Cumulant approximations and renormalized Wigner-Kirkwood expansion for quantum Boltzmann densities

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The logarithm of the quantum Boltzmann density $\rho_V(X)=\langle X|e^{-\beta H_V}|X\rangle$, where $H_V=p^2/2m+V$, is expressed as a cumulant expansion in powers of $v=V-W$, where $W(x)=V(X)+V'(X)(x-X)+\frac{1}{2}V''(X)(x-X)^2$ is the local quadratic approximant to $V(x)$ at the point X. Where $V''(X)>0$, this expansion behaves "nonsecularly" as $\beta\to\infty$ (all its terms $\sim\beta$), and thus remains a useful approximation scheme even as the temperature $\beta^{-1}\to 0$ (in that limit, it yields Rayleigh-Schrödinger perturbation expansions of the ground state of H_V). By Taylor expanding $v(x)$ about X in the cumulant expansion, we obtain an expansion which is a *resummation* over powers of $V''(X)$ of the Wigner-Kirkwood (WK) expansion of $\ln\rho_V$; this "renormalized" WK expansion, whose coefficients are simple functions of $V''(X)$, is as simple to use as the ordinary WK expansion, yet more accurate where $V''(X)\neq 0$, and usable down to zero temperature where $V''(X)>0$ (yielding, in that limit, WK-type expansions for the ground state of H_V). In lowest order, it yields an approximation initially proposed by Miller.

I. INTRODUCTION

The quantum Boltzmann density

$$\rho_V(X)=\langle X|e^{-\beta H_V}|X\rangle,\quad H_V=\frac{p^2}{2m}+V\;, \tag{1.1}$$

where β^{-1} is the temperature and H_V is the Hamiltonian for a particle of mass m moving in one dimension over a potential $V(x)$, is of considerable practical importance, but usually difficult to compute. Simple approximations are thus most welcome. A basic approximation, valid in the high-temperature limit ($\beta\to 0$) is the classical

$$\rho_{V,\mathrm{cl}}(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}e^{-\beta V(X)}\;, \tag{1.2}$$

where

$$\lambda=\left[\frac{\beta\hbar^2}{2m}\right]^{1/2} \tag{1.3}$$

is the thermal wavelength (i.e., the de Broglie wavelength at energy β^{-1}). Various improvements to $\rho_{V,\mathrm{cl}}$ have been proposed,[1] notably expansions of $\rho_V(X)$, or of its logarithm, in powers of $\hbar$ (Wigner-Kirkwood expansions),[2–6] and classical path approximations.[7,8]

In this paper, we obtain a new set of approximations by applying cumulant expansion methods as used in the theory of stochastic processes[9] and the theory of relaxation.[10] We use the path-integral representation[11] to facilitate our intuitive understanding. Our main result of practical interest is a resummation over powers of $V''(X)$ [$V(x)\equiv d^2V/dx^2$] of the Wigner-Kirkwood (WK) expansion, providing systematic corrections to an approximation initially proposed by Miller.[7] This "renormalized" WK expansion has been succinctly presented elsewhere;[12] here we give the details of the derivation, and a more elaborate physical discussion. The general approach follows a previous paper.[13]

We start from the observation that at high temperatures, and also at low temperatures in certain cases, $\rho_V(X)$ is mostly determined by the values of $V(x)$ within a *limited* interval $(\Delta x)_{V,\beta,X}$ around the point X. A useful approximation may thus be obtained by substituting for $V(x)$ another potential $W(x)$, chosen such that $W(x)\cong V(x)$ inside the interval Δx, yet simple enough that $\rho_W(X)$ is known exactly, i.e.,

$$\rho_V(X)\cong\rho_W(X)\;. \tag{1.4}$$

Three different forms for $W(x)$ naturally suggest themselves: (a) a constant, (b) a linear approximant, and (c) a quadratic approximant. The first choice yields the classical approximation (1.2), while the other two yield approximations initially introduced by Miller.[7]

To obtain corrections to the approximation (1.4), the straightforward procedure is to expand $\rho_V(X)$ in powers of the "perturbation"

$$v(x)=V(x)-W(x)\;.$$

The terms of that expansion, however, behave secularly (i.e., nth term $\sim\beta^n$) as $\beta\to\infty$, so that the expansion is useless for getting approximations at low temperatures.

The difficulty is similar to that met in the theory of relaxation,[10] and the same solution obtains; viz., expand $\ln\rho_V(X)$, rather than $\rho_V(X)$, in powers of v, thereby getting a *cumulant* expansion.[10,14] Because of the properties of cumulants, that expansion behaves properly (all terms $\sim\beta$) as $\beta\to\infty$, provided the ground state of H_W is *isolated*. The latter condition assures that the stochastic processes associated with $\rho_W(X)$ have *finite memories*. In the limit $\beta\to\infty$, the above cumulant expansion in powers of v becomes the Rayleigh-Schrödinger perturbation expansion of $2\ln\phi_V^0(X)-\beta E_V^0$, where $\phi_V^0(x)$ and E_V^0 are the ground-state wave function and energy of H_V.[13]

The terms of the cumulant expansion are of the form

$$\int_{-\infty}^{\infty} d^n x\, v(x_1)v(x_2)\cdots v(x_n)\int_0^T d^n t\, P_n^c(x_1,t_1;\ldots;x_n,t_n) \tag{1.5}$$

($T=\beta\hbar$) where the functions P_n^c are combinations of propagators over the potential $W(x)$. With $W(x)$ given by one of the three choices indicated earlier [$W(x)$ at most quadratic in x], the functions P_n^c are known in closed form. The integrals (1.5), however, can be evaluated in closed form only if $v(x)$ is a *polynomial* in x. Otherwise, (1.5) must be evaluated numerically; although this is not impracticable for the lowest-order terms, much of the simplicity of the initial approximation (1.4) (known exactly) is lost.

But the fact that (1.5) is exactly calculable for $v(x)$ a polynomial suggests that closed-form corrections to (1.4) be gotten by Taylor-series expanding each factor $v(x_i)$ about X in (1.5). We thereby get a generalized Wigner-Kirkwood type of expansion of $\ln\rho_V(X)$. In the case $W(x)=\text{const}$, this is the ordinary WK expansion[2–6] in powers, formally, of

$$\lambda^2(d/dX)^2 \text{ and } \beta V(X)\,. \tag{1.6}$$

Because λ and β tend to infinity as the temperature tends to zero, this expansion is not usable at low temperatures. However, in the case where $W(x)$ is a quadratic approximant, the above procedure yields a renormalized WK expansion (i.e., a partial resummation of the ordinary WK expansion) which is in powers of

$$\Lambda^2(d/dX)^2 \text{ and } \mathscr{B}\,V(X)\,, \tag{1.7}$$

where the renormalized parameters Λ and $\mathscr{B}$ tend to λ and β as $\beta\to 0$, but stay finite as $\beta\to\infty$, provided $V''(X)>0$. This expansion, whose coefficients are simple functions of $V''(X)$, is as simple to use as the ordinary WK expansion, yet more accurate [where $V''(X)\neq 0$], and applicable down to zero temperature where $V''(X)>0$. It is our main result of practical interest.

The above treatment could be extended to the case of more than one dimension and to nondiagonal elements of the thermal density matrix

$$\rho_V(X,X')=\langle X'|e^{-\beta H_V}|X\rangle\,. \tag{1.8}$$

The evaluation of the terms of the resummed WK expansion would then be much more involved, however. Formulas for the terms of the *ordinary* WK expansion in this general context have recently been given in Ref. 5, and in Ref. 6 if a magnetic field is present.

In Sec. II, we motivate in a heuristic manner the approximation $\rho_V\cong\rho_W$ where $W(x)$ is a local approximant to $V(x)$. In Secs. III and IV, the direct and cumulant expansions of $\rho_V(X)$ in powers of $V-W$ are written down and analyzed. In Sec. V, we study some general features pertaining to the cases where $W(x)$ is quadratic. In Sec. VI, the generalized Wigner-Kirkwood expansions are constructed. The specific cases where $W(x)$ is a constant, a linear approximant and a quadratic approximant are treated in Secs. VII, VIII, and IX, respectively. We end with a short discussion in Sec. X, pointing out that many of the results obtained also apply to the nondiagonal elements of the density matrix (1.8), provided some trivial modifications are done. An appendix contains technical details.

II. APPROXIMATIONS TO $\rho_V(X)$ VIA LOCAL APPROXIMANTS TO $V(x)$

Classically, the relative probability for a particle over a potential $V(x)$ to be found at the point X is given by the Boltzmann factor $e^{-\beta V(X)}$, and depends solely on the value of $V(x)$ *at the point* X. By contrast, the quantum $\rho_V(X)$ is influenced by the values of $V(x)$ *everywhere*, as evidenced by its path-integral representation[7,11]

$$\rho_V(X)=\int_{X,0}^{X,T}\mathscr{D}x(t)\,e^{-\hbar^{-1}S_V[x(t)]}\,,\quad T=\beta\hbar \tag{2.1}$$

where the functional

$$S_V[x(t)]=\int_0^T dt\left[\tfrac{1}{2}m\dot{x}(t)^2+V(x(t))\right] \tag{2.2}$$

is the action for motion over *minus* the potential $V(x)$, and the integral (2.1) is over all paths $x(t)$, $0\le t\le T$, with $x(0)=x(T)=X$.

However, at high temperatures, and also at low temperatures in certain cases, it is essentially the values of $V(x)$ inside a *limited* interval $(\Delta x)_{V,\beta,X}$ about X which determine $\rho_V(X)$. Indeed, at large temperatures, the time T in (2.1) is small, so that trajectories which wander far from X must have large kinetic energies,[11] whence small weights $e^{-S/\hbar}$; the interval Δx is here determined mostly by the kinetic part of the action, and a rough estimate may be gotten from the uncertainty relation $\Delta p\,\Delta x\cong\hbar$ with $(\Delta p)^2/(2m)\cong\beta^{-1}$, yielding $\Delta x\cong(\beta\hbar^2/2m)^{1/2}=\lambda$. In the high-temperature limit $\beta\to 0$, Δx shrinks to zero and the classical approximation (1.2) obtains.

At low temperatures, the time T is large, so that the kinetic part of the action is small [note that $\int_0^T dt\,\dot{x}(t)^2\sim T^{-1}$]; here it is mostly the potential part the action which determines Δx, which thus consists mostly of regions "downhill" of X. If X is near a minimum of $V(x)$, then Δx is again a relatively small interval around X.

The above suggest that if $W(x)$ is another potential such that $\beta|W(x)-V(x)|\ll 1$ for $x\in\Delta x$, then one can approximate $\rho_V(X)\cong\rho_W(X)$. This will be of practical utility if the local approximant $W(x)$ is such that $\rho_W(x)$ is known exactly. Three different such choices of $W(x)$ will be considered (see Fig. 1). (a) The simplest choice is the constant approximant

$$W_X^f(x)\equiv V(X) \tag{2.3a}$$

(the superscript f is for "free particle;" the subscript X, emphasizing the dependence on X, will usually be omitted to simplify notation); this yields the classical approximation [Eq. (1.2)]

$$\rho_V^{f0}(X)\equiv\rho_{W^f}(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}e^{-\beta V(X)}\,. \tag{2.4}$$

The superscript 0 indicates that this approximation is of zeroth order in the "perturbation" $v^f(x)=V(x)-W^f(x)$; higher-order approximations $\rho_V^{fn}(X)$, $n=1,2,\ldots$ will be constructed later on. (b) The linear approximant

$$W_X^l(x)=V(X)+V'(X)(x-X) \tag{2.3b}$$

yields the approximation

$$\rho_V^{l0}(X)\equiv\rho_{W^l}(X)$$
$$=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp[-\beta V(X)+\tfrac{1}{12}\beta^2\lambda^2V'(X)^2]\ . \tag{2.5}$$

(c) The quadratic approximant

$$W_X^q(x)=V(X)+V'(X)(x-X)+\tfrac{1}{2}m\omega_X^2(x-X)^2\ , \tag{2.3c}$$

$$\omega_X^2\equiv V''(X)/m$$

yields the approximation

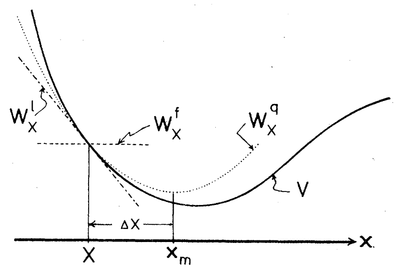

FIG. 1. Potential $V(x)$ and its constant, linear, and quadratic approximants at X.

$$\rho_V^{q0}(X)\equiv\rho_{W^q}(X)=\rho_{\omega_X}(\Delta X)\ , \tag{2.6}$$

where (setting $\Omega=\beta\hbar\omega$, $\widetilde{X}=X/\lambda$)

$$\rho_\omega(x)\equiv\langle x\,|\,e^{-\beta H_\omega}\,|\,x\rangle=\begin{cases}\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\left[\dfrac{\Omega}{\sinh\Omega}\right]^{1/2}\exp[-\tfrac{1}{2}\widetilde{X}^2\Omega\tanh(\tfrac{1}{2}\Omega)] & \text{if } \Omega^2>-\pi^2\\ \infty \quad \text{if } \Omega^2\le-\pi^2\end{cases} \tag{2.7}$$

is the quantum Boltzmann density for the harmonic oscillator

$$H_\omega=\frac{p^2}{2m}+V_\omega,\quad V_\omega(x)=\tfrac{1}{2}m\omega^2x^2\ . \tag{2.8}$$

In (2.6), the argument

$$\Delta X\equiv V'(X)/V''(X)=X-x_m \tag{2.9}$$

is the distance between the point X and the bottom, or top, x_m of the harmonic approximant (2.3c) (see Fig. 1). When $V''(X)$ is negative, ω is imaginary and the hyperbolic functions in (2.7) become circular functions; if, moreover,

$$\Omega^2=(\beta\hbar\omega_X)^2=2\lambda^2\beta V''(X)\le-\pi^2 \tag{2.10}$$

then (2.6)-(2.7) diverges and cannot be used.

The approximations (2.5) and (2.6) were proposed by Miller.[7,15] Approximation (2.6) may, unlike (2.4) and (2.5), be expected to often be usable down to zero temperature, since $\rho_V(X)$ then concentrates near the bottom of $V(x)$, where the latter is usually well approached by its harmonic approximant.[7]

III. EXPANSION IN POWERS OF $V-W$

Introducing $V=W+v$ into (2.1), we rewrite it as

$$\rho_V(X)=\rho_W(X)\left\langle\exp\left[-\hbar^{-1}\int_0^T dt\, v(\hat{x}(t))\right]\right\rangle_W\ , \tag{3.1}$$

where the averaging operation $\langle\ \rangle_W$ is defined by[16]

$$\langle F[\hat{x}(t)]\rangle_W=\frac{\int_{X,0}^{X,T}\mathscr{D}x(t)e^{-\hbar^{-1}S_W[x(t)]}F[x(t)]}{\int_{X,0}^{X,T}\mathscr{D}x(t)e^{-\hbar^{-1}S_W[x(t)]}} \tag{3.2}$$

for any functional $F[x(t)]$ (we shall usually omit the subscript W on $\langle\ \rangle$ when there is no risk of ambiguity). The statistical average (3.2) completely characterizes the *stochastic process*[9] $\hat{x}(t)$ (random variables and processes will always be identified with a caret). Expanding the exponential in (3.1), we obtain the "perturbation expansion"

$$\rho_V(X)=\rho_W(X)\left[1-\hbar^{-1}\int_0^T dt\langle\hat{v}(t)\rangle_W+\tfrac{1}{2}\hbar^{-2}\int_0^T dt_1\int_0^T dt_2\langle\hat{v}(t_1)\hat{v}(t_2)\rangle_W+\cdots\right] \tag{3.3a}$$

$$=\rho_W(X)\left[1-\hbar^{-1}\int_0^T dt\int_{-\infty}^{\infty}dx\, v(x)P_1(x,t)+\tfrac{1}{2}\hbar^{-2}\int_0^T d^2t\int d^2x\, v(x_1)v(x_2)P_2(x_1,t_1;x_2,t_2)+\cdots\right]\ , \tag{3.3b}$$

where we use the abbreviations

$$\int_0^T d^nt=\int_0^T dt_1\int_0^T dt_2\cdots\int_0^T dt_n\ ,$$
$$\int d^nx=\int_{-\infty}^{\infty}dx_1\cdots\int_{-\infty}^{\infty}dx_n\ ,$$
$$\hat{v}(t)=v(\hat{x}(t))\ .$$

In (3.3b), we introduced the *joint probability densities*

$$P_n(x_1,t_1;\ldots;x_n,t_n)$$
$$=\text{Prob}\{\hat{x}(t_i)=x_i,\ i=1,2,\ldots,n\} \tag{3.4}$$
$$=\langle\delta(\hat{x}(t_1)-x_1)\delta(\hat{x}(t_2)-x_2)\cdots\delta(\hat{x}(t_n)-x_n)\rangle \tag{3.4'}$$

$$= \frac{\langle X,0 \mid x_1,t_1 \rangle \langle x_1,t_1 \mid x_2,t_2 \rangle \cdots \langle x_n,t_n \mid X,T \rangle}{\langle X,0 \mid X,T \rangle} . \tag{3.5}$$

In (3.5) we assumed $0 \le t_1 \le t_2 \le \cdots \le t_n \le T$, and denoted by

$$\langle x',t' \mid x'',t'' \rangle = \langle x' \mid e^{-(t''-t')H_W/\hbar} \mid x'' \rangle \tag{3.6}$$

$$= \int_{x',t'}^{x'',t''} \mathscr{D}x(t) e^{-S_W[x(t)]/\hbar} \tag{3.6'}$$

the relative probability for a path to go through x'' at time t'', if it was at x' at t'. We have

$$\langle F(\hat{x}(t_1),\ldots,\hat{x}(t_n)) \rangle = \int d^n x\, F(x_1,\ldots,x_n) P_n(x_1,t_1;\ldots;x_n,t_n) \tag{3.7}$$

for any function $F(x_1,\ldots,x_n)$, and (abbreviating $x_i,t_i = i$)

$$\int_{-\infty}^{\infty} dx_j P_n(1;\ldots;n) = P_{n-1}(1;\ldots;j-1;j+1;\ldots;n),\quad j=1,2,\ldots,n$$
$$\int d^n x P_n(\{x_i,t_i\}) = 1 . \tag{3.8}$$

A typical $P_1(x,t)$ is shown in Fig. 2. Using an overbar to indicate time averaging, i.e.,

$$\overline{f(t_1,\ldots,t_n)} \equiv T^{-n} \int_0^T dt_1 \cdots \int_0^T dt_n f(t_1,\ldots,t_n) \tag{3.9}$$

we denote, for any function $F(x_1,\ldots,x_n)$,

$$\langle\langle F(\hat{x}_1,\ldots,\hat{x}_n) \rangle\rangle \equiv \overline{\langle F(\hat{x}(t_1),\ldots,\hat{x}(t_n)) \rangle} = \int_{-\infty}^{\infty} d^n x\, F(x_1,\ldots,x_n) \mathscr{P}_n(x_1,\ldots,x_n) , \tag{3.10}$$

where the time-averaged density

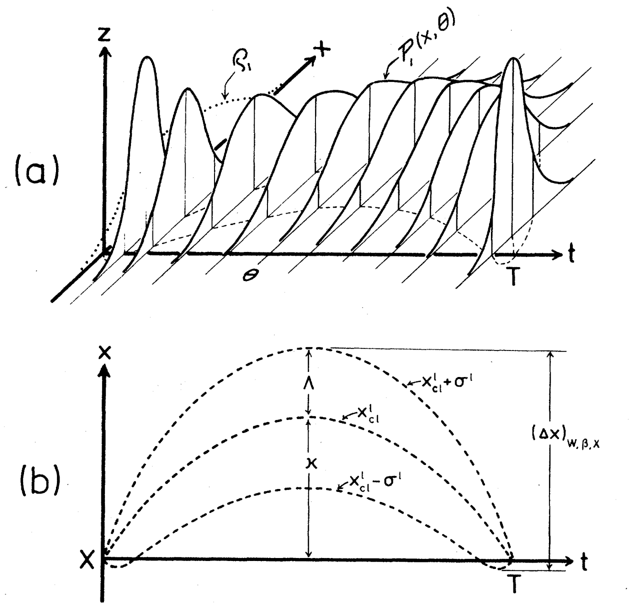

FIG. 2. Shape of the densities $P_1(x,t)$ and $\mathscr{P}_1(x)$ for the case $W(x) = W^l(x)$ linear in x. Note that $P_1(x,t) \to \delta(x)$ as $t \to 0$ or $t \to T$. Dashed curves in the (x,t) plane in both (a) and (b) are the maximum value and (maximum value)/e contours of $P_1(x,t)$ [i.e., the middle curve is $x^l_{cl}(t)$, and the other two are $x^l_{cl}(t) \pm \sigma^l(t)$ (see Sec. V)]. Dotted curve in the (z,x) plane in (a) is $z = \mathscr{P}_1(x)$, and the full curve in the plane $t = \theta$ is $z = P_1(x,\theta)$. [The dashed contours in (a) and (b), and the corresponding values of $P_1(x,t)$, are calculated; the other values of $P_1(x,t)$, and the curve $z = \mathscr{P}_1(x)$, are rough estimates.]

$$\mathscr{P}_n(x_1,\ldots,x_n) \equiv \overline{P_n(x_1,t_1;\ldots;x_n,t_n)} = \left\langle\left\langle \prod_{i=1}^{n} \delta(\hat{x}_i - x_i) \right\rangle\right\rangle \tag{3.11}$$

is obviously symmetric in its arguments, and satisfies relations similar to (3.8). Equations (3.3) may then be written as

$$\rho_V(X) = \rho_W(X)[1 - \beta\langle\langle v(\hat{x}) \rangle\rangle + \tfrac{1}{2}\beta^2 \langle\langle v(\hat{x}_1) v(\hat{x}_2) \rangle\rangle + \cdots] \tag{3.3c}$$

$$= \rho_W(X) \left[1 - \beta \int dx\, v(x) \mathscr{P}_1(x) + \tfrac{1}{2}\beta^2 \int dx_1 \int dx_2 v(x_1) v(x_2) \mathscr{P}_2(x_1,x_2) + \cdots \right] . \tag{3.3d}$$

At first glance, one would expect to improve the approximation $\rho_V \cong \rho_W$ by truncating expansion (3.3) later than its first term. This, however, is true only at high temperatures; at low temperatures, the "secular" behavior (where $\sim$ means "of *roughly* the same size as")

$$\left.\begin{aligned} &\int_0^T d^n t \langle \hat{v}(t_1) \hat{v}(t_2) \cdots \hat{v}(t_n) \rangle \sim T^n \\ &\langle\langle v(\hat{x}_1) v(\hat{x}_2) \cdots v(\hat{x}_n) \rangle\rangle \sim \langle\langle \mid v(\hat{x}) \mid \rangle\rangle^n \end{aligned}\right\} T \to \infty \tag{3.12}$$

i.e., the fact that (3.3) is roughly in powers of $\beta\langle\langle \mid v(\hat{x}) \mid \rangle\rangle_W$, renders that expansion useless when β is large.

The situation is similar to that met in the theory of relaxation.[10] There, the remedy is to perform a cumulant expansion,[14] which is "nonsecular," provided that the stochastic processes involved have finite memories. But this is also the case here if the ground state of H_W is isolated, the memory of the stochastic process $\{\hat{x}(t), \langle\ \rangle_W\}$ then being

$$\tau_W \cong \hbar/\Delta E_W^0 , \tag{3.13}$$

where ΔE_W^0 is the energy gap between the ground and first excited states of H_W; indeed we have, from (3.6) (ϕ_W^n and E_W^n the eigenstates and energies of H_W),[17]

$$\langle x',t'|x'',t''\rangle = \sum_n \phi_W^n(x')\phi_W^n(x'')e^{-(t''-t')E_W^n/\hbar}$$

$$\cong \phi_W^0(x')\phi_W^0(x'')e^{-(t''-t')E_W^0/\hbar}$$

$$\text{for } |t''-t'| \gg \hbar/\Delta E_W^0$$

from which we readily deduce (abbreviating $x_i,t_i \equiv i$)

$$P_n(1;\ldots;n) \cong P_m(1;\ldots;m)P_{n-m}(m+1;\ldots;n)$$
$$\text{if } |t_{m+1}-t_m| \gg \tau_W,\ n\geq 2,\ m=2,\ldots,n-1 \quad (3.14)$$

which is the habitual characterization of a finite memory process.[9]

IV. CUMULANT EXPANSIONS

Expanding $\ln\langle \exp[\int dt\, \hat{v}(t)]\rangle$ in powers of v, we rewrite (3.1) as

$$\rho_V(X) = \rho_W(X)\exp\left[\left\langle \exp\left[-\hbar^{-1}\int_0^T dt\,\hat{v}(t)\right]-1\right\rangle_{c\{v\}}\right]$$
$$= \rho_W(X)\exp\left[-\hbar^{-1}\int_0^T dt\langle\hat{v}(t)\rangle + \tfrac{1}{2}\hbar^{-2}\int_0^T dt_1\int_0^T dt_2\langle\hat{v}(t_1)\hat{v}(t_2)\rangle_{c\{v\}} + \cdots\right] \quad (4.1a)$$
$$= \rho_W(X)\exp\left[-\hbar^{-1}\int_0^T dt\int_{-\infty}^{\infty} dx\, v(x)P_1(x,t) + \tfrac{1}{2}\hbar^{-2}\int_0^T d^2t\int d^2x\, v(x_1)v(x_2)P_2^c(x_1,t_1;x_2,t_2) + \cdots\right], \quad (4.1b)$$

where $\langle\ \rangle_{c\{v\}}$ denotes the cumulant "average",[10] i.e.,

$$\langle\hat{v}\rangle_{c\{v\}} = \langle\hat{v}\rangle,\ \langle\hat{v}_1\hat{v}_2\rangle_{c\{v\}} = \langle\hat{v}_1\hat{v}_2\rangle - \langle\hat{v}_1\rangle\langle\hat{v}_2\rangle,$$
$$\langle 123\rangle_c = \langle 123\rangle - \langle 12\rangle\langle 3\rangle - \langle 1\rangle\langle 23\rangle$$
$$-\langle 13\rangle\langle 2\rangle + 2\langle 1\rangle\langle 2\rangle\langle 3\rangle, \quad (4.2)$$
$$\ldots .$$

The brackets { } contain the *cumulant arguments*, i.e., the variables with respect to which the cumulants are built (e.g., if $\hat{v}_1=\hat{x}^2$ and $\hat{v}_2=\hat{x}$, then $\langle\hat{v}_1\hat{v}_2\rangle_{c\{v\}} = \langle\hat{v}_1\hat{v}_2\rangle - \langle\hat{v}_1\rangle\langle\hat{v}_2\rangle = \langle\hat{x}^3\rangle - \langle\hat{x}^2\rangle\langle\hat{x}\rangle$, while $\langle\hat{v}_1\hat{v}_2\rangle_{c\{x\}} = \langle\hat{x}^3\rangle - 3\langle\hat{x}^2\rangle\langle\hat{x}\rangle + 2\langle\hat{x}\rangle^3$). In cases where the cumulant arguments are the blocks of all similarly indexed factors, we shall also use the notation $\langle\ \rangle_{c*}$; e.g.,

$$\langle\hat{x}_1\hat{x}_2\hat{y}_1\rangle_{c*} \equiv \langle\hat{x}_1\hat{x}_2\hat{y}_1\rangle_{c\{x_1y_1,x_2\}}$$
$$= \langle\hat{x}_1\hat{x}_2\hat{y}_1\rangle - \langle\hat{x}_1\hat{y}_1\rangle\langle\hat{x}_2\rangle,$$
$$\left\langle\prod_{i=1}^n \hat{x}_i^{m_i}\right\rangle_{c*} = \left\langle\prod_{i=1}^n \hat{x}_i^{m_i}\right\rangle_{c\{x^m\}}, \quad (4.3)$$
$$\left\langle\prod_{i=1}^n f_i(\hat{x}_i)\right\rangle_{c*} = \left\langle\prod_{i=1}^n f_i(\hat{x}_i)\right\rangle_{c\{f\}}.$$

In (4.1b), we introduced cumulant "densities"

$$P_n^c(x_1,t_1;\ldots;x_n,t_n) = \left\langle\prod_{i=1}^n \delta(\hat{x}(t_i)-x_i)\right\rangle_{c\{\delta\}} \quad (4.4)$$

or, in terms of the densities P_n [Eq. (3.4)],

$$P_1^c(x,t) = P_1(x,t),$$
$$P_2^c(1,2) = P_2(1,2) - P_1(1)P_1(2),$$
$$P_3^c(1,2,3) = P_3(1,2,3) - P_1(1)P_2(2,3) - P_2(1,2)P_1(3) - P_2(1,3)P_1(2) + 2P_1(1)P_1(2)P_1(3), \quad (4.4')$$
$$\ldots .$$

For any set of functions $f_i(x)$, we have

$$\left\langle\prod_{i=1}^n f_i(\hat{x}(t_i))\right\rangle_{c\{f\}} = \int d^nx\prod_{i=1}^n f_i(x_i)P_n^c(\{x_i,t_i\}). \quad (4.5)$$

In general, we shall append a subscript or superscript c to identify objects constructed with the cumulant algorithm (4.2) or (4.4′) from an initial family of objects. For example,

$$\mathscr{P}_n^c(x_1,\ldots,x_n) \equiv \overline{P_n^c(x_1,t_1;\ldots;x_n,t_n)}$$
$$= \left\langle\!\left\langle\prod_{i=1}^n \delta(\hat{x}_i-x_i)\right\rangle\!\right\rangle_{c\{\delta\}} \quad (4.6)$$

is related to the time-averaged densities $\mathscr{P}_n$ [Eq. (3.11)] in the same manner as P_n^c is related to the P_n, and Eq. (4.1) may be written

$$\rho_V(X) = \rho_W(X)\exp[-\beta\langle\!\langle v(\hat{x})\rangle\!\rangle + \tfrac{1}{2}\beta^2\langle\!\langle v(\hat{x}_1)v(\hat{x}_2)\rangle\!\rangle_{c*} + \cdots] \quad (4.1c)$$
$$= \rho_W(X)\exp\left[-\beta\int dx\, v(x)\mathscr{P}_1^c(x) + \tfrac{1}{2}\beta^2\int dx_1\int dx_2 v(x_1)v(x_2)\mathscr{P}_2^c(x_1,x_2) + \cdots\right]. \quad (4.1d)$$

We have [compare (3.8)]

$$\int_{-\infty}^{\infty} dx\, P_1^c(x,t) = 1,\quad \int_{-\infty}^{\infty} dx\, \mathscr{P}_1^c(x) = 1; \quad (4.7)$$

$$\left.\begin{array}{l}\int_{-\infty}^{\infty} dx_j P_n^c(x_1,t_1;\ldots;x_n,t_n) = 0\\ \int_{-\infty}^{\infty} dx_j \mathscr{P}_n^c(x_1,\ldots,x_n) = 0\end{array}\right\} j=1,2,\ldots,n,\ n\geq 2. \quad (4.8b)$$

Equations (4.8) follow from the basic property of cumulants of vanishing if their arguments separate into two or more independent subsets:[10] thus, e.g.,

$$\int dx_1 \left\langle \prod_{i=1}^{n} \delta(\hat{x}(t_i)-x_i) \right\rangle_{c\{\delta\}} = \left\langle \hat{1} \prod_{i=2}^{n} \delta(\hat{x}(t_i)-x_i) \right\rangle_{c\{1,\delta\}} = 0 \; ;$$

they imply that the $\mathscr{P}_n^c$, $n \geq 2$, assume both positive and negative values. We therefore expect the cumulant integrals in (4.1d) to usually be less, due to the oscillations of $\mathscr{P}_n^c(x_1,\ldots,x_n)$, than the moment integrals in (3.3d) [note that $\mathscr{P}_n(x_1,\ldots,x_n) \geq 0$], and accordingly approximations obtained by truncating the cumulant expansion (4.1) to be better than approximations obtained by truncating the moment expansion (3.3).

But more importantly, in the cases where the stochastic process $\{\hat{x}(t), \langle\;\rangle_W\}$ has a finite memory τ_W, the basic property of cumulants mentioned above implies that

$$\left.\begin{array}{l} \langle \hat{v}(t_1)\hat{v}(t_2)\cdots\hat{v}(t_n)\rangle_{c\{v\}} \to 0 \\ P_n^c(x_1,t_1;\ldots;x_n,t_n) \to 0 \end{array}\right\} \text{ for } t_n - t_1 \gg n\tau_W \;\; (0 \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq T) \tag{4.9}$$

since when $(t_n-t_1) \gg n\tau_W$, there is at least one gap $(t_{j+1}-t_j) \gg \tau_W$, i.e., the set $\{\hat{x}(t_1),\ldots,\hat{x}(t_n)\}$ separates into at least two mutually independent subsets. The fact that the quantities in (4.9) are sizable only if the times $t_1,\ldots,t_n$ are clustered together implies [compare (3.12)]

$$\left.\begin{array}{l} \int_0^T d^n t \langle \hat{v}(t_1)\hat{v}(t_2)\cdots\hat{v}(t_n)\rangle_{c\{v\}} \sim T\tau_W^{n-1} \\ \langle\!\langle v(\hat{x}_1)v(\hat{x}_2)\cdots v(\hat{x}_n)\rangle\!\rangle_{c\{v\}} \\ \quad \sim (\tau_W/T)^{n-1} \langle\!\langle\, |v(\hat{x})| \,\rangle\!\rangle^n \end{array}\right\} \; T \to \infty \; . \tag{4.10}$$

Hence, when τ_W is finite, all the terms of the cumulant expansion (4.1) grow linearly with β as $\beta \to \infty$, so that (4.1) stays a usable perturbation expansion even as the temperature $\beta^{-1} \to 0$. In that limit, it becomes the Rayleigh-Schrödinger expansion of $2\ln\phi_V^0(X) - \beta E_V^0$, as is clear from considering

$$\rho_V(X) = \sum_n [\phi_V^n(X)]^2 e^{-\beta E_V^n} \to [\phi_V^0(X)]^2 e^{-\beta E_V^0} \;\; \text{as } \beta \to \infty \; , \tag{4.11}$$

where $\phi_V^n(x)$ and E_V^n are the eigenstates and energies of H_V.

For discussion purposes, it is convenient to combine (4.10) with the corresponding relation for small T as [generalizing to any set $\{f_i(x)\}$]

$$\left\langle\!\!\left\langle \prod_{i=1}^{n} f_i(\hat{x}_i) \right\rangle\!\!\right\rangle_{c\{f\}} \sim (\mathscr{B}/\beta)^{n-1} \prod_{i=1}^{n} \langle\!\langle\, |f_i(\hat{x})| \,\rangle\!\rangle \; , \tag{4.12}$$

where $\mathscr{B}$ is a (smooth) function of β chosen such that $\mathscr{B} \to \beta$ as $\beta \to 0$ and $\mathscr{B} \to \tau_W/\hbar$ as $\beta \to \infty$; a natural choice is

$$\mathscr{B}^{-1} = \bar{E}_{W,\beta} \equiv \mathrm{Tr}(H_W e^{-\beta H_W})/\mathrm{Tr}e^{-\beta H_W} - W_{\min} \; , \tag{4.13}$$

where $\bar{E}_{W,\beta}$ is the mean thermal energy measured relative to the bottom $W_{\min}$ of $W(x)$ (we indeed have $\bar{E} \sim \beta^{-1}$ as $\beta \to 0$ and $\bar{E} \sim E_W^0 - W_{\min} \cong \Delta E_W^0 = \hbar/\tau_W$ as $\beta \to \infty$). In the quadratic case (2.3c), we have (for ω real)

$$\bar{E}_{\omega,\beta} = \tfrac{1}{2}\hbar\omega \coth(\tfrac{1}{2}\beta\hbar\omega) \to \begin{cases} \tfrac{1}{2}\hbar\omega & \text{as } \beta \to \infty \\ \beta^{-1} & \text{as } \beta \to 0 \; . \end{cases} \tag{4.14}$$

Equation (4.12) can be made to also cover the infinite memory cases if we define more generally

$$\mathscr{B} = \begin{cases} \bar{E}_{W,\beta}^{-1} & \text{if } E_W^0 \text{ is isolated} \\ \beta & \text{otherwise} \; . \end{cases} \tag{4.15}$$

According to (4.12), the cumulant expansion (4.1) is roughly in powers of $\mathscr{B}\langle\!\langle\, |v(x)| \,\rangle\!\rangle$.

V. GAUSSIAN CASES

When the potential $W(x)$ is at most quadratic in x, the densities P_n and P_n^c are exactly calculable, and have remarkable properties. For studying these, it is convenient to introduce an auxiliary stochastic process.

A. The process $\{\hat{y}(t), \langle\;\rangle_W^{\sim}\}$

We shall denote by $x_{\mathrm{cl}}^W(x',t';x'',t'';t)$ the classical trajectory from (x',t') to (x'',t'') over *minus* the potential $W(x)$. Let us denote concisely by

$$x_{\mathrm{cl}}(t) \equiv x_{\mathrm{cl}}^W(X,0;X,T;t)$$

the classical trajectory from $(X,0)$ to (X,T), and set

$$\hat{y}(t) \equiv \hat{x}(t) - x_{\mathrm{cl}}(t) \; . \tag{5.1}$$

We identify with a tilde the average over the stochastic process $\hat{y}(t)$; thus,

$$\begin{aligned} \langle F[\hat{y}(t)]\rangle^{\sim} &= \langle F[\hat{x}(t) - x_{\mathrm{cl}}(t)]\rangle \; , \\ \langle F[\hat{x}(t)]\rangle &= \langle F[x_{\mathrm{cl}}(t) + \hat{y}(t)]\rangle^{\sim} \end{aligned} \tag{5.2}$$

for any functional $F[\;]$. Equivalently,

$$\langle F[\hat{y}(t)]\rangle^{\sim} = \frac{\int_{0,0}^{0,T} \mathscr{D}y(t) e^{-S_{\tilde{W}}[y(t)]} F[y(t)]}{\int_{0,0}^{0,T} \mathscr{D}y(t) e^{-S_{\tilde{W}}[y(t)]}} \; , \tag{5.3}$$

where the integrals are over all paths $y(t)$, $0 \leq t \leq T$, with $y(0) = y(T) = 0$ [compare (3.2)], and the (time-dependent) potential

$$\tilde{W}(y,t) = W(x_{\mathrm{cl}}(t)+y) - W(x_{\mathrm{cl}}(t)) - yW'(x_{\mathrm{cl}}(t)) \; . \tag{5.4}$$

We associate with the process $\{\hat{y}(t), \langle\;\rangle_{\tilde{W}}\}$ the same objects and operations, identified with tildes ($\tilde{P}_n$, $\tilde{\mathscr{P}}_n$,

$\langle\!\langle\ \rangle\!\rangle^{\sim}$, etc.) as were associated with $\hat{x}(t)$; the tilded densities possess all the properties of their untilded counterparts [(3.8), (4.7), (4.8), etc.].

In view of (5.2), the densities $P_n(\{x_i,t_i\})$ are expressible in terms of the densities $\widetilde{P}_n(\{y_i,t_i\})$ as

$$P_n(\{x_i,t_i\})=\widetilde{P}_n(\{x_i-x_{\rm cl}(t_i),t_i\}) . \qquad (5.5)$$

Also, for any function $F(x_1,\ldots,x_n)$

$$\langle\!\langle F(\{\hat{x}_i\})\rangle\!\rangle=\langle\!\langle F(\{x_{\rm cl}(t_i)+\hat{y}_i\})\rangle\!\rangle^{\sim} = \int d^n y\, F(\{x_{\rm cl}(t_i)+y_i\})\widetilde{P}_n(\{y_i,t_i\}) . \qquad (5.6)$$

In the special cases where $x_{\rm cl}(t)\equiv X$ is stationary, the time-integrated density $\mathscr{P}_n$ is simply expressible in terms of $\widetilde{\mathscr{P}}_n$ (but not otherwise), and we have

$$\mathscr{P}_n(x_1,\ldots,x_n)=\widetilde{\mathscr{P}}_n(x_1-X,\ldots,x_n-X), \qquad (5.7a)$$

$$\langle\!\langle F(\hat{x}_1,\ldots,\hat{x}_n)\rangle\!\rangle=\int d^n y\, F(\{X+y_i\})\widetilde{\mathscr{P}}_n(y_1,\ldots,y_n) . \qquad (5.7b)$$

B. $W(x)$ quadratic

We now consider features specific to the cases where $W(x)$ is quadratic. Henceforth, in this section, all quantities refer to the potential

$$W(x)=a+bx+\tfrac{1}{2}m\omega^2x^2,\quad \widetilde{W}(y)=\tfrac{1}{2}m\omega^2y^2 . \qquad (5.8)$$

Here $\widetilde{W}(y)$ [Eq. (5.4)] is free of $x_{\rm cl}(t)$, implying that the operation $\langle\ \rangle^{\sim}$ [Eq. (5.3)] is independent of X and of the constants a and b.

With $W(x)$ quadratic, the propagator (3.6) is given by[18]

$$\langle x',t'\,|\,x'',t''\rangle=(2\pi\hbar)^{-1/2}\left[\frac{\partial^2 S_{\rm cl}}{\partial x'\partial x''}\right]^{1/2} \times\exp[-\hbar^{-1}S_{\rm cl}(x',t';x'',t'')] , \qquad (5.9)$$

$$S_{\rm cl}(x',t';x'',t'')\equiv S[x^{W}_{\rm cl}(x',t';x'',t'';t)] . \qquad (5.10)$$

More precisely, (5.9) holds if the classical trajectory *minimizes* the action S, i.e., if S is bounded below; otherwise, $\langle x',t'\,|\,x'',t''\rangle$ is infinite.

The classical action (5.10) is a quadratic form in x' and x''. It then follows from (5.9) and (3.5) that the densities $P_n(\{x_i,t_i\})$ are exponentials of quadratic forms in the x_i; this defines $\hat{x}(t)$ as a *Gaussian stochastic process.*[9,10] A basic property of such processes is that

$$\langle \hat{x}(t_1)\hat{x}(t_2)\cdots\hat{x}(t_n)\rangle_{c\{x\}}=0 \quad\text{for } n\geq 3 . \qquad (5.11)$$

The densities $\widetilde{P}_n$ (for W quadratic, again) are easily shown to have the expressions

$$\widetilde{P}_n(y_1,t_1;\ldots;y_n,t_n) =\pi^{-n/2}(\det{}^nA)^{1/2}\exp\left[-\sum_{i=1}^{n}{}^nA_{ii}y_i^2-2\sum_{i=1}^{n}{}^nA_{i,i+1}y_iy_{i+1}\right] , \qquad (5.12)$$

where ${}^nA$ is a symmetric matrix of elements (we set $t_0=0$, $t_{n+1}=T$, $y_0=y_{n+1}=0$, and abbreviate $y_i,t_i=i$)

$$\begin{aligned}{}^nA_{ii}&=\tfrac{1}{2}\hbar^{-1}\frac{\partial^2}{\partial y_i^2}[\widetilde{S}_{\rm cl}(i-1;i)+\widetilde{S}_{\rm cl}(i;i+1)] ,\\ {}^nA_{i,i+1}&={}^nA_{i+1,i}=\tfrac{1}{2}\hbar^{-1}\frac{\partial^2}{\partial y_i\partial y_{i+1}}\widetilde{S}_{\rm cl}(i;i+1) ,\end{aligned} \qquad (5.13)$$

and $\widetilde{S}_{\rm cl}(y',t';y'',t'')$ is the classical action from (y',t') to (y'',t'') over the potential $-\widetilde{W}(y)$. The elements of the matrix ${}^nA$ not displayed in (5.13) are zero. Note that ${}^nA$ does not depend on the y_i, since the classical actions are quadratic in the latter.

The Gaussian densities $\widetilde{P}_n$ [Eq. (5.12)], and also their time integrals $\widetilde{\mathscr{P}}_n$, have the symmetry

$$\begin{aligned}&\widetilde{P}_n(-y_1,t_1;\ldots;-y_n,t_n)=\widetilde{P}_n(y_1,t_1;\ldots;y_n,t_n) ,\\ &\widetilde{\mathscr{P}}_n(-y_1,\ldots,-y_n)=\widetilde{\mathscr{P}}_n(y_1,\ldots,y_n)\end{aligned} \qquad (5.14)$$

implying

$$\left.\begin{aligned}&\left\langle\prod_{i=1}^{n}[\hat{y}(t_i)]^{m_i}\right\rangle^{\sim}=0\\ &\langle\!\langle \hat{y}_1^{m_1}\hat{y}_2^{m_2}\cdots\hat{y}_n^{m_n}\rangle\!\rangle^{\sim}=0\end{aligned}\right\}\ \text{for } \sum_{i=1}^{n}m_i \text{ odd} . \qquad (5.15)$$

The associated cumulant densities $\widetilde{P}_n^{\,c}$ and $\widetilde{\mathscr{P}}_n^{\,c}$ inherit the symmetry (5.14), whence relations similar to (5.15); combining these with the Gaussian property (5.11), we have

$$\left.\begin{aligned}&\left\langle\prod_{i=1}^{n}[\hat{y}(t_i)]^{m_i}\right\rangle^{\sim}_{c\{y^m\}}=0\\ &\langle\!\langle \hat{y}_1^{m_1}\hat{y}_2^{m_2}\cdots\hat{y}_n^{m_n}\rangle\!\rangle^{\sim}_{c\{y^m\}}=0\end{aligned}\right\}\ \text{for } \left[\sum_{i=1}^{n}m_i \text{ odd}\right] \text{ or } \{m_i=1,\ i=1,2,\ldots,n,\ n\geq 3\} . \qquad (5.16)$$

1. Discussion

The probability density $P_1(x,t)=\text{Prob}\{\hat{x}(t)=x\}$ may be written in the suggestive form

$$P_1(x,t)=\pi^{-1/2}\sigma(t)^{-1}\exp\{-[x-x_{\rm cl}(t)]^2/\sigma(t)^2\} , \qquad (5.17)$$

where the "thermal quantum dispersion function" $\sigma(t)={}^1A_{11}^{-1/2}$ is given by

$$[\sigma(t)]^{-2}=\tfrac{1}{2}\hbar^{-1}\frac{\partial^2}{\partial x^2}[\widetilde{S}_{\rm cl}(0,0;x,t)+\widetilde{S}_{\rm cl}(x,t;0,T)] . \qquad (5.18)$$

A typical shape of $P_1(x,t)$ was shown in Fig. 2. We shall denote

$$\kappa=\max_{0\le t\le T}|x_{\rm cl}(t)-X| \ , \quad \Lambda=\max_{0\le t\le T}|\sigma(t)| \ . \tag{5.19}$$

These may be regarded as two components of the interval $(\Delta x)_{W,\beta,X}$ (discussed in Sec. II) spanned by the thermal quantum wanderings over the potential $W(x)$: κ is the extension of the mean wandering, and Λ the dispersion about that mean [see Fig. 2(b)].

The densities $P_n(x_1,t_1;\ldots;x_n,t_n)$ are centered about $(x_{\rm cl}(t_1),\ldots,x_{\rm cl}(t_n))$, and of extent roughly Λ in each x_i. Let us consider $[y_i\equiv x_i-x_{\rm cl}(t_i)]$

$$P_2(x_1,t_1;x_2,t_2)=\pi^{-1}(\det{}^2A)^{1/2} \times\exp(-{}^2A_{11}y_1^2-2\,{}^2A_{12}y_1y_2-{}^2A_{22}y_2^2) \ . \tag{5.20}$$

Because P_2 is integrable [Eq. (3.8)], the curves in the (x_1,x_2) plane corresponding to constant values of the exponent in (5.20), i.e., the *contours* of P_2, must be ellipses [see Fig. 3(a)] (if they were parabolas or hyperbolas, P_2 would not be integrable). These ellipses are centered at $(x_{\rm cl}(t_1),x_{\rm cl}(t_2))$, and tilted relative to the x_1 and x_2 axes due to the cross term ${}^2A_{12}y_1y_2$; because ${}^2A_{12}<0$ in general [see Eqs. (7.3) and (9.11)], the major axes point from the $--$ to the $++$ quadrants of the (y_1,y_2) plane.

Thus, $P_2(x_1,t_1;x_2,t_2)$ is maximum when x_1 and x_2 lie on the classical trajectory $x_{\rm cl}(X,0;X,T;t)$. As x_1 and x_2 depart from $x_{\rm cl}$, P_2 decreases, faster if x_1 and x_2 are on opposite sides of $x_{\rm cl}$ (because trajectories passing through x_1 and x_2 must then have larger kinetic energies, hence smaller weights), and slower if x_1 and x_2 are on the same side of $x_{\rm cl}$; that is, x_1 and x_2 are *correlated* (due to ${}^2A_{12}$).

The cumulant "density" $P_2^c(x_1,t_1;x_2,t_2)$ [Eq. (4.4)] [see Fig. 3(b)] is a measure of this correlation, being the difference between $P_2(x_1,t_1;x_2,t_2)$ and the uncorrelated product $P_1(x_1,t_1)P_1(x_2,t_2)$, whose contours are ellipses with axes *parallel* to the x_1 and x_2 axes [Fig. 3(a)].

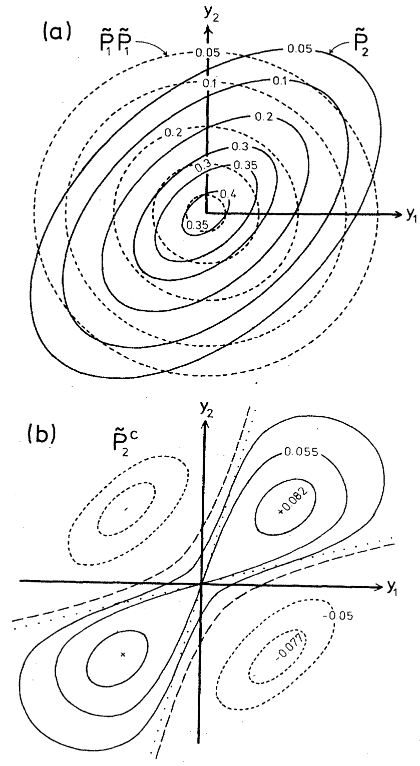

FIG. 3. Contours of $\tilde P_2(y_1,t_1;y_2,t_2)$, $\tilde P_1(y_1,t_1)\tilde P_1(y_2,t_2)$, and $\tilde P_2^c(y_1,t_1;y_2,t_2)$ for the case $\tilde W(x)\equiv 0$, at $t_1=T/3$, $t_2=2T/3$ ($\lambda\equiv 1$). (a) Full ellipses are contours of $\tilde P_2(y_1,t_1;y_2,t_2)$, dashed circles are contours of $\tilde P_1(y_1,t_1)\tilde P_1(y_2,t_2)$. For the special values of t_1,t_2 chosen here, the contours of $\tilde P_2$ are tilted by 45°, and the contours of $\tilde P_1\tilde P_1$ are circles (in general, the tilt of $\tilde P_2$ can be any angle, and the contours of $\tilde P_1\tilde P_1$ are ellipses with axes parallel to the y_1,y_2 axes). At (0,0), $\tilde P_2=0.41$ and $\tilde P_1\tilde P_1=0.36$. (b) Contours of $\tilde P_2^c(y_1,t_1;y_2,t_2)$ [i.e., the difference of the contours in (a)]. Solid curves are positive values, dashed curves negative values; the long-dashed hyperbola, whose asymptotes are the dotted straight lines, is $\tilde P_2^c=0$. [The curve $\tilde P_2^c=0$, and the minima and maxima, are calculated; the other (approximate) contours were deduced from the intersections of the contours of $\tilde P_2$ and $\tilde P_1\tilde P_1$ in a denser version of (a).]

VI. GENERALIZED WIGNER-KIRKWOOD EXPANSION

Let us introduce the dimensionless quantities [see (5.19)]

$$\hat z(t)\equiv\hat y(t)/\Lambda, \quad \Delta x_{\rm cl}(t)=[x_{\rm cl}(t)-X]/\kappa \ . \tag{6.1}$$

We identify with an acute accent (′) the statistical averages, densities, etc., associated with the process $\hat z(t)$; we have, e.g.,

$$\acute P_n(\{z_i,t_i\})=\Lambda^n\tilde P_n(\{\Lambda z_i,t_i\}) \ ,$$
$$\acute{\mathscr P}_n(\{z_i\})=\Lambda^n\tilde{\mathscr P}_n(\{\Lambda z_i\}) \ . \tag{6.2}$$

Using (5.6) in the form

$$\left\langle\!\left\langle\prod_i v(\hat x_i)\right\rangle\!\right\rangle_{c\{v\}}=\left\langle\!\left\langle\prod_i v(x_{\rm cl}(t_i)+\Lambda\hat z_i)\right\rangle\!\right\rangle'_{c\{v\}} \tag{6.3}$$

in (4.1c), and Taylor series expanding in powers of Λ, we get

$$\rho_V(X)=\rho_W(X)\exp\left[\sum_{n=1}^{\infty}\frac{(-\beta)^n}{n!}\sum_{\{m_i\ge 0\}}\frac{\Lambda^{\sum_i m_i}}{\prod_i m_i!}\prod_{i=1}^{n}[v_{\rm cl}^{m_i'}(t_i)]\left\langle\prod_{i=1}^{n}[\hat z(t_i)]^{m_i}\right\rangle'_{c*}\right] \tag{6.4}$$

$$=\rho_W(X)\exp\{-\beta\overline{v_{\rm cl}(t)}-\tfrac{1}{2}\Lambda^2[\beta\overline{v_{\rm cl}''(t)\langle\hat z(t)^2\rangle'}-\beta^2\overline{v_{\rm cl}'(t_1)v_{\rm cl}'(t_2)\langle\hat z(t_1)\hat z(t_2)\rangle'}]+\cdots\} \ , \tag{6.4'}$$

($v^{m\prime} \equiv d^m v/dx^m$) where we denote

$$v_{\rm cl}^{m\prime}(t) \equiv v^{m\prime}(x_{\rm cl}(t)) = v^{m\prime}(X+\kappa\,\Delta x_{\rm cl}(t)) \ . \tag{6.5}$$

Equation (6.4′) pertains only to the case of $W(x)$ quadratic, as we invoked (5.16) to eliminate a number of terms of (6.4); in particular, only *even* powers of Λ appear [by (5.15) also, a number of cumulants have become ordinary moments, e.g., $\langle \hat{z}(t_1)\hat{z}(t_2)\rangle'_c = \langle \hat{z}(t_1)\hat{z}(t_2)\rangle'$]. The cumulants $\langle \prod_i [\hat{z}(t_i)]^{m_i}\rangle'_{c*}$ are all calculable in closed form (for W quadratic). Since the dispersion of the process $\hat{y}(t)$ is of order Λ, that of $\hat{z}(t)$ is of order 1, so that by (4.12), expansion (6.4) may be viewed as in powers of $\Lambda^2(d/dx)^2$ and $\mathscr{B}v(x)$. Note the intuitively appealing "classical path" approximation

$$\rho_V(X) \cong \rho_W(X) e^{-\overline{\beta v(x_{\rm cl}(t))}} \ . \tag{6.6}$$

We now expand each $v_{\rm cl}^{m\prime}(t)$ in (6.4) in powers of κ; we get

$$\rho_V(X) = \rho_W(X)\exp\left[\sum_{n=1}^{\infty}\frac{(-\beta)^n}{n!}\sum_{\{m_i+r_i\geq 0\}}\Lambda^{\sum_i m_i}\kappa^{\sum_i r_i}\prod_{i=1}^{n}\frac{v^{(m_i+r_i)\prime}(X)}{m_i!\,r_i!}\overline{\prod_{i=1}^{n}[\Delta x_{\rm cl}(t_i)]^{r_i}\left\langle\prod_{i=1}^{n}[\hat{z}(t_i)]^{m_i}\right\rangle'_{c*}}\right]$$

$$= \rho_W(X)\exp\{-\beta v(X) - \kappa\beta v'(X)\overline{\Delta x_{\rm cl}(t)} - \tfrac{1}{2}\Lambda^2[\beta v''(X)\overline{\langle[\hat{z}(t)]^2\rangle'} - \beta^2 v'(X)^2\overline{\langle\hat{z}(t_1)\hat{z}(t_2)\rangle'}]$$

$$-\tfrac{1}{2}\kappa^2\beta v''(X)\overline{[\Delta x_{\rm cl}(t)]^2} - \tfrac{1}{6}\kappa^3\beta v'''(X)\overline{[\Delta x_{\rm cl}(t)]^3}$$

$$-\tfrac{1}{2}\kappa\Lambda^2[\beta v'''(X)\overline{\Delta x_{\rm cl}(t)\langle[\hat{z}(t)]^2\rangle'} - 2\beta^2 v'v''\overline{\Delta x_{\rm cl}(t_1)\langle\hat{z}(t_1)\hat{z}(t_2)\rangle'}] + \cdots\} \ . \tag{6.7}$$

Since $|\Delta x_{\rm cl}(t)| \leq 1$, this expansion may be viewed as in powers of

$$\kappa(d/dX),\quad \Lambda^2(d/dX)^2,\quad \mathscr{B}v(X) \ . \tag{6.8}$$

VII. THE CASE $W(x) \equiv V(X)$

In this section, we consider the case $W(x) = W^f(x) \equiv V(X)$. The classical action from (x',t') to (x'',t'') over the potential $-\widetilde{W}^f(x) \equiv 0$ [see (5.4)] is

$$\widetilde{S}_{\rm cl}^f(x',t';x'',t'') = \tfrac{1}{2}m(x''-x')^2/(t''-t') \ . \tag{7.1}$$

The classical trajectory from $(X,0)$ to (X,T) is just $x_{\rm cl}^f(t) \equiv X$, and the thermal quantum dispersion function [Eq. (5.18)]

$$\sigma^f(t) = 2\lambda[t(T-t)/T^2]^{1/2} \ , \tag{7.2}$$

where λ is the thermal wavelength (1.3). Thus, $\kappa^f = 0$, $\Lambda^f = \lambda$. The elements of the matrix ${}^2A^f$ [Eq. (5.13)] are (for $t_2 \geq t_1$)

$$\begin{aligned} {}^2A_{11}^f &= \frac{1}{4}\lambda^{-2}\frac{Tt_2}{t_1(t_2-t_1)} \ , \\ {}^2A_{22}^f &= \frac{1}{4}\lambda^{-2}\frac{T(T-t_1)}{(T-t_2)(t_2-t_1)} \ , \\ {}^2A_{12}^f &= -\frac{1}{4}\lambda^{-2}\frac{T}{(t_2-t_1)} \ . \end{aligned} \tag{7.3}$$

Note that the "correlation coefficient" ${}^2A_{12}^f$ (see Sec. V B 1) does not become much smaller than ${}^2A_{11}^f$ and ${}^2A_{22}^f$ as $|t_2-t_1| \to \infty$, i.e., the stochastic process $\hat{x}^f(t)$ has an infinite memory.

The cumulant expansion (4.1d) may be written as [using (5.7) and (6.2)]

$$\rho_V(X) = \tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp\left[-\beta\int dz\, V(X+\lambda z)\mathscr{P}_1^f(z) + \tfrac{1}{2}\beta^2\int dz_1\int dz_2 v(X+\lambda z_1)v(X+\lambda z_2)\mathscr{P}_2^{fc}(z_1,z_2) + \cdots\right] . \tag{7.4}$$

We denote by $\rho_V^{fn}(X)$ the cumulant approximation of order n in v. The zeroth-order approximation $\rho_V^{f0}(X)$ is just the classical approximation (2.4). The first-order approximation may be written in the intuitively appealing form

$$\rho_V^{f1}(X) = \tfrac{1}{2}\pi^{-1/2}\lambda^{-1}e^{-\beta\overline{V}(X)} \ , \tag{7.5}$$

where

$$\overline{V}(X) \equiv \langle\langle V(\hat{x})\rangle\rangle^f = \int dz\, V(X+\lambda z)\mathscr{P}_1^f(z) \ . \tag{7.6}$$

The dimensionless density

$$\mathscr{P}_1^f(z) = \tfrac{1}{2}\pi^{-1/2}\int_0^1 ds[s(1-s)]^{-1/2} \times\exp\{-\tfrac{1}{4}z^2/[s(1-s)]\} \tag{7.7}$$

is more or less similar[19] to the Gaussian $(3/2\pi)^{1/2}e^{-3z^2/2}$. The approximation (7.5) is analogous to the classical approximation (2.4), but with $V(X)$ replaced by its average over the "zeroth-order" thermal quantum wandering

$\hat{x}^f(t)$, which amounts to a local average over a spread λ. This allows one to visualize nicely how the quantum effects alter $\rho_{V,\mathrm{cl}}(X)$ (see Fig. 4).

The approximation (7.5) may be hoped to usually be a substantial improvement over $\rho_{V,\mathrm{cl}}(X)$, for the terms neglected in expansion (7.4) are expected to be relatively small, not only on account of their higher order in v, but also because of the oscillatory nature of the densities $\mathscr{P}_n^c$ $(n\geq 2)$. For example, let $V(x)=\frac{1}{2}m\omega^2x^2$. The exact $\rho_\omega(X)$ is then given by (2.7), or, in expanded form

$$\rho_\omega(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp[-(\tfrac{1}{12}\Omega^2-\tfrac{1}{360}\Omega^4-\cdots)-\tilde{X}^2(\tfrac{1}{4}\Omega^2-\tfrac{1}{48}\Omega^4+\tfrac{1}{480}\Omega^6+\cdots)]\ . \tag{7.8}$$

The approximation (7.5) yields (being obviously exact to first order in Ω^2)

$$\rho_\omega^{f1}(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp(-\tfrac{1}{12}\Omega^2-\tfrac{1}{4}\Omega^2\tilde{X}^2)=\rho_{\omega,\mathrm{cl}}(X)\exp(-\tfrac{1}{12}\Omega^2)\ . \tag{7.9}$$

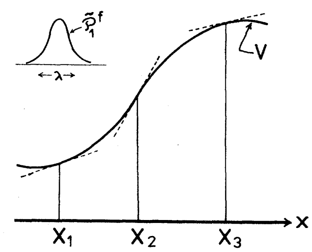

FIG. 4. Typical segment of a potential $V(x)$ and probability density $\tilde{\mathscr{P}}_1^f(x)$. With $\bar{V}(X)=\int_{-\infty}^{\infty}dx\,V(x)\tilde{P}_1^f(x-X)$, it is easy to see that $\bar{V}(X_1)>V(X_1)$, whence $\rho_V^{f1}(X_1)<\rho_{V,\mathrm{cl}}(X_1)$ [case $V''(X)>0$], $\bar{V}(X_2)\cong V(X_2)$, whence $\rho_V^{f1}(X_2)\cong\rho_{V,\mathrm{cl}}(X_2)$ [case $V''(X)=0$], and $\bar{V}(X_3)<V(X_3)$, whence $\rho_V^{f1}(X_3)>\rho_{V,\mathrm{cl}}(X_3)$ [case $V''(X)<0$]. The first-order effect of the curvature $V''(X)$ on $\rho_V(X)$ is displayed explicitly in the WK expansion (7.11). The slope $V'(X)$ clearly has no effect on $\bar{V}(X)$, and thus affects $\rho_V(X)$ to only second order, as seen in (7.11).

The linear potential $V_k(x)=kx$ is a case where (7.5) brings no improvement over $\rho_{V,\mathrm{cl}}$, since $\bar{V}_k(X)=V_k(X)$. However, because of the Gaussian property (5.11), the *second*-order cumulant approximation is *exact* here, i.e.,

$$\rho_k^{f2}(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp\left[-\beta\bar{V}_k(X)+\tfrac{1}{2}\beta^2\int_0^T dt_1\int_0^T dt_2\langle\hat{v}_k^f(t_1)\hat{v}_k^f(t_2)\rangle_{c\{v\}}\right]=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp(-\beta kX+\tfrac{1}{12}\beta^2\lambda^2k^2)=\rho_k^{\mathrm{exact}}(X) \tag{7.10}$$

$[v_k^f(x)=k(x-X)]$. By contrast, all the terms of even order in expansion (3.3) are nonzero; here the superiority of the cumulant expansion is manifest.

The expansion (6.7) ($W=W^f$) is the ordinary Wigner-Kirkwood expansion:[20,21]

$$\begin{aligned}\rho_V(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp\{&-\beta V(X)+\lambda^2[-\tfrac{1}{6}\beta V''+\tfrac{1}{12}\beta^2(V')^2]+\lambda^4[-\tfrac{1}{60}\beta^3(V')^2V''+\tfrac{1}{30}\beta^2V'V'''+\tfrac{1}{90}\beta^2(V'')^2-\tfrac{1}{60}\beta V^{\mathrm{IV}}]\\&+\lambda^6[\tfrac{17}{5040}\beta^4(V')^2(V'')^2+\tfrac{1}{840}\beta^4(V')^3V'''-\tfrac{29}{2520}\beta^3V'V''V'''-\tfrac{1}{280}\beta^3(V')^2V^{\mathrm{IV}}\\&-\tfrac{4}{2835}\beta^3(V'')^3+\tfrac{23}{5040}\beta^2(V''')^2+\tfrac{1}{280}\beta^2V'V^{\mathrm{V}}+\tfrac{1}{210}\beta^2V''V^{\mathrm{IV}}-\tfrac{1}{840}\beta V^{\mathrm{VI}}]+\cdots\}\end{aligned} \tag{7.11}$$

[all derivatives of V evaluated at X; $V^{\mathrm{V}}\equiv d^5V/dx^5$, etc.]. This expansion may be viewed as in powers of the parameters in (6.8), or in (1.6) since $\kappa=0$, $\Lambda=\lambda$, and $\mathscr{B}=\beta$ here.

VIII. THE CASE $W(x)=V(x)+(x-X)V'(X)$

With $W(x)=W^l(x)$ [Eq. (2.3b)], we have $\tilde{W}^l=\tilde{W}^f$, so that the process $\hat{y}^l(t)=\hat{y}^f(t)$, $\sigma^l(t)=\sigma^f(t)$, etc.; the difference between the processes $\hat{x}^l(t)$ and $\hat{x}^f(t)$ resides solely in the classical trajectories, here given by

$$x_{\mathrm{cl}}^l(t)=X+\lambda^2\beta V'(X)[t(T-t)/T^2]\ . \tag{8.1}$$

The density $P_1^l(x,t)$ [Eq. (5.17) with (8.1) and (7.2)] is that shown in Fig. 2. We have

$$\Lambda^l=\Lambda^f=\lambda,\quad \kappa^l=\tfrac{1}{4}\lambda^2\beta\,|\,V'(X)\,|\ . \tag{8.2}$$

In the case $V(x)=\frac{1}{2}m\omega^2x^2$, we have

$$\rho_\omega^{l0}(X)=\rho_{\omega,\mathrm{cl}}(X)\exp(\tfrac{1}{48}\tilde{X}^2\Omega^2)\ ,$$

while

$$\rho_\omega^{l1}(X)=\rho_\omega^{l0}(X)\exp(-\tfrac{1}{12}\Omega^2-\tfrac{1}{480}\tilde{X}^2\Omega^6)$$

[compare (7.8)]. It is instructive to contrast this with the classical path approximation (6.6), which yields ρ_ω^{l1} but without the term $-\frac{1}{12}\Omega^2$, showing that the latter stems from deviations of the process $\hat{x}^l(t)$ from the classical path (8.1).

The generalized WK expansion (6.7) ($W=W^l$) is identical to the ordinary WK expansion (7.11), and simply corresponds to viewing the latter as in powers of the three parameters in (6.8) ($W=W^l$) rather than of the two in (1.6); it gives, however, information on the physical and mathematical structure of (7.11), showing, e.g., that the factors $V'(X)$ (i.e., κ^l) in (7.11) originate in the x_{cl}^l part of the thermal quantum wanderings.

IX. THE CASE $W(x)=W^q(x)$

We now consider the case (2.3c) (Fig. 1). The classical action from (x',t') to (x'',t'') over the potential $-\tilde{W}^q(x)=-\frac{1}{2}m\omega^2x^2$ [see (5.8)] is $(\Delta t=t''-t')$

$$\tilde{S}^q_{\rm cl}(x',t';x'',t'')=\frac{1}{2}\left[\frac{m\omega}{\sinh(\omega\,\Delta t)}\right]$$
$$\times\{[(x')^2+(x'')^2]\cosh(\omega\,\Delta t)-2x'x''\}\;. \tag{9.1}$$

If $V''(X)<0$, then ω is imaginary and the hyperbolic functions in (9.1) become circular functions. If moreover $(\omega\Delta t)^2\le-\pi^2$, then (9.1) is not a minimum, but only a stationary point of $S^q[x(t)]^{t''}_{t'}$. The latter is in fact *unbounded below*[22] when $(\omega\Delta t)^2\le-\pi^2$, and it then follows from (3.6′) that[23]

$$\langle x',t'\,|\,x'',t''\rangle=\infty \quad \text{if } \omega^2(t''-t')^2\le-\pi^2\;. \tag{9.2}$$

Hence, $\rho_{W^q}(X)$ [Eq. (2.6)] and the operation $\langle\;\rangle_{W^q}$ [Eq. (3.2)] are undefined when (2.10) holds.

The classical trajectory from $(X,0)$ to (X,T) over the potential $-W^q(x)$ is [see (2.9) for notation]

$$x^q_{\rm cl}(X,0;X,T;t)=x_m+\Delta X\frac{\sinh(\omega t)+\sinh[\omega(T-t)]}{\sinh(\omega T)} \tag{9.3}$$

and the dispersion function [Eq. (5.18)]

$$\sigma^q(t)=2^{1/2}\lambda_\omega\left[\frac{\sinh(\omega t)\sinh[\omega(T-t)]}{\sinh(\omega T)}\right]^{1/2}, \tag{9.4}$$

where we denote

$$\lambda_\omega=\left[\frac{\hbar}{m\omega}\right]^{1/2}=\lambda(2/\Omega)^{1/2}\;. \tag{9.5}$$

Since $\sigma^q(t)$ and $|x^q_{\rm cl}(t)-X|$ are maximum at $t=\frac{1}{2}T$, we have [see Eqs. (5.19)]

$$\kappa^q=|\Delta X|\;|\operatorname{sech}(\tfrac{1}{2}\Omega)-1|\;,$$
$$\Lambda^q=\lambda_\omega[\tanh(\tfrac{1}{2}\Omega)]^{1/2}\;. \tag{9.6}$$

When $\Omega^2\le-\pi^2$, κ^q and Λ^q are undefined (the thermal quantum wanderings being infinitely spread out). At small Ω,

$$\kappa^q=\tfrac{1}{4}\lambda^2\beta\,|V'(X)|\,(1-\tfrac{5}{48}\Omega^2+\tfrac{61}{5760}\Omega^4-\cdots)\;,$$
$$\Lambda^q=\lambda(1-\tfrac{1}{12}\Omega^2+\tfrac{1}{120}\Omega^4-\cdots)\;, \tag{9.7}$$

whence $\kappa^q\to\kappa^l\to 0$ and $\Lambda^q\to\lambda\to 0$ in the high-temperature limit $\beta\to 0$. In the low-temperature limit $\beta\to\infty$, and provided $V''(X)>0$, we have

$$\kappa^q\to|\Delta X|,\quad \Lambda^q\to\lambda_\omega \quad \text{as } \beta\to\infty\;\;[V''(X)>0]\;. \tag{9.8}$$

Thus, in contrast to the free-particle and linear-potential cases, κ^q and Λ^q stay finite as $\beta\to\infty$ [if $V''(X)>0$]. Note that λ_ω is the width, or "wavelength," of the ground state

$$\phi^0_\omega(x)=\pi^{-1/4}\lambda_\omega^{-1/2}e^{-(x/\lambda_\omega)^2/2} \tag{9.9}$$

of the harmonic oscillator H_ω [Eq. (2.8)]. More generally, Λ^q at *any* temperature is the de Broglie wavelength corresponding to the mean thermal energy of the oscillator, i.e. [compare (1.3)],

$$\Lambda^q=\frac{\hbar}{(2m\bar{E}_{\omega,\beta})^{1/2}}=\left[\frac{\mathscr{B}\hbar^2}{2m}\right]^{1/2}, \tag{9.10}$$

where $\mathscr{B}$ and $\bar{E}_{\omega,\beta}$ are given in (4.13) and (4.14).

The parameters of the two-point joint density $P^q_2(x_1,t_1;x_2,t_2)$, $t_2\ge t_1$, are [these go to (7.3) as $\omega\to 0$]

$${}^2A_{11}=\tfrac{1}{2}\lambda_\omega^{-2}\frac{\sinh(\omega t_2)}{\sinh(\omega t_1)\sinh[\omega(t_2-t_1)]}\;,$$
$${}^2A_{12}=-\tfrac{1}{2}\lambda_\omega^{-2}\frac{1}{\sinh[\omega(t_2-t_1)]}\;, \tag{9.11}$$
$${}^2A_{22}=\tfrac{1}{2}\lambda_\omega^{-2}\frac{\sinh[\omega(T-t_1)]}{\sinh[\omega(t_2-t_1)]\sinh[\omega(T-t_2)]}\;.$$

If ω is real and positive $[V''(X)>0]$ we have ${}^2A_{12}\cong 0$, ${}^2A_{11}\cong\sigma(t_1)^{-2}$, and ${}^2A_{22}\cong\sigma(t_2)^{-2}$ when $|t_2-t_1|\gg\omega^{-1}$; whence (3.14) $(n=2,\ m=1)$ with

$$\tau_W=\tau_\omega=\omega^{-1} \tag{9.12}$$

in accord with (3.13), since $\Delta E^0_W=\hbar\omega$ here.

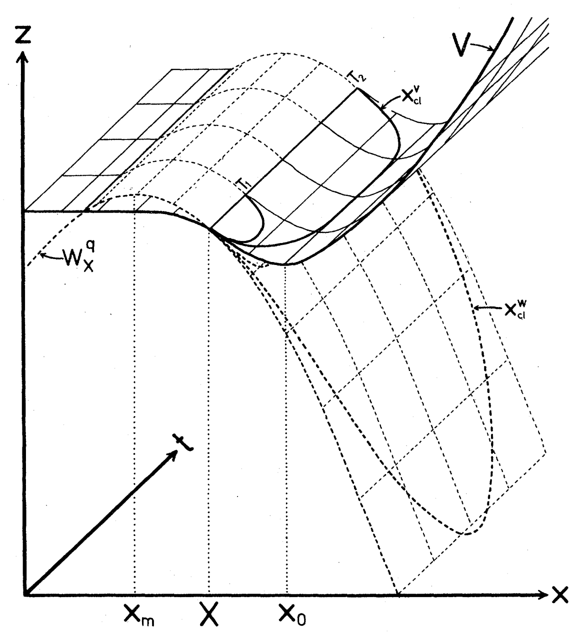

FIG. 5. Potential $V(x)$ and its harmonic approximant $W^q_X(x)$ at X are displaced along the time axis to generate sheets on which the classical trajectories $(X,0)\to(X,T)$ are drawn. In the case $T=T_1$, the trajectories $x^V_{\rm cl}(t)$ and $x^W_{\rm cl}(t)$ are not very different, although the latter extends a bit farther since its potential energy decreases faster. But in the case $T=T_2$, $x^W_{\rm cl}(t)$ extends much farther than $x^V_{\rm cl}(t)$.

A. Cumulant approximations (discussion)

In view of (9.2), and as already mentioned in Sec. II, the approximation $\rho_V^{q0}(X)$ [Eq. (2.6)], and likewise $\rho_V^{q1}, \rho_V^{q2}, \ldots$, are undefined when (2.10) holds. To see what happens, let us refer to Fig. 5, and consider $\rho_V(X)$. For X as in Fig. 5, we have $\rho_V(X) > \rho_{V,\text{cl}}(X)$ because quantum paths can wander *below* $V(X)$, thereby decreasing the action S_V via its potential term. The larger $T = \beta\hbar$ is, the farther paths can wander, such as to decrease $S_{V,\text{pot}}$ without unduly increasing $S_{V,\text{kin}}$; however, there is no advantage for paths to go beyond the minimum x_0. Hence, at large T, the important paths $(X,0) \to (X,T)$ over $V(x)$ first relax from X to the vicinity of x_0, hover there for a while, and then climb back to X (the important paths are more or less clustered about the classical paths; the latter are shown in Fig. 5).

But if we now replace $V(x)$, which is bounded below, by its harmonic approximant $W_X^q(x)$ at X, which is unbounded below (Fig. 5), paths then have advantage in going ever lower, i.e., farther from X, as T increases; and, in fact, once $\Omega^2 \le -\pi^2$, they have advantage in going right to $\pm\infty$, thereby making the action S_W infinitely negative[22] [note that when $\Omega^2 \leqq -\pi^2$, $x_{\text{cl}}^q(t)$, the classical trajectory over $-W^q(x)$, is an *oscillation*, which obviously does not minimize S]. Thus, in replacing V by W^q, we *overdo* the quantum wandering effect, and infinitely so if $\Omega^2 \leqq -\pi^2$.

We therefore expect the approximations $\rho_V^{qn}(X)$, $n = 0,1,2,\ldots$ to be good when β is such that the important quantum paths over $V(x)$ or $W^q(x)$ extend not farther than halfway to x_0, say; to get worse as β increases further; and to be completely erratic at $\Omega^2 \leqq -\pi^2$. However, because regions $V''(X) < 0$ are usually high-potential regions, it should usually happen that when β is so large that $\Omega^2 \leqq -\pi^2$, then $\rho_V(X)$ is small and of minor import. Hence the approximations ρ_V^{qn} should usually be usable down to zero temperature. In that limit, they become Rayleigh-Schrödinger approximations.[13]

B. Renormalized Wigner-Kirkwood expansion

All the terms of the generalized WK expansion (6.7) ($W = W^q$) can be calculated in closed form; we get

$$\begin{aligned}\rho_V(X) = (2\pi)^{-1/2}\lambda_\omega^{-1}(\sinh\Omega)^{-1/2}\exp[&-(\Delta X/\lambda_\omega)^2\tanh(\tfrac{1}{2}\Omega) - \tfrac{1}{6}\beta V'''(\Delta X)^3 F_1(\Omega) - \beta V''' \Delta X\, \lambda_\omega^2 F_2(\Omega) \\ &- \tfrac{1}{4}\beta V^{\text{IV}}(\Delta X)^2\lambda_\omega^2 F_3(\Omega) - \tfrac{1}{8}\beta V^{\text{IV}}\lambda_\omega^4 F_4(\Omega) - \tfrac{1}{8}\beta V^{\text{V}}\,\Delta X\,\lambda_\omega^4 F_5(\Omega) \\ &- \tfrac{1}{48}\beta V^{\text{VI}}\lambda_\omega^6 F_6(\Omega) + \tfrac{1}{36}\beta^2 V'''^2\lambda_\omega^6\Omega^{-1}F_7(\Omega) + \cdots\,]\end{aligned} \tag{9.13}$$

(all derivatives of V evaluated at X), where the $F_n(\Omega)$ are simple functions:

$$\begin{aligned}
F_1(\Omega) &= (\Omega\sinh^3\Omega)^{-1}\{\Omega[-\tfrac{1}{4}\sinh(3\Omega) - \tfrac{3}{2}\sinh(2\Omega) + \tfrac{15}{4}\sinh(\Omega)] + [\tfrac{11}{12}\cosh(3\Omega) - \tfrac{1}{2}\cosh(2\Omega) - \tfrac{25}{4}\cosh(\Omega)] + \tfrac{35}{6}\}\,, \\
F_2(\Omega) &= (\Omega\sinh^2\Omega)^{-1}[\tfrac{7}{12}\cosh(2\Omega) - \tfrac{4}{3}\cosh(\Omega) - \tfrac{1}{4}\Omega\sinh(2\Omega) + \tfrac{3}{4}]\,, \\
F_3(\Omega) &= (\Omega\sinh^3\Omega)^{-1}\{-\tfrac{19}{48}\sinh(3\Omega) + \tfrac{23}{24}\sinh(2\Omega) - \tfrac{35}{48}\sinh(\Omega) + \Omega[\tfrac{1}{8}\cosh(3\Omega) + \tfrac{1}{4}\cosh(2\Omega) - \tfrac{7}{8}\cosh(\Omega) + \tfrac{1}{2}]\}\,, \\
F_4(\Omega) &= (\Omega\sinh^2\Omega)^{-1}\{\Omega[\tfrac{1}{4} + \tfrac{1}{8}\cosh(2\Omega)] - \tfrac{3}{16}\sinh(2\Omega)\}\,, \\
F_5(\Omega) &= (\Omega\sinh^3\Omega)^{-1}\{[\tfrac{77}{480}\cosh(3\Omega) - \tfrac{2}{5}\cosh(2\Omega) + \tfrac{87}{96}\cosh(\Omega)] - \tfrac{1}{16}\Omega[\sinh(3\Omega) + 3\sinh(\Omega)] - \tfrac{2}{3}\}\,, \\
F_6(\Omega) &= (8\Omega\sinh^3\Omega)^{-1}\{\Omega[\tfrac{1}{4}\cosh(3\Omega) + \tfrac{9}{4}\cosh(\Omega)] - \tfrac{11}{24}\sinh(3\Omega) - \tfrac{9}{8}\sinh(\Omega)\}\,, \\
F_7(\Omega) &= (\Omega\sinh^3\Omega)^{-1}\{-\tfrac{167}{192}\cosh(3\Omega) + 2\cosh(2\Omega) - \tfrac{371}{64}\cosh(\Omega) + \Omega[\tfrac{11}{32}\sinh(3\Omega) + \tfrac{57}{32}\sinh(\Omega)] + \tfrac{14}{3}\}\,.
\end{aligned} \tag{9.14}$$

At small Ω, the F_n may be expanded in powers of Ω [see (A3) in the Appendix], and (9.13) converts into the ordinary WK expansion (7.11). At large Ω (real), we have [see (A4)]

$$F_n(\Omega) \to (\text{const})\Omega^{-1} + \text{const}, \quad \Omega \to \infty \tag{9.15}$$

so that *all* the terms of (9.13) become linear in β as $\beta \to \infty$, in accord with (4.10). The terms Ω^{-1} and Ω^0 in (9.15) lead to terms independent of β, and proportional to β, respectively, in expansion (9.13) as $\beta \to \infty$; in view of (4.11), these two classes of terms constitute WK expansions of $2\ln[\phi_V^0(X)]$ and of $-\beta E_V^0$, respectively. Explicitly [we display the terms coming from F_1, F_2, and F_7 in (9.13)],

$$\begin{aligned}
\ln[\phi_V^0(X)] &= \ln[\phi_\omega^0(\Delta X)] - \tfrac{11}{36}(\hbar\omega)^{-1}V'''(\Delta X)^3 \\
&\quad - \tfrac{7}{12}(\hbar\omega)^{-1}V'''\,\Delta X\,\lambda_\omega^2 \\
&\quad - \tfrac{167}{3456}(\hbar\omega)^{-2}(V''')^2\lambda_\omega^6 + \cdots\,, \\
E_V^0 &= \tfrac{1}{2}\hbar\omega - \tfrac{1}{6}V'''(\Delta X)^3 - \tfrac{1}{2}V'''\,\Delta X\,\lambda_\omega^2 \\
&\quad + \tfrac{11}{288}(\hbar\omega)^{-1}(V''')^2\lambda_\omega^6 + \cdots
\end{aligned} \tag{9.16}$$

[$\phi_\omega^0(x)$ is given in (9.9)]. Observe how the combinations $\beta V = (T/\hbar)V$ in (9.13) have become $(\hbar\omega)^{-1}V = (\tau_\omega/\hbar)V$ in (9.16), as announced by (4.10). Expansions (9.16) are what one would obtain if one Taylor-series expanded the perturbation $v^q = V - W^q$ around X in the Rayleigh-Schrödinger expansions of $\ln[\phi_V^0(X)]$ and E_V^0 [Eqs. (9.16), of course, pertain only to the case $\omega>0$ real, since $V''(X)<0$ with $\beta\to\infty$ implies $\Omega^2\leqq-\pi^2$, and $\omega=0$ implies $\tau_\omega=\omega^{-1}=\infty$].

Expansion (9.13) may be viewed as in powers of the three parameters in (6.8) ($W=W^q$), or, because $\kappa^q\sim|(\Lambda^q)^2\mathscr{B}V'(X)|$ [since $\kappa^q\to|\frac{1}{4}\lambda^2\beta V'|$ as $\beta\to 0$, $\kappa^q\to|V'/V''|\ =|\frac{1}{2}\lambda_\omega^2(\hbar\omega)^{-1}V'|$ as $\beta\to\infty$], as in powers of just the two parameters in (1.7). Observe that the limit of (6.8) ($\omega^2>0$) is

$$|\Delta X|\,d/dX,\ \ \lambda_\omega^2(d/dX)^2\,,\ \ (\hbar\omega)^{-1}v^q(X) \tag{9.17}$$

i.e., the expansion parameters of (9.16).

Expansion (9.13) is a resummation over powers of $V''(X)$ of the ordinary WK expansion (7.11), i.e., all the terms of the form

$$\prod_i V^{m_i'}(V')^p(V'')^n,\ \ m_i\geq 3,\ p,n \text{ integers}$$

are resummed over n [e.g., $(\beta/6)V'''(V'/V'')^3F_1(\Omega)$ in (9.13) resums all the terms of the form $V'''(V')^3(V'')^n$ in (7.11)]. The resummation over p, i.e., over powers of $V'(X)$, may also be performed by simply regrouping terms, as it is easy to see [from the fact that the expansion parameters are (9.17) and $v^{q\prime}(X)=v^{q\prime\prime}(X)=0$] that $p\leqq\sum_i m_i$, i.e., in (9.13), each combination $\prod_i V^{m_i'}$ ($m_i\geqq 3$) comes multiplied by a polynomial in V'/V'' of *finite* degree $\leqq\sum_i m_i$.

The results of this section have until now been considered as pertaining only to the case $\Omega^2>-\pi^2$, since otherwise the averaging operation $\langle\ \rangle_{W^q}$ [Eq. (3.2)] is undefined. But nothing prevents us from formally extending the domain of expansion (9.13) to the range $\Omega^2<-\pi^2$, as its terms are all finite there [except at the discrete values $\Omega^2=-(n\pi)^2$, $n=1,2,\ldots$]. In fact, it is clear that (9.13) is the resummation of the ordinary WK expansion (7.11) over powers of $V''(X)$ *also* at $\Omega^2<-\pi^2$, simply because (9.13) ($\Omega^2<\pi^2$) is the *analytic continuation* of (9.13) ($\Omega^2>-\pi^2$). However, this analytic continuation lacks, because $(\Delta x)_{W^q}=\infty$ at $\Omega^2<-\pi^2$, the physical grounding whereby the original expansion was motivated (in Sec. II), and it is not expected to yield useful approximations [a truncation of (9.13) when $(\beta\hbar\omega)^2<-\pi^2$ yields an approximation which oscillates with β, and tends to no definite limit, as $\beta\to\infty$].

X. CONCLUSION

The renormalized Wigner-Kirkwood expansion (9.13) is our main result of practical interest. It is as simple to use, yet more accurate than the ordinary WK expansion, which is already known to often be very good;[4] moreover, (9.13) is usable down to zero temperature near well bottoms, where $\rho_V(X)$ concentrates.

From a conceptual point of view, the renormalization of the WK expansion (7.11), with the sharp contrast between the cases $\Omega^2>-\pi^2$ and $\Omega^2\leqq-\pi^2$ [where $\Omega^2=\beta^2\hbar^2V''(X)/m$], constitutes a nice example of a resummation procedure which in one case is physically motivated, and leads to useful approximations, and in the other case, is purely formal and yields no useful approximations.

We considered three types of cumulant expansions: (4.1) in powers of $\mathscr{B}v$; (6.4) in powers of $\Lambda^2(d/dX)^2$ and $\mathscr{B}v$; and (6.7) in powers of $\kappa\, d/dX$, $\Lambda^2(d/dX)^2$, and $\mathscr{B}v$. These expansions also apply to the off-diagonal elements of the density matrix $\rho_V(X,X')$ [Eq. (1.8)], if only we replace (X,T) by (X',T) in (3.2), (3.5), etc., let $x_{\rm cl}(t)$ be the classical trajectory from $(X,0)$ to (X',T), and replace $\rho_V(X)$ and $\rho_W(X)$ by $\rho_V(X,X')$ and $\rho_W(X,X')$, respectively, in (4.1), (6.4), and (6.7) [the processes $\hat{y}(t)$ and $\hat{z}(t)$ remain unchanged]. The expansion (4.1) ($X'\neq X$) has been discussed in Ref. 13, for any W. Expansions (4.1) and (6.4) ($X'\neq X$) with $W(x)\equiv 0$ are identical to the expansions derived in Ref. 5 (the multidimensional case is treated there, and extended to the presence of a magnetic field in Ref. 6). With $W(x)=W^0(x)\equiv 0$, the classical trajectory from $(X,0)$ to (X',T) is[24]

$$x_{\rm cl}^0(t)=X+(X'-X)(t/T),\ \ \kappa^0=|X'-X|$$

and expansion (6.7) ($X'\neq X$) is then in powers of $|X'-X|\,d/dX$, $\lambda^2(d/dX)^2$, and $\beta V(X)$; this expansion, which may be found in Eqs. (7)—(10) of Ref. 4, is thus usable only for $|X'-X|$ sufficiently small [indeed, if $|X'-X|$ is large on the scale of variation of $V(x)$, the latter cannot be replaced by a local approximant at X, because $\rho_V(X,X')$ is determined by the values of $V(x)$ within an interval $(\Delta x)_{V,\beta,X,X'}$ which *contains* the interval (X,X')]. This circumstance precludes, in particular, the applicability of WK expansions to the exchange effect in a gas of strongly interacting particles.[25] Expansion (6.7) [$X'\neq X$, $W(x)\equiv 0$] may nevertheless be useful because $\rho_V(X,X')$ is sizable only for $|X'-X|\lesssim\lambda$ at high temperatures; it may be resummed over powers of $V''(X)$ by letting $W(x)=W_X^q(x)$ be the quadratic approximant to $V(x)$ at X. To deal with $|X'-X|$ large, one may use expansions (4.1) or (6.4), with $W(x)\equiv 0$ as in Refs. 5 and 6, or with $W(x)$ equal to some quadratic approximant [chosen, e.g., as that best fitting $V(x)$ inside the interval (X,X')].

APPENDIX: EXPANSION (9.13)

We here give the details of expansion (9.13). We display the terms required for exactness to sixth order in λ [from Eqs. (9.7), $\Delta x_{\rm cl}(t)$ (or κ) is of order λ^2, and $\hat{y}(t)$ (or Λ) is of order λ]. Taking account of $v^q(X)=v^{q\prime}(X)=v^{q\prime\prime}(X)=0$, we have

$$\rho_V(X)=\tfrac{1}{2}\pi^{-1/2}\lambda^{-1}\exp\{-\tfrac{1}{2}\ln[(\sinh\Omega)/\Omega]-(\Delta X/\lambda_\omega)^2\tanh(\tfrac{1}{2}\Omega)+B_1+B_2+\cdots+B_7+\cdots\}\,, \tag{A1}$$

where

$$B_1=-\tfrac{1}{6}\beta V'''\overline{[\Delta x_{\rm cl}(t)]^3}=-\tfrac{1}{6}\beta V'''(\Delta X)^3F_1(\Omega)\,,$$

$$B_2=-\tfrac{1}{2}\beta V'''\overline{\Delta x_{\rm cl}(t)\langle[\hat{y}(t)]^2\rangle^{\sim}}=-\tfrac{1}{2}\beta V'''\,\Delta X\,\lambda_\omega^2F_2(\Omega)\,,$$

$$B_3=-\tfrac{1}{4}\beta V^{\rm IV}\overline{[\Delta x_{\rm cl}(t)]^2\langle[\hat{y}(t)]^2\rangle^{\sim}}$$

$$= -\tfrac{1}{4}\beta V^{\mathrm{IV}}(\Delta X)^2\lambda_\omega^2 F_3(\Omega)\ ,$$

(A2)

$$B_4 = -\frac{1}{4!}\beta V^{\mathrm{IV}}\overline{\langle[\hat{y}(t)]^4\rangle^{\sim}} = -\tfrac{1}{8}\beta V^{\mathrm{IV}}\lambda_\omega^4 F_4(\Omega)\ ,$$

$$B_5 = -\frac{1}{4!}\beta V^{\mathrm{V}}\overline{\Delta x_{\mathrm{cl}}(t)\langle[\hat{y}(t)]^4\rangle^{\sim}}$$

$$= -\tfrac{1}{8}\beta V^{\mathrm{V}}\Delta X\,\lambda_\omega^4 F_5(\Omega)\ ,$$

$$B_6 = -\frac{1}{6!}\beta V^{\mathrm{VI}}\overline{\langle\hat{y}(t)^6\rangle^{\sim}} = -\tfrac{1}{48}\beta V^{\mathrm{VI}}\lambda_\omega^6 F_6(\Omega)\ ,$$

$$B_7 = \tfrac{1}{72}\beta^2 V'''^2\overline{\langle[\hat{y}(t_1)]^3[\hat{y}(t_2)]^3\rangle^{\sim}}$$

$$= \tfrac{1}{36}\beta^2(V''')^2\lambda_\omega^6\Omega^{-1}F_7(\Omega)$$

[see (3.9), (2.9), and (9.5) for the notation], where the functions $F_n(\Omega)$ were displayed in (9.14). At small Ω,

$$F_1(\Omega) = -\tfrac{1}{1120}\Omega^6 + \tfrac{1}{8064}\Omega^8 + \cdots\ ,$$

$$F_2(\Omega) = -\tfrac{1}{60}\Omega^3 + \tfrac{29}{10080}\Omega^5 + \cdots\ ,$$

$$F_3(\Omega) = \tfrac{1}{560}\Omega^5 + \cdots,\quad F_4(\Omega) = \tfrac{1}{30}\Omega^2 - \tfrac{1}{210}\Omega^4 + \cdots\ , \tag{A3}$$

$$F_5(\Omega) = -\tfrac{1}{280}\Omega^4 + \cdots,\quad F_6(\Omega) = \tfrac{1}{140}\Omega^3 + \cdots\ ,$$

$$F_7(\Omega) = \tfrac{23}{1120}\Omega^4 + \cdots\ ,$$

and as $\Omega^2 \to +\infty$,

$$F_1(\Omega) \to -1 + \tfrac{11}{3}\Omega^{-1},\quad F_2(\Omega) \to -\tfrac{1}{2} + \tfrac{7}{6}\Omega^{-1}\ ,$$

$$F_3(\Omega) \to \tfrac{1}{2} - \tfrac{19}{12}\Omega^{-1},\quad F_4(\Omega) \to \tfrac{1}{4} - \tfrac{3}{8}\Omega^{-1}\ , \tag{A4}$$

$$F_5(\Omega) \to -\tfrac{1}{4} + \tfrac{77}{120}\Omega^{-1},\quad F_6(\Omega) \to \tfrac{1}{8} - \tfrac{11}{48}\Omega^{-1}\ ,$$

$$F_7(\Omega) \to \tfrac{11}{8} - \tfrac{167}{48}\Omega^{-1}\ .$$

By introducing into (A1) the expansions (A3) and

$$\tanh z = z - \tfrac{1}{3}z^3 + \tfrac{2}{15}z^5 - \tfrac{17}{315}z^7 + \cdots\ ,$$

$$\ln[(\sinh z)/z] = \tfrac{1}{6}z^2 - \tfrac{1}{180}z^4 + \tfrac{1}{2835}z^6 + \cdots \tag{A5}$$

and using the relations

$$\Omega^2 = 2\lambda^2\beta V'',\quad \Delta X = 2\beta(\lambda/\Omega)^2 V',\quad \lambda_\omega^2 = 2\lambda^2/\Omega \tag{A6}$$

one readily verifies that the terms displayed in (A3) and (A5) lead to the terms displayed in the ordinary WK expansion (7.11). By using (A4) and $\tanh(\tfrac{1}{2}\Omega)\to 1$, $(\Omega/\sinh\Omega)^{1/2} \to (2\Omega)^{1/2}e^{-\Omega/2}$ as $\Omega\to\infty$ in (A1), we get (4.11) and (9.16).

1. Sketch of calculations

To evaluate the first six terms in the list (A2), we need the formula

$$\langle[\hat{y}(t)]^n\rangle^{\sim} = \pi^{-1/2}[\sigma(t)]^{-1}\int_{-\infty}^{\infty} dy\, y^n e^{-y^2/[\sigma(t)]^2}$$

$$= \begin{cases} 0, & n \text{ odd} \\ 2^{-n/2}[(n-1)!!][\sigma(t)]^n, & n \text{ even} \end{cases} \tag{A7}$$

$[(n-1)!! = 1\times 3\times 5\times\cdots\times(n-1)]$. To evaluate B_7, we will use the result

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, x^3 y^3 e^{-ax^2-2bxy-cy^2}$$

$$= -\tfrac{3}{8}\pi(b/\Delta^{5/2})[3+5(b^2/\Delta)]\ , \tag{A8}$$

where

$$\Delta = ac - b^2 = \det\begin{bmatrix} a & b \\ b & c\end{bmatrix}\ . \tag{A9}$$

We now have, from Eqs. (9.3), (9.4), and (9.11) ($\alpha = \omega t$, $\Omega = \omega T$),

$$\Delta x_{\mathrm{cl}}(t) = \Delta X\, f(\omega t)\ ,$$

$$\sigma(t) = 2^{1/2}\lambda_\omega g(\omega t)\ , \tag{A10}$$

$$\Delta = \det{}^2 A$$

$$= \tfrac{1}{4}\lambda_\omega^{-4}\frac{\sinh\Omega}{\sinh(\alpha_1)\sinh(\alpha_2-\alpha_1)\sinh(\Omega-\alpha_2)}\quad (\alpha_2 \geq \alpha_1)\ , \tag{A11}$$

where

$$f(\alpha) = [\sinh(\alpha) + \sinh(\Omega-\alpha) - \sinh(\Omega)]/\sinh(\Omega)\ ,$$

$$g(\alpha) = [\sinh(\alpha)\sinh(\Omega-\alpha)/\sinh(\Omega)]^{1/2}\ . \tag{A12}$$

Thus, for n even,

$$\overline{[\Delta x_{\mathrm{cl}}(t)]^m\langle[\hat{y}(t)]^n\rangle^{\sim}} = 2^{-n/2}[(n-1)!!]\overline{[\Delta x_{\mathrm{cl}}(t)]^m[\sigma(t)]^n}$$

$$= (n-1)!!(\Delta X)^m\lambda_\omega^{n/2}F(\Omega)\ , \tag{A13}$$

$$F(\Omega) = \Omega^{-1}\int_0^{\Omega} d\alpha[f(\alpha)]^m[g(\alpha)]^n\ . \tag{A14}$$

This formula covers the first six terms in (A2). As for the seventh, we have, on using (A8) with $a = {}^2A_{11}$, $b = {}^2A_{12}$, $c = {}^2A_{22}$ [Eqs. (9.11)], and (A11), for $t_2 \geq t_1$,

$$\langle[\hat{y}(t_1)]^3[\hat{y}(t_2)]^3\rangle^{\sim} = -\tfrac{3}{8}({}^2A_{12}/\Delta)[3+5({}^2A_{12}^2/\Delta)]$$

$$= \lambda_\omega^3 G(\omega t_1, \omega t_2)\ , \tag{A15}$$

where

$$G(\alpha_1,\alpha_2)$$

$$= (\sinh\Omega)^{-3}[9\sinh^2\alpha_1\sinh(\alpha_2-\alpha_1)$$

$$\times\sinh^2(\Omega-\alpha_2)\sinh\Omega$$

$$+ 15\sinh^3\alpha_1\sinh^3(\Omega-\alpha_2)]\ . \tag{A16}$$

Whence

$$\overline{\langle[\hat{y}(t_1)]^3[\hat{y}(t_2)]^3\rangle^{\sim}} = 2\lambda_\omega^3\Omega^{-1}F_7(\Omega)\ , \tag{A17}$$

where

$$\Omega^{-1}F_7(\Omega) = \Omega^{-2}\int_0^{\Omega} d\alpha_2\int_0^{\alpha_2} d\alpha_1 G(\alpha_1,\alpha_2) \tag{A18}$$

[we used $\overline{f(t_1,t_2)} = 2T^{-2}\int_0^T dt_2\int_0^{t_2} dt_1 f(t_1,t_2)$, hence the factor 2 in (A17)].

[1]For a review of semiclassical methods in statistical mechanics, see Y. Singh and S. K. Sinha, Phys. Rep. **79**, 213 (1981).

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[9]See, e.g., N. G. Van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

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[14]Another widely used approach is the "memory-function" method, with its attendant projection-operator techniques [R. Zwanzig, in *Boulder Lectures in Theoretical Physics* (Wiley, New York, 1961), Vol. III; H. Mori, Prog. Theor. Phys. **33**, 423 (1965); **34**, 399 (1965)]. However, the cumulant expansion method is much preferable in the present situation, especially since Gaussian stochastic processes are involved, with their special cumulant properties (see Refs. 9 and 10).

[15]Three-dimensional versions of these approximations were derived by M. Durand, M. Brack, and P. Schuck, Z. Phys. A **286**, 381 (1978), by a somewhat different approach from ours, more closely related to the WKB method, and applied to Fermion systems (nuclei).

[16]The path-integral representation, although the most convenient, notationally and heuristically, is not at all indispensable. Thus, by denoting (a)

$$\hat{a}(t)\equiv e^{-tH_W/\hbar}\hat{a}e^{tH_W/\hbar}$$

for any operator $\hat{a}$, and using (b)

$$e^{-\beta H_V}e^{\beta H_W}=T_{\rightarrow}\exp\left[-\int_0^T dt\,\hat{v}(t)/\hbar\right],$$

where $T_{\rightarrow}$ (time) orders operators such that time increases from left to right, we have again (3.1), but with $\hat{v}(t)=v(\hat{x}(t))$ having the meaning (a), and the operation $\langle\ \rangle_W$ defined by (Ref. 13) (c)

$$\langle F[\hat{x}(t)]\rangle_W\equiv\langle X\,|\,T_{\rightarrow}F[\hat{x}(t)]e^{-\beta H_W}\,|\,X\rangle/\langle X\,|\,e^{-\beta H_W}\,|\,X\rangle$$

[the momentum operator $p=(\hbar/i)(d/dX)$ in $H_W=p^2/2m+W_X$ must be understood as not acting on the *subscript X* in W_X]. The ordering operator $T_{\rightarrow}$ is part of the averaging operation, so that everything commutes inside $\langle\ \rangle$. [Note that the caret identifies $\hat{x}(t)$ as a stochastic process on the left-hand side of (c), and as a Heisenberg operator on the right-hand side.]

[17]That is, when $|t''-t'|\gg\tau_W$, the (relative) probability density for the value x'' at time t'' is independent of the value x' at t', and is simply given by the ground-state wave function. From a more intuitive point of view, $\Delta E_W^0\neq 0$ normally implies that $W(x)$ possesses at least one well whose bottom is an absolute minimum (assuming that W is bounded below). Thus, a path starting at x' at time t' will, provided $t''-t'$ is sufficiently large, aim for such a well bottom, hover there for a while, such as to minimize $S_W[x(t)]$ (via the potential term), and thereby "forget" its initial position x', before aiming for x''. By contrast, in the free-particle case $W(x)=$const, where the action consists of only a kinetic part, a path always remembers its initial position, since it does not wish to move away from there, in order to minimize $\int dt\frac{1}{2}m\dot{x}(t)^2$. In the case of a linear potential $W(x)=kx$ (k constant), the memory is also infinite, since we then have an everlasting downhill drift, with no potential minimum where the path can stabilize and "forget."

[18]See, e.g., L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

[19]If we denote by $\mu_n=\int_{-\infty}^{\infty}dz\,z^n\mathscr{P}_1^f(z)$ the moments of the density (7.7), then we have $\mu_n=0$ for n odd, and $\mu_2=\frac{1}{3}$, $\mu_4=\frac{2}{5}$. The "kurtosis," defined such that it vanishes for a Gaussian (see Ref. 9, p. 14), is $(\mu_4/\mu_2^2)-3=0.6$, indicating that $\mathscr{P}_1^f(z)$ is more spread out in the wings and narrower in its center than is a Gaussian having the same second moment.

[20]From Eqs. (3.12)—(3.16) of Ref. 3, adapted to the one-dimensional case.

[21]The physical significance of the terms of order λ^2 in (7.11) is easily understood: the slope $V'(X)$, because it generates no net change in the mean potential energy under the zeroth-order thermal quantum wandering $\hat{x}^f(t)$ (see Fig. 4), affects $\rho_V(X)$ only in second order, by acting in two steps: first, it modifies the quantum wanderings, skewing them downhill; second, it generates a *loss* in mean potential energy under these skewed wanderings. Thus, a nonzero slope, whatever its sign, causes an *increase* of $\rho_V(X)$ relative to $\rho_{V,\mathrm{cl}}(X)$ [as it allows wanderings *below* $V(X)$]. By contrast, the curvature $V''(X)$ leads, under the wandering $\hat{x}^f(t)$, to a net change in mean potential energy, loss if $V''(X)<0$, gain if $V''(X)>0$ (see Fig. 4), and correspondingly increases or decreases $\rho_V(X)$, in first order.

[22]One can see intuitively that $S_\omega[x(t)]_0^T$, with $\omega^2<0$, becomes unbounded below when T exceeds some value ($\pi/|\omega|$ specifically) as follows: let $V_\omega(x)=V_{i\nu}(x)=-\frac{1}{2}m\nu^2x^2$ ($\nu^2>0$). Then a path $(X,0)\rightarrow(X,T)$ which wanders up to a maximum distance $x=Y$, where $Y\gg X$, has a mean potential energy $S_{\mathrm{pot}}\sim -m\nu^2Y^2$, and a mean kinetic energy $S_{\mathrm{kin}}\sim mY^2/T^2$, so that the action $S=S_{\mathrm{kin}}+S_{\mathrm{pot}}\sim(a-b\nu^2T^2)Y^2$ (a,b constants). Thus, when $\nu^2T^2>a/b$, S can be made as negative as desired by letting Y be sufficiently large [this argument can be made quantitative (showing that $a/b=\pi^2$) by expressing the quantum paths as Fourier series; see Ref. 23].

[23]A. Royer, J. Math. Phys. **25**, 2873 (1984).

[24]With $W(x)\equiv 0$, expansion (3.3) is in powers of βV. But because cumulants of order ≥ 2 are unaltered if constants are added to their arguments, one may, in expansion (4.1), replace $v(x)=V(x)$ by $V(x)-V(X)$, or $V(x)-\langle\langle V(x)\rangle\rangle$ [except in the first term], which will usually be much smaller than $V(x)$ in magnitude. This shows again the superiority of the cumulant expansion over the moment expansion.

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