldsymbol{y}_\nu}{\sqrt{E}}\right\rangle = \int_{\mathbb{R}^D} \frac{d\boldsymbol{q}}{(2\pi)^D} \frac{\exp\left(i\boldsymbol{q}\frac{\boldsymbol{y}_{\nu+1}-\boldsymbol{y}_\nu}{\sqrt{E}}\right)}{E+\frac{\hat{\boldsymbol{q}}^2}{2}} \overset{\boldsymbol{q}\to\sqrt{E}\boldsymbol{q}}{=} E^{D/2-1} \langle \boldsymbol{y}_{\nu+1}| \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} |\boldsymbol{y}_\nu\rangle. \quad \text{(A4)}$$

This explicitly decouples E, giving rise to

$$\widetilde{Q}(E) = E^{D/2-n-1-(|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|)/2} \int_{\mathbb{R}^D} d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \times \prod_{\nu=0}^{n} \langle \boldsymbol{y}_{\nu+1}| \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} |\boldsymbol{y}_\nu\rangle \boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}. \quad \text{(A5)}$$

Now, the inverse Laplace transform can be performed and evaluated at $s_{n+1} = 1$. With the help of the formula $\int_0^\infty ds\, s^\nu e^{-sE} = \Gamma(\nu+1)E^{-\nu-1}$, we obtain

$$Q = K \int_{\mathbb{R}^D} d\boldsymbol{y}_1\ldots d\boldsymbol{y}_n \prod_{\nu=0}^{n} \langle \boldsymbol{y}_{\nu+1}| \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} |\boldsymbol{y}_\nu\rangle \boldsymbol{y}_\nu^{\boldsymbol{m}_\nu}, \quad \text{(A6)}$$

where the multiplicative factor

$$K = \frac{1}{\Gamma\left(n+1-\frac{D}{2}+\frac{|\boldsymbol{m}_1|+\cdots+|\boldsymbol{m}_n|}{2}\right)}. \quad \text{(A7)}$$

In the second step, we invoke a resolution of unity $\int_{\mathbb{R}^D} d\boldsymbol{y}_\nu |\boldsymbol{y}_\nu\rangle\langle\boldsymbol{y}_\nu| = \mathbb{I}$, which brings Q to the form

$$Q = K \langle \boldsymbol{y}_{n+1}| \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} \hat{\boldsymbol{y}}^{\boldsymbol{m}_n} \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} \hat{\boldsymbol{y}}^{\boldsymbol{m}_{n-1}} \cdots \times \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} \hat{\boldsymbol{y}}^{\boldsymbol{m}_1} \frac{1}{1+\frac{\hat{\boldsymbol{q}}^2}{2}} |\boldsymbol{y}_0\rangle. \quad \text{(A8)}$$

With the use of the algebraic identity

$$[\hat{y}_j, F(\hat{\boldsymbol{q}})] = i\frac{\partial F(\boldsymbol{q})}{\partial q_j}|_{\boldsymbol{q}=\hat{\boldsymbol{q}}}, \tag{A9}$$

and the fact that $\hat{y}_j|\boldsymbol{y}_0\rangle = 0\,(j = 1,\ldots,D)$, we can bring (A8) to the form (recall the definition $\boldsymbol{y}_0 = \boldsymbol{y}_{n+1} = \boldsymbol{0}$)

$$Q = K\langle \boldsymbol{y}_{n+1}|G(\hat{\boldsymbol{q}})\,|\boldsymbol{y}_0\rangle = K\int_{\mathbb{R}^D}\frac{d\boldsymbol{q}}{(2\pi)^D}G(\boldsymbol{q}), \tag{A10}$$

with $G(\boldsymbol{q})$ defined as

$$G(\boldsymbol{q}) = \left(\frac{i^{|\boldsymbol{m}_n|}}{1+\frac{\boldsymbol{q}^2}{2}}\frac{\partial^{|\boldsymbol{m}_n|}}{\partial \boldsymbol{q}^{\boldsymbol{m}_n}}\right)\cdots\left(\frac{i^{|\boldsymbol{m}_1|}}{1+\frac{\boldsymbol{q}^2}{2}}\frac{\partial^{|\boldsymbol{m}_1|}}{\partial \boldsymbol{q}^{\boldsymbol{m}_1}}\right)\frac{1}{1+\frac{\boldsymbol{q}^2}{2}}. \tag{A11}$$

Note that we could arrive at the same conclusion by employing in (A6) the spectral expansion of the position operator (or better, its power) in both position and momentum representations, i.e.,

$$\hat{\boldsymbol{y}}^{\boldsymbol{m}} = \int_{\mathbb{R}^D} d\boldsymbol{y}_\nu|\boldsymbol{y}_\nu\rangle\boldsymbol{y}_\nu^{\boldsymbol{m}}\langle\boldsymbol{y}_\nu| = \int_{\mathbb{R}^D} d\boldsymbol{q}_\nu|\boldsymbol{q}_\nu\rangle i^{|\boldsymbol{m}|}\frac{\partial^{|\boldsymbol{m}|}}{\partial \boldsymbol{q}_\nu^{\boldsymbol{m}}}\langle\boldsymbol{q}_\nu|\,. \tag{A12}$$

Ensuing lack of one δ function then causes the residual $\boldsymbol{q}$ integration in (A10).

APPENDIX B: STRUCTURE OF $Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$

In this Appendix, we show that the number of terms involved in evaluating $Q(\boldsymbol{m}_1,\ldots,\boldsymbol{m}_n)$ via (15) grows as (46). We start by observing that the function $G(\boldsymbol{q})$ in (A11) can be written as a sum

$$G(\boldsymbol{q}) = \sum_{\boldsymbol{r},s} a_{\boldsymbol{r},s}\frac{\boldsymbol{q}^{\boldsymbol{r}}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^s}, \tag{B1}$$

with combinatorial factors $a_{\boldsymbol{r},s}$ whose explicit form is not relevant for the arguments to follow. The components of multi-index $\boldsymbol{r}$ satisfy $0 \leqslant r^j \leqslant m_1^j + \cdots + m_n^j$ for all $j = 1,\ldots,D$ since each differentiation $\partial/\partial q_j$ can produce at most one power of q_j.

The summation index s in (B1) is not an independent variable but it is fully specified once $\boldsymbol{r}$ is known. To see this, consider an elementary differentiation step

$$\frac{\partial}{\partial q^j}\frac{\boldsymbol{q}^{\boldsymbol{r}}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^s} = \frac{r^j\boldsymbol{q}^{\boldsymbol{r}-\boldsymbol{e}_j}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^s} - \frac{s\boldsymbol{q}^{\boldsymbol{r}+\boldsymbol{e}_j}}{\left(1+\frac{\boldsymbol{q}^2}{2}\right)^{s+1}}, \tag{B2}$$

where $e_j^i = \delta_{ij}$, and define Δ to be the difference between the degree of the polynomial in the denominator and the numerator. The derivative shifts Δ from $2s - |\boldsymbol{r}|$ to $2s - |\boldsymbol{r}| + 1$, and this is common to both terms on the right-hand side. Hence, the nonzero terms in sum (B1) must satisfy the condition $2s - |\boldsymbol{r}| = |\boldsymbol{m}_1| + \cdots + |\boldsymbol{m}_n| + 2n + 2$. This is also evident on the dimensional ground.

We also note that due to (B2) r^j in (B1) has, for all j, the same even parity as the total degree of differentiation $m_1^j + \cdots + m_n^j$ because otherwise the integral in (A10) would vanish. Altogether, we see that there are only

$$\sum_{\boldsymbol{r},s} 1 = \prod_{j=1}^{D}\sum_{r^j=0}^{m_1^j+\cdots+m_n^j} 1 = \prod_{j=1}^{D}\left[\left(m_1^j + \cdots + m_n^j\right)/2 + 1\right], \tag{B3}$$

nontrivially contributing terms in (B1).

Let us close this Appendix by proving the inequality (47). To this end, we observe that one can write

$$\begin{aligned}(2\mathfrak{m}-1)!! = \frac{2\mathfrak{m}!}{2^{\mathfrak{m}}\mathfrak{m}!} &= \frac{1}{\sqrt{\pi}}\Gamma\left[1/2 + \sum_{j=1}^{D}\left(m_1^j + \cdots + m_n^j\right)\right] \\ &\quad\times\prod_{j=1}^{D} 2^{m_1^j+\cdots+m_n^j} \\ &\geqslant \prod_{j=1}^{D} 2^{m_1^j+\cdots+m_n^j} \geqslant \prod_{j=1}^{D}\left[1 + \left(m_1^j + \cdots + m_n^j\right)/2\right].\end{aligned} \tag{B4}$$

On the first line, we have used the duplication formula [45] $\Gamma(z)\Gamma(z+1/2) = \sqrt{\pi}\Gamma(2z)2^{1-2z}$. On the second line, the use was made of the inequality $\Gamma(1/2+z) \geqslant \sqrt{\pi}$ (valid for $z \geqslant 2$) and the convexity inequality $2^z - 1 \geqslant z\ln 2 > z/2$ (valid for $z \geqslant 0$).

[1] E. Wigner, Phys. Rev. **40**, 749 (1932).
[2] J. G. Kirkwood, Phys. Rev. **44**, 31 (1933).
[3] B. Simon, *Functional Integration and Quantum Physics* (Academic, New York, 1979).
[4] Z. Haba, *Feynman Integral and Random Dynamics in Quantum Physics; A Probabilistic Approach to Quantum Dynamics* (Kluwer, London, 1999).
[5] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th ed. (World Scientific, London, 2009).
[6] J. Zinn-Justin, *Path Integrals in Quantum Mechanics* (Oxford University Press, Oxford, 2005).
[7] W. Fischer, H. Leschke, and P. Müller, J. Phys. A: Math. Gen. **25**, 3835 (1992).
[8] E. W. Brown, B. K. Clark, J. L. DuBois, and D. M. Ceperley, Phys. Rev. Lett. **110**, 146405 (2013).
[9] W. Krauth, *Statistical Mechanics: Algorithms and Computations* (Oxford University Press, Oxford, 2006).
[10] F. T. Hioe and E. W. Montroll, J. Math. Phys. **16**, 1945 (1975).
[11] F. T. Hioe, D. Machlillen, and E. W. Montroll, Phys. Rep. **43**, 305 (1978).
[12] K. Banerjee, P. Bhatnager, V. Choudry, and S. S. Kanwal, Proc. R. Soc. London, Ser. A **360**, 575 (1978).
[13] W. Witschel, Chem. Phys. **56**, 265 (1980).

[14] M. Schwartz, Jr., J. Stat. Phys. **15**, 255 (1976).
[15] W. H. Miller, J. Chem. Phys. **55**, 3146 (1971).
[16] V. S. Jorish and V. Yu. Zitserman, Chem. Phys. Lett. **34**, 378 (1975).
[17] H. J. Korsch, J. Phys A: Math. Gen. **12**, 1521 (1979).
[18] P. Brantut *et al*., Science **337**, 1069 (2012).
[19] Ch. Grenier, C. Kollath, and A. Georges, arXiv:1209.3942.
[20] G. Chabrier, D. Saumon, and A. Potekhin, J. Phys. A **39**, 4411 (2006).
[21] A. Alastuey and Ph. A. Martin, Phys. Rev. A **40**, 6485 (1989); B. Jancovici, Mol. Phys. **32**, 1177 (1976); M. M. Gombert and D. Léger, Phys. Rev. E **57**, 3962 (1998).
[22] M. E. Boyd, S. Y. Larsen, and J. E. Kilpatrick, J. Chem. Phys. **50**, 4034 (1969).
[23] J. Cao and G. A. Voth, J. Chem. Phys. **101**, 6168 (1994).
[24] B. Militzer and D. M. Ceperley, Phys. Rev. E **63**, 066404 (2001).
[25] C. Predescu, D. Sabo, and J. D. Doll, J. Chem. Phys. **119**, 4641 (2003).
[26] R. P. Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).
[27] R. Giachetti and V. Tognetti, Phys. Rev. Lett. **55**, 912 (1985).
[28] S. Paulin, A. Alastuey, and T. Dauxois, J. Stat. Phys. **128**, 1391 (2007).
[29] C. Schubert, Phys. Rep. **355**, 73 (2001).
[30] D. Fliegner, M. G. Schmidt, and C. Schubert, Z. Phys. C: Part. Fields **64**, 111 (1994).
[31] D. Fliegner, P. Haberl, M. G. Schmidt, and C. Schubert, Ann. Phys. (NY) **264**, 51 (1998).
[32] A. A. Belkov, D. Ebert, A. V. Lanyov, and A. Schaale, Int. J. Mod. Phys. A **8**, 1313 (1993).
[33] L. Carson, Phys. Rev. D **42**, 2853 (1990).
[34] K. Kikkawa, Prog. Theor. Phys. **56**, 947 (1976).
[35] R. MacKenzie, F. Wilczek, and A. Zee, Phys. Rev. Lett. **53**, 2203 (1984).
[36] C. M. Fraser, Z. Phys. C: Part. Fields **28**, 101 (1985).
[37] W. G. Gibson, J. Phys. A: Math. Gen. **17**, 1891 (1984).
[38] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[39] B. Simon, *Functional Integration and Quantum Physics* (Academic, New York, 1979).
[40] E. Onofri, Am. J. Phys. **46**, 379 (1978).
[41] J. A. Zuk, J. Phys. A: Math. Gen. **18**, 1795 (1985).
[42] See, e.g., V. S. Vladimirov, *Equations of Mathematical Physics* (Marcel Dekker, New York, 1971).
[43] T. Kihara, Y. Midzuno, and T. Shizume, J. Phys. Soc. Jpn. **10**, 249 (1955).
[44] L. D. Landau and E. Lifschitz, *Statistical Physics* (Pergamon, Elmsford, 1980).
[45] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 7th ed. (Elsevier, New York, 2007).
[46] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.89.012135 for WOLFRAM MATHEMATICA notebook.
[47] Z. Bern and D. A. Kosower, Phys. Rev. Lett. **66**, 1669 (1991); Nucl. Phys. B **379**, 451 (1992).
[48] M. J. Strassler, Nucl. Phys. B **385**, 145 (1992).
[49] M. Blasone, P. Jizba, and G. Vitiello, *Quantum Field Theory and its Macroscopic Manifestations* (Imperial College Press, London, 2011).
[50] D. Fliegner, P. Haberl, M. G. Schmidt, and C. Schubert, Ann. Phys. (NY) **264**, 51 (1998).
[51] D. Fliegner, M. G. Schmidt, and C. Schubert, Z. Phys. C: Part. Fields **64**, 111 (1994).
[52] B. Jancovici, Phys. A (Amsterdam) **91**, 152 (1978).
[53] A. Alastuey and B. Jancovici, Phys. A (Amsterdam) **97**, 349 (1979).
[54] L. Wang, Plasma Phys. Controlled Fusion **29**, 395 (1987).
[55] J. Caro, E. Ruiz Arriola, and L. L. Salcedo, J. Phys. G: Nucl. Part. Phys. **22**, 981 (1996).
[56] T. A. Osborn and F. H. Molzahn, Phys. Rev. A **34**, 1696 (1986).
[57] M. Durand, P. Schuck, and X. Viñas, Phys. Rev. A **36**, 1824 (1987).
[58] H. Kleinert, Phys. Lett. A **173**, 332 (1993).
[59] C. M. Bender, K. A. Milton, M. Moshe, S. S. Pinsky and L. M. Simmons Jr., Phys. Rev. Lett. **58**, 2615 (1987).
[60] P. M. Stevenson, Phys. Rev. D **23**, 2916 (1981).