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N-body Green's functions and their semiclassical expansion

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A new semiclassical expansion for quantum mechanics is developed. The high-energy asymptotic expansion for the coordinate-space matrix elements of the N-body Green's function is derived. The asymptotic series is characterized by its coefficient functions, P_n. It is shown that the coefficient of the nth term in the expansion, P_n, satisfies a simple recursion relation. The functions, P_n, turn out to be polynomials in Planck's constant h of order $2(n-1)$. In terms of the interaction, the P_n are also polynomials of the potential and its derivatives. If all the P_n are truncated to some common power M in h, one generates a natural Mth order semiclassical approximation to the Green's function. This semiclassical expansion is given a physical interpretation which is particularly simple in terms of state density. By relating the asymptotic series to the Born series, a closed form for the functions P_n is derived.

I. INTRODUCTION

This paper proposes a new semiclassical expansion for quantum mechanics. The basic scale factor for quantum effects is

$$q=\hbar^2/2m\,, \tag{1.1}$$

where $\hbar$ is the rationalized value of Planck's constant and m is the mass of a particle. If H is the full N-particle Hamiltonian of a system, interacting via a sum of pair-wise potentials, then for complex energies z the Green's function is the operator $G(z)=(H-z)^{-1}$. Knowledge of $G(z)$ determines almost all of the behavior of the quantum system. Given $G(z)$, one can determine the N-particle transition amplitude for scattering, the bound-state energy spectrum, and the bound-state wave functions that characterize system H. The goal of this paper is to find a series expansion in q of the coordinate space matrix elements of $G(z)$.

The quantum parameter q enters the Schrödinger equation through the form assumed by the kinetic energy operator H_0. Let $\vec{x}$ denote the $3N$-dimensional vector giving the location of the N three-dimensional, mass m particles. If Δ_x is the Laplacian associated with $\vec{x}$ then

$$H_0=-q\Delta_x\,. \tag{1.2}$$

The fully interacting system is then defined by

$$H=H_0+V\,. \tag{1.3}$$

The interaction operator V is given as multiplication by the potential field $v(\vec{x})$. The detailed expressions which we develop for our semiclassical approximation require only that H_0 be a Laplacian and that $v(\vec{x})$ is a local potential with bounded derivatives with respect to $\vec{x}$ to all orders. Thus our theory is a semiclassical expansion for Hamiltonian problems with smooth potential fields.

The approach we take to this problem is to examine the asymptotic expansions of the closely related pair of operators $G(z)$ and $e^{-\beta H}$. The parameter β is the inverse temperature. It will be shown that the expansion of $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ in powers of β and of $\langle\vec{x}|G(z)|\vec{x}'\rangle$ in powers of $z^{-1/2}$ are determined by a common set of coefficient functions $P_n(\vec{x},\vec{x}';q)$, where n takes on positive integer values. Further study of the P_n shows that it is a polynomial in q of order $n-1$. Thus the functions P_n provide a natural interpolation between the classical solution ($q=0$) and the quantum solution ($q=\hbar^2/2m$). In addition, this interpolation is smooth in the variable q, since P_n is constructed of just powers of $v(\vec{x})$ and its derivatives.

In Sec. II we describe the interrelationship between the high-energy expansion of $G(z)$ and the high-temperature expansion of $e^{-\beta H}$. The unifying role played by the $P_n(\vec{x},\vec{x}';q)$ is emphasized and the recursion relation defining $P_n(\vec{x},\vec{x}';q)$ is found. Section III states the definition of our semiclassical expansion. The Weyl transform is used to obtain the classical phase-space counterpart to $G(z)$. The semiclassical limit $\hbar\to 0$ is discussed and the implications for both classical and quantum state density are derived. In Sec. IV we continue the investigation of $P_n(\vec{x},\vec{x}';q)$. A general closed form of $P_n(\vec{x},\vec{x}';q)$ based on comparing the asymptotic expansion with the Born series is obtained. A summary of our conclusions is given in Sec. V. Appendix A contains the derivation of an integral representation of the coordinate-space matrix elements of the Nth Born term. Appendix B quotes explicit formulas for the functions $P_n(\vec{x},\vec{x}';q)$.

The methods used in this paper have been strongly influenced by the analysis used to understand the Korteweg-de-Vries (KdV) equation and its soliton solutions. It is well known that the one-dimensional (1D) KdV equation has an infinite number of constants of motion. These constants of motion can be constructed by an integral over all

$\vec{x}$ of an invariant density which is a function of $v(\vec{x})$. In fact, the invariant density is just the diagonal value ($\vec{x}=\vec{x}'$) of $P_n(\vec{x},\vec{x}';q)$. The work[1] of Gardner, Greene, Kruskal, and Miura catalogs $P_n(\vec{x},\vec{x};q)$ (up to a total derivative factor) expressions for $n=1,\ldots,11$. In this paper we will determine P_n for a space of any dimensionality and will find both the off-diagonal and on-diagonal values of P_n. The literature that is of particular relevance to the semiclassical approximation developed here is the study of the asymptotic form of $\langle\vec{x}|G(z)|\vec{x}'\rangle$ in 1D by Gelfand and Dikii[2]; the study of the asymptotic form of $\langle\vec{x}|G(z)|\vec{x}'\rangle$ in 3D by Buslaev,[3] and the generalization of P_n from 1D to ND found by Perelomov.[4] To the best of our knowledge, our work is the first to take seriously the idea that the $P_n(\vec{x},\vec{x}';q)$ provides the natural semiclassical interpolation between quantum and classical solutions.

This paper is the first of two related papers on the semiclassical expansion suggested by the functions $P_n(\vec{x},\vec{x}';q)$. One may renormalize the expansions we find for the Green's function by explicitly summing up all the classical terms. In this way, one can describe problems with strong interactions $v(\vec{x})$, provided that the quantum effects proportional to q can be treated perturbatively. This is the basic idea behind the Wigner-Kirkwood[5] semiclassical expansion. A standard form of the Wigner-Kirkwood expansion is

$$\langle\vec{x}|e^{-\beta H}|\vec{x}\rangle=\langle\vec{x}|e^{-\beta H_0}|\vec{x}\rangle \times e^{-\beta v(\vec{x})}[1+q(\cdots)+q^2(\cdots)+\cdots]. \quad (1.4)$$

The coefficients of q, q^2, etc., are functions of $v(\vec{x})$ and their derivatives. The appearance of $v(x)$ in the exponential means that classical interaction has been summed to infinite order. The classical renormalization program is possible with the semiclassical expansion implied by the $P_n(\vec{x},\vec{x}';q)$. Since the analysis of this renormalization is a substantial problem in its own right, we shall place it in a separate paper.

II. ASYMPTOTIC EXPANSIONS

In this section we compare the asymptotic expansions for fixed $\vec{x},\vec{x}'$ of the matrix elements $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ and $\langle\vec{x}|G(z)|\vec{x}'\rangle$. The Bloch equation describing the function $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ is used to obtain the recursion relation that defines the functions $P_n(\vec{x},\vec{x}';q)$. In the following analysis we will carry out explicit calculations of the series expansions of $\langle\vec{x}|G(z)|\vec{x}'\rangle$. These calculations are formal in the sense that we will freely interchange orders of summation and integration. We will not determine convergence properties of these series. Estimating the convergence behavior will depend on the growth properties of the functions $P_n(\vec{x},\vec{x}';q)$ in the index n for fixed $\vec{x}$, $\vec{x}'$, and q. It would take us far afield to determine the bounds on P_n sufficient to control the convergence characteristic of the many series we write down. However, the few rigorous results that do exist[2,3] in $d=1$ and 3 indicate that the convergence estimates for the asymptotic series given below should not be too difficult to obtain. On the other hand, all the representations we derive for $P_n(\vec{x},\vec{x}';q)$ in Sec. IV are rigorous. The basic purpose of this paper is to obtain a balanced overview of the many ways the representations of the heat kernel $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ and the Green's function $\langle\vec{x}|G(z)|\vec{x}'\rangle$ are linked together, the fundamental role the functions P_n play in describing these two matrix elements, and the manner in which the functions P_n lead inevitably to a semiclassical expansion.

We take d as the dimensionality of $\vec{x}$. In quantum mechanics, operators are linear transformations acting on the Hilbert space $\mathcal{H}=L^2(\mathbb{R}^d)$. Let $\sigma(H)$ be the spectrum of H. For $\mathrm{Re}\,z<\sigma(H)$, the Laplace transform relates $G(z)$ to $e^{-\beta H}$,

$$G(z)=\int_0^\infty e^{z\beta}e^{-\beta H}d\beta\,. \quad (2.1)$$

If we use the Dirac notation to specify the kernel representation of the operators $G(z)$ and $e^{-\beta H}$, Eq. (2.1) becomes

$$\langle\vec{x}|G(z)|\vec{x}'\rangle=\int_0^\infty e^{z\beta}\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle\,d\beta. \quad (2.2)$$

Consider the asymptotic expansion $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle/\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ in powers of β. We define $P_n(\vec{x},\vec{x}';q)$ as the functions satisfying

$$\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle\sim\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\beta^n P_n(\vec{x},\vec{x}';q)\,, \quad (2.3)$$

where ~ signifies an asymptotic expansion[6] in variable β for fixed $\vec{x},\vec{x}'$.

Because of the Laplace transform Eq. (2.2) relating $G(z)$ to $e^{-\beta H}$, any expansion of $e^{-\beta H}$ implies a related expansion for $G(z)$. Placing (2.3) in (2.2) gives

$$\langle\vec{x}|G(z)|\vec{x}'\rangle\sim\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}P_n(\vec{x},\vec{x}';q)\times\int_0^\infty e^{z\beta}\beta^n\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle\,d\beta$$
$$\sim\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}P_n(\vec{x},\vec{x}';q)\left(\frac{\partial}{\partial z}\right)^n\langle\vec{x}|G_0(z)|\vec{x}'\rangle\,, \quad (2.4)$$

where $G_0(z)$ is the free Green's function $(H_0-z)^{-1}$. For z belonging to $\mathbb{C}\setminus\{\sigma(H)\}$, $(\partial/\partial z)^n\langle\vec{x}|G_0(z)|\vec{x}'\rangle$

are independent analytic functions of z. Taken together, expansions (2.3) and (2.4) show us that knowledge of the coefficient functions $P_n(\vec{x},\vec{x}';q)$ is sufficient to determine either expansion.

The next step is to recall the recursion relations, discovered by Perelomov,[4] which define the $P_n(\vec{x},\vec{x}';q)$ in terms of $v(\vec{x})$. The kernel of $e^{-\beta H}$ may be constructed from the solution of the heat (or Bloch) equation

$$\left(\frac{\partial}{\partial\beta}+H\right)\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle=0\,, \tag{2.5}$$

that satisfies the δ-function boundary condition

$$\lim_{\beta\to 0}\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle=\delta(\vec{x}-\vec{x}')\,. \tag{2.6}$$

Associated with the full-heat Eq. (2.5) is the free-heat equation that results when $v(\vec{x})=0$, viz.,

$$\left(\frac{\partial}{\partial\beta}+H_0\right)\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle=0\,. \tag{2.7}$$

Again, $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ satisfies the δ-function boundary condition. The well-known solution of Eq. (2.7) is

$$\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle=(4\pi\beta q)^{-d/2}\exp\left(-\frac{(\vec{x}-\vec{x}')^2}{4\beta q}\right)\,. \tag{2.8}$$

The square $(\vec{x}-\vec{x}')^2$ denotes the metric length squared of the vector $\vec{x}-\vec{x}'$.

Our method of studying $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ is to systematically work with the configurational function $F(\vec{x},\vec{x}';\beta,q)$ defined by

$$\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle=\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle F(\vec{x},\vec{x}';\beta,q)\,, \tag{2.9}$$

where

$$\lim_{\beta\to 0}F(\vec{x},\vec{x}';\beta,q)=1\,. \tag{2.10}$$

The configurational function F is of obvious physical importance since it is the density whose $d\vec{x}$ integral constructs the quantum partition function of the N-particle system in volume Σ, viz.,

$$Q_N(\Sigma)=\mathrm{Tr}_\Sigma e^{-\beta H}\equiv\frac{1}{(4\pi\beta q)^{3N/2}}\int_\Sigma d\vec{x}\,F(\vec{x},\vec{x};\beta,q)\,. \tag{2.11}$$

We construct $F(\vec{x},\vec{x}';\beta,q)$ in two stages. The first is to find the differential equation that F satisfies. The second is to solve the differential equation by a series expansion in β.

Substitute (2.9) into the heat Eq. (2.5). We find

$$\left(\frac{\partial}{\partial\beta}-2q\vec{\nabla}_x(\ln\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle)\cdot\vec{\nabla}_x+v(\vec{x})-q\Delta_x\right)\times F(\vec{x},\vec{x}';\beta,q)=0\,. \tag{2.12}$$

In this formula, $\vec{\nabla}_x$ represents the d-dimensional gradient. The explicit form of the free-heat equation solution (2.3) allows us to write

$$\vec{\nabla}_x\ln\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle=-\frac{1}{2\beta q}(\vec{x}-\vec{x}')\,. \tag{2.13}$$

Thus, the partial differential equation for F is

$$\left(\frac{\partial}{\partial\beta}+\frac{1}{\beta}(\vec{x}-\vec{x}')\cdot\vec{\nabla}_x+v(\vec{x})-q\Delta_x\right)F(\vec{x},\vec{x}';\beta,q)=0\,. \tag{2.14}$$

The boundary condition for F is given by Eq. (2.10). Represent F by an asymptotic series expansion in β,

$$F(\vec{x},\vec{x}';\beta,q)\sim\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}P_n(\vec{x},\vec{x}';q)\,. \tag{2.15}$$

Normalization condition (2.10) implies $P_0(\vec{x},\vec{x}';q)=1$.

Now determine the coefficient functions P_n. Insert the expansion (2.15) into (2.14). Equating the coefficient of the same power of β gives

$$\left(1+\frac{1}{n}(\vec{x}-\vec{x}')\cdot\vec{\nabla}_x\right)P_n(\vec{x},\vec{x}';q)=[v(\vec{x})-q\Delta_x]P_{n-1}(\vec{x},\vec{x}';q)\,. \tag{2.16}$$

Equation (2.16) may be simplified. Take ξ to be any positive parameter, and g to be any differentiable function with argument in the Euclidean space E_d. Then, for any $\vec{x}$ and $\vec{y}$ in E_d,

$$\frac{d}{d\xi}g(\vec{x}+\xi\vec{y})=\vec{y}\cdot\vec{\nabla}_x g(\vec{x}+\xi\vec{y})\,. \tag{2.17}$$

So, the left-hand side of Eq. (2.16) takes the form

$$\left(1+\frac{\xi}{n}\frac{d}{d\xi}\right)P_n(\vec{x}'+\xi\vec{y},\vec{x}';q)=\frac{1}{n\xi^{n-1}}\frac{d}{d\xi}[\xi^nP_n(\vec{x}'+\xi\vec{y};\vec{x}';q)]\,, \tag{2.18}$$

where $\xi\vec{y}=\vec{x}-\vec{x}'$. Equation (2.18) shows that the left-hand side of (2.16) has an exact integrating factor $n\xi^{n-1}$. Multiply (2.16) by $n\xi^{n-1}$ and replace $\vec{x}=\vec{x}'+\xi\vec{y}$. Then integration with respect to $\xi\in[0,1]$ gives us, after the replacement of $\vec{y}=\vec{x}-\vec{x}'$,

$$P_n(\vec{x},\vec{x}';q)=n\int_0^1 d\xi\,\xi^{n-1}v([\xi])P_{n-1}([\xi],\vec{x}';q)-nq\int_0^1 d\xi\,\xi^{n-1}\Delta_yP_{n-1}(\vec{y},\vec{x}';q)\,|_{\vec{y}=[\xi]}\,, \tag{2.19}$$

where the square bracket notation means

$$[\xi]=\xi\vec{x}+(1-\xi)\vec{x}'\,. \tag{2.20}$$

The notation in the last term on the right-hand side of (2.19) means that, first the Laplacian of P_{n-1} with respect to $\vec{y}$ is to be calculated, then $\vec{y}$ is to be set equal to $[\xi]$. The iteration of recursion relation is well defined if the potential $v(\vec{x})$ is infinitely differentiable.

Equation (2.19) is Perelomov's recursion relation[7] for $P_n(\vec{x},\vec{x}';q)$. Independent of the dimensionality E_d, it requires only a one-dimensional integration in parameter ξ. It is apparent that $P_n(\vec{x},\vec{x}';q)$ is the nth-order polynomial in $v(\vec{x})$ and its derivatives. Further, note that $P_n(\vec{x},\vec{x}';q)$ must be invariant with respect to the interchange of variables $\vec{x}\leftrightarrow\vec{x}'$. This follows since both $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ and $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ are real-valued matrix elements of functions of the Hermitian operators H and H_0. So the $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$, $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ are symmetric and this symmetry must be shared by the coefficient functions $P_n(\vec{x},\vec{x}';q)$.

The iterative structure of the recursion relation also implies that P_n is a polynomial of degree $n-1$ in the variable q. So it is natural, if $n\geq 1$, to represent P_n as

$$P_n(\vec{x},\vec{x}';q)=\sum_{m=0}^{n-1} q^m D_{m,n}(\vec{x},\vec{x}')\,. \tag{2.21}$$

The functions $D_{m,n}$ have no dependence on q. Formula (2.21) displays explicitly the semiclassical interpolation generated by the functions P_n. A recursion relation for the function $D_{m,n}$ follows by substituting (2.21) in (2.19) and equating the coefficients of the common power q. Thus, we have

$$D_{m,n}(\vec{x},\vec{x}')=n\int_0^1 d\xi\,\xi^{n-1}v([\xi])D_{m,n-1}([\xi],\vec{x}') -n\int_0^1 d\xi\,\xi^{n-1}\Delta_y D_{m-1,n-1}(\vec{y},\vec{x}')\,|_{\vec{y}=[\xi]}\,. \tag{2.22}$$

The functions $D_{m,n}$ are understood to be zero if $m\geq n$ or if either m or n are negative. $D_{0,0}(\vec{x},\vec{x}')=1$. In particular, note the first iterate of (2.19) or (2.22) gives

$$P_1(\vec{x},\vec{x}';q)=D_{0,1}(\vec{x},\vec{x}')=\int_0^1 d\xi\,v([\xi])\,. \tag{2.23}$$

Integral (2.23) is just the average value of v summed along a straight line joining $\vec{x}$ and $\vec{x}'$. When $\vec{x}=\vec{x}'$, then $P_1(\vec{x},\vec{x}';q)$ is just $v(\vec{x})$. In Sec. IV we will derive a closed integral form for $D_{m,n}(\vec{x},\vec{x}')$.

At the outset of this section, we mentioned that several rigorous studies of convergence criteria for expansion (2.4) are known. Typical of what one expects to find in general are the results holding for $d=3$. Buslaev has proved[3] the following. If the potential is a real function possessing derivatives to all orders such that the potential and all its derivatives decrease faster than any power of $|\vec{x}|^{-1}$ as $|\vec{x}|\to\infty$, then for z in the cut plane $\mathbb{C}\setminus\{\mathbb{R}_+\}$,

$$\langle\vec{x}|G(z)|\vec{x}'\rangle=\sum_{n=0}^{L}\frac{(-1)^n}{n!}P_n(\vec{x},\vec{x}';q)\left(\frac{\partial}{\partial z}\right)^n\langle\vec{x}|G_0(z)|\vec{x}'\rangle +R_L(\vec{x},\vec{x}';z)\,. \tag{2.24}$$

L may be any positive integer and the remainder term is estimated by

$$|R_L(\vec{x},\vec{x}';z)|\leq\frac{C_L}{|\sqrt{z}\,|^{L+1}}(1+|\vec{x}|+|\vec{x}'|)^{M(L)}\,, \tag{2.25}$$

where $M(L)>0$ is a finite number. The structure of the estimate (2.25) means that series (2.24) is asymptotically convergent (for all $\vec{x},\vec{x}'$) as $|z|\to\infty$. Series (2.24) is not exactly the same as the one Buslaev used, but the difference in the two descriptions can be absorbed in the remainder term estimate. More general asymptotic expansions with remainder term estimates of the Green's functions for elliptic operators in any dimension can be found in Agmon and Kannai.[8]

III. THE SEMICLASSICAL LIMIT

In this section we examine the nature of the semiclassical limit $q\approx 0$ inherent in the functions P_n. We discuss two rather distinct situations. The first case is the behavior of the limit when $\vec{x}=\vec{x}'$. Since the imaginary part of the Green's function for $\vec{x}=\vec{x}'$ is proportional to quantum state density, it is possible to make a detailed comparison with associated classical state density for the same system H. In the more general case $\vec{x}\neq\vec{x}'$, there is an additional phase oscillation in our expansion which is a manifestation of the essential singularity in the limit $\hbar\to 0$. The purpose of this section is to provide the correct physical interpretation of our formalism.

We first collect several formulas that are useful in discussing the semiclassical limit. If the free-heat kernel Eq. (2.8) is Laplace transformed by Eq. (2.2) and the resultant expression analytically continued to all $z\in\mathbb{C}\setminus\mathbb{R}_+$ the free Green's function takes the standard form

$$\langle\vec{x}|G_0(z)|\vec{x}'\rangle=\frac{i\pi}{(4\pi q)^{d/2}}z^{d/2-1}\left(\frac{q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|}{2}\right)^{1-d/2} \times H^{(1)}_{d/2-1}(q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)\,. \tag{3.1}$$

In this formula, $H^{(1)}$ denotes the Bessel function of the third kind. Note that as $\vec{x}'\to\vec{x}$, the Green's function has the characteristic singularity

$$\langle\vec{x}|G_0(z)|\vec{x}'\rangle\sim\frac{\Gamma(d/2-1)}{(4\pi q)^{d/2}}\left(\frac{4q}{|\vec{x}-\vec{x}'|^2}\right)^{d/2-1}, \tag{3.2}$$

where Γ is the gamma function. Only for $d=1$ is this singularity absent. Setting $d=3$ gives us the conventional expression

$$\langle\vec{x}|G_0(z)|\vec{x}'\rangle=\frac{1}{4\pi q}\frac{\exp(iq^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)}{|\vec{x}-\vec{x}'|}\,. \tag{3.3}$$

The nth partial derivative of the free Green's function with respect to z is just

$$\left(\frac{\partial}{\partial z}\right)^n \langle \vec{x}\,|G_0(z)|\,\vec{x}'\rangle = \frac{i\pi}{(4\pi q)^{d/2}} z^{d/2-1-n}\left(\frac{q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|}{2}\right)^{n+1-d/2} H^{(1)}_{d/2-1-n}(q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)\,, \tag{3.4}$$

which has the characteristic singularity as $\vec{x}'\to\vec{x}$,

$$\left(\frac{\partial}{\partial z}\right)^n \langle \vec{x}\,|G_0(z)|\,\vec{x}'\rangle \sim \frac{\Gamma(d/2-1-n)}{(4\pi q)^{d/2}}\left(\frac{4q}{|\vec{x}-\vec{x}'|^2}\right)^{d/2-1-n} \tag{3.5}$$

for $n\le[d/2-1]$, where $[x]$ stands for the largest integer $\le x$. Combining expression (3.4) with (2.4) gives us the expansion

$$\langle\vec{x}|G(z)\,|\,\vec{x}'\rangle \sim \frac{i\pi}{(4\pi q)^{d/2}} z^{d/2-1}\sum_{n=0}^{\infty}\frac{(-)^n}{n!}\,\frac{P_n(\vec{x},\vec{x}';q)}{z^n}\left(\frac{q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|}{2}\right)^{n+1-d/2} H^{(1)}_{d/2-1-n}(q^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)\,. \tag{3.6}$$

Consider the behavior of the Green's function in the neighborhood of the diagonal. In view of the characteristic singularity as $\vec{x}'\to\vec{x}$ as given by (3.5), one has to resort to a regularization procedure in order to give the diagonal a well-defined meaning. The regularized Green's function obtained by subtracting all the first $[d/2-1]$ singular terms is

$$\langle\vec{x}\,|G^R(z)\,|\,\vec{x}'\rangle = \langle\vec{x}\,|G(z)\,|\,\vec{x}'\rangle - \sum_{n=0}^{[d/2-1]}(-)^n\frac{P_n(\vec{x},\vec{x}';q)}{n!}\left(\frac{\partial}{\partial z}\right)^n\langle\vec{x}\,|G_0(z)\,|\,\vec{x}'\rangle\,. \tag{3.7}$$

Specializing to the three-dimensional case ($d=3$), the regularized Green's function will now be explicitly given by

$$\langle\vec{x}\,|G^R(z)\,|\,\vec{x}'\rangle = \langle\vec{x}|G(z)-G_0(z)\,|\,\vec{x}'\rangle \sim -i\frac{\exp(iq^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)}{8\pi q^{3/2}}\sum_{n=1}^{\infty}\frac{P_n(\vec{x},\vec{x}';q)}{z^{n-1/2}}\sum_{k=0}^{n-1}a(n,k)(-2iq^{-1/2}\sqrt{z}\,|\vec{x}-\vec{x}'|)^k\,, \tag{3.8}$$

where

$$a(n,k)=\frac{(2n-2-k)!}{2^{2n-2}n!\,(n-1-k)!\,k!}\,. \tag{3.9}$$

The diagonal limit ($\vec{x}'\to\vec{x}$), gives one the result

$$\langle\vec{x}\,|G^R(z)\,|\vec{x}\rangle \sim -\frac{i}{8\pi q^{3/2}}\sum_{n=1}^{\infty}a(n,0)\frac{P_n(\vec{x},\vec{x};q)}{z^{n-1/2}}\,. \tag{3.10}$$

Coming back to the general case, setting $z=s+i\mu$ and taking the limit $\mu\to0+$, the imaginary part of (3.6) reduces to

$$\mathrm{Im}\langle\vec{x}|G(s+i0)\,|\,\vec{x}'\rangle \sim \pi\frac{s^{d/2-1}}{(4\pi q)^{d/2}}\sum_{n=0}^{\infty}\frac{(-)^n}{n!}\,\frac{P_n(\vec{x},\vec{x}';q)}{s^n}\left(\frac{q^{-1/2}\sqrt{s}\,|\vec{x}-\vec{x}'|}{2}\right)^{n+1-d/2} J_{d/2-1-n}(q^{-1/2}\sqrt{s}\,|\vec{x}-\vec{x}'|)\,, \tag{3.11}$$

which is regular on the diagonal limit ($\vec{x}'\to\vec{x}$) with the result

$$\mathrm{Im}\langle\vec{x}|G(s+i0)\,|\vec{x}\rangle \sim \frac{\pi s^{d/2-1}}{(4\pi q)^{d/2}\Gamma(d/2)}\sum_{n=0}^{\infty}(-)^n\binom{d/2-1}{n}\frac{P_n(\vec{x},\vec{x};q)}{s^n}\,, \tag{3.12}$$

where

$$\binom{\nu}{n}=\frac{\Gamma(\nu+1)}{n!\,\Gamma(\nu+1-n)} \tag{3.13}$$

is the generalized binomial coefficient.

To begin our interpretation of the nature of the semiclassical content, consider first the diagonal case as it appears in expansion (3.7). Consider the definition of state density for system H. Take $\{e(\lambda)\}$ and $\{e_0(\lambda)\}$ to be the spectral projectors that are defined by the self-adjoint operators H and H_0. The projector $e(\lambda)$ is defined as the projection operator onto all states in $\mathcal{H}$ with energy λ or less. These projectors diagonalize H, via the spectral representation,

$$H=\int_{-\infty}^{\infty}\lambda\,de(\lambda)\,. \tag{3.14}$$

In terms of $\{e(\lambda)\}$, the operator Green's function has the representation

$$G(z)=\int_{-\infty}^{\infty}\frac{1}{\lambda-z}\,de(\lambda)\,, \tag{3.15}$$

with a similar form expression $G_0(z)$ in terms of $\{e_0(\lambda)\}$. The matrix element (or kernel) form of Eq. (3.15) is

$$\langle \vec{x}|G(z)|\vec{x}'\rangle = \int_{\infty}^{\infty} \frac{1}{\lambda - z} d\langle \vec{x}|e(\lambda)|\vec{x}'\rangle . \qquad (3.16)$$

Note the adjoint property $e^\dagger(\lambda) = e(\lambda)$ plus symmetry (in $\vec{x} \leftrightarrow \vec{x}'$) means that $\langle \vec{x}|e(\lambda)|\vec{x}'\rangle$ is a real function. Thus, if we take the imaginary part of Eq. (3.16) and set $z = s + i\mu$, then limit $\mu \to 0+$ gives us[9]

$$\mathrm{Im}\langle \vec{x}|G(s+i0)|\vec{x}'\rangle = \pi \frac{d}{ds}\langle \vec{x}|e(s)|\vec{x}'\rangle . \qquad (3.17)$$

Note that on the diagonal ($\vec{x}' = \vec{x}$) the right-hand side is π times the state density at energy s and position $\vec{x}$. For example, if Σ is an arbitrary volume in E_d, then the total number of states in Σ with energy less than s is given by

$$\mathrm{Tr}_\Sigma e(s) = \int_\Sigma d\vec{x} \langle \vec{x}|e(s)|\vec{x}\rangle . \qquad (3.18)$$

Of course, as $\Sigma \to \mathbb{R}^d$, the divergence of (3.18) reflects the fact that H has a continuous spectrum. Recalling (3.11) one obtains

$$\frac{d}{ds}\langle \vec{x}|e(s)|\vec{x}'\rangle \sim \frac{s^{d/2-1}}{(4\pi q)^{d/2}} \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \frac{P_n(\vec{x},\vec{x}';q)}{s^n} \left(\frac{q^{-1/2}\sqrt{s}\,|\vec{x}-\vec{x}'|}{2}\right)^{n+1-d/2} J_{d/2-1-n}(q^{-1/2}\sqrt{s}\,|\vec{x}-\vec{x}'|) , \qquad (3.19)$$

from which the state density at energy s and position x becomes

$$\frac{d}{ds}\langle \vec{x}|e(s)|\vec{x}\rangle \sim \frac{s^{d/2-1}}{(4\pi q)^{d/2}\Gamma(d/2)} \times \sum_{n=0}^{\infty} (-)^n \binom{d/2-1}{n} \frac{P_n(\vec{x},\vec{x};q)}{s^n} . \qquad (3.20)$$

In this way we have found an asymptotic expansion for the state density at $\vec{x}$ produced by the effect of the potential $v(\vec{x})$.

State density is a concept that is well defined in classical mechanics, so one can expect to find the classical analog to expansion (3.20). In addition, we will show that there is a unique classical Green's function defined as a complex valued function on phase space. Recall that observables in quantum mechanics are represented by self-adjoint operators in Hilbert space $\mathcal{H}$, whereas observables in classical mechanics are represented by functions on the phase space Γ. We seek the phase-space function that corresponds to the quantum Green's function. A standard way to transform the kernels of quantum operators to a phase-space form is given by the Weyl transform.[10] We determine the phase-space image of the resolvent identity for the Green's function. The classical limit is then found by letting $h \to 0$.

It is useful to start by noting that the classical definition of the differential number of states in phase space Γ is

$$\frac{d\vec{p}\,d\vec{x}}{h^d} . \qquad (3.21)$$

So, if $H(\vec{x},\vec{p})$ is the classical Hamiltonian, the number of states at $\vec{x}$ with energy s or less is

$$\tilde{e}(s,\vec{x}) = \int \Theta(s - H(\vec{x},\vec{p})) \frac{d\vec{p}}{h^d} , \qquad (3.22)$$

where Θ denotes the Heaviside function. Clearly, $\tilde{e}(s,\vec{x})$ is the classical counterpart to the matrix elements of the spectral projector $\langle \vec{x}|e(s)|\vec{x}\rangle$.

Now, let us consider the resolvent identity satisfied by the quantum Green's function. In operator form, one has

$$G(z) = G_0(z) - G_0(z)VG(z) . \qquad (3.23)$$

The kernel representation of this equation is the integral equation,

$$\langle \vec{x}|G(z)|\vec{x}'\rangle = \langle \vec{x}|G_0(z)|\vec{x}'\rangle - \int \langle \vec{x}|G_0(z)|\vec{x}''\rangle v(\vec{x}'')\langle \vec{x}''|G(z)|\vec{x}'\rangle\, d\vec{x}'' . \qquad (3.24)$$

The Weyl transform for an arbitrary operator A in $\mathcal{H}$ with kernel $\langle \vec{x}|A|\vec{x}'\rangle$ is defined by

$$A_W(\tau) = \int e^{i\vec{p}\cdot\vec{y}/\hbar}\langle \vec{x} - \tfrac{1}{2}\vec{y}|A|\vec{x} + \tfrac{1}{2}\vec{y}\rangle\, d\vec{y} , \qquad (3.25)$$

where $\tau = \{\vec{p},\vec{x}\}$ is a point in the $2d$-dimensional phase space Γ. The transform of the operator given by the product AB is[11]

$$(AB)_W(\tau) = A_W(\tau)e^{+i\hbar\Lambda/2}B_W(\tau) , \qquad (3.26)$$

where Λ is the Poisson bracket operation

$$\Lambda = \overleftarrow{\nabla}_x \cdot \overrightarrow{\nabla}_p - \overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_x , \qquad (3.27)$$

so that

$$A_W \Lambda B_W = \{A_W, B_W\} \qquad (3.28)$$

is the standard classical Poisson bracket.

First, observe that the Weyl transforms of both $G_0(z)$ and V are independent of h, viz.,

$$V_W(\tau) = v(z) , \qquad (3.29)$$

$$G_0(z)_W(\tau) = \frac{1}{(\vec{p}^2/2m - z)} . \qquad (3.30)$$

We define the formal limiting value of $G(z)_W$ to be

$$\tilde{G}(z)_W(\tau) = \lim_{h\to 0} G(z)_W(\tau). \tag{3.31}$$

With this notation, the transform of the product $G_0(z)VG(z)$ is

$$[G_0(z)VG(z)]_W(\tau) = G_0(z)_W(\tau)e^{i\hbar\Lambda/2}V_W(\tau)e^{i\hbar\Lambda/2}G(z)_W(\tau). \tag{3.32}$$

Taking the formal limit $h\to 0$, we find

$$\lim_{h\to 0}[G_0(z)VG(z)]_W(\tau) = G_0(z)_W(\tau)V_W(\tau)\tilde{G}(z)_W(\tau). \tag{3.33}$$

In this manner we see that the resolvent identity (3.23) has the classical limit

$$\tilde{G}(z)_W(\tau) = G_0(z)_W(\tau) - G_0(z)_W(\tau)V_W(\tau)\tilde{G}(z)_W(\tau). \tag{3.34}$$

This last equation is an algebraic equation in phase space with solution

$$\tilde{G}(z)_W(\vec{p},\vec{x}) = \frac{1}{\vec{p}^2/2m + v(\vec{x}) - z}. \tag{3.35}$$

Thus, it is seen that the obvious choice for the definition of the classical Green's function is also the one implied by the $h\to 0$ limit of the Weyl transform of the resolvent identity. From here on we will take expression (3.35) as the definition of the classical Green's function.

One important structural feature of the quantum Green's function is the identity (3.17) that related the state density at $\vec{x}$ to the imaginary part of $G(s+i0)$. It is a straightforward calculation to show that a similar relationship exists for the classical Green's function. Taking the imaginary part of (3.35) in the $\mathrm{Im}z\to 0+$ limit, one has

$$\mathrm{Im}\tilde{G}(s+i0)_W(\vec{p},\vec{x}) = \pi\delta(H(\vec{p},\vec{x}) - s). \tag{3.36}$$

The variable $\vec{p}$ does not occur in the quantum state density at $\vec{x}$ so, as in Eq. (3.22), we define a momentum-summed equivalent of (3.36) by

$$\mathrm{Im}\tilde{G}(s+i0,\vec{x}) = \int \mathrm{Im}\tilde{G}(s+i0)_W(\vec{p},\vec{x})\frac{d\vec{p}}{h^d} = \pi\int\delta(H(\vec{p},\vec{x}) - s)\,\frac{d\vec{p}}{h^d}. \tag{3.37}$$

But, according to (3.22), this can be rewritten as

$$\mathrm{Im}\tilde{G}(s+i0,\vec{x}) = \pi\frac{d}{ds}\tilde{e}(s,\vec{x}). \tag{3.38}$$

This is the precise counterpart to the quantum relation (3.17). The approximation of using $d\tilde{e}(s,\vec{x})/ds$ for the quantum density $d\langle\vec{x}|e(s)|\vec{x}\rangle/ds$ is the basis of the Thomas-Fermi formula used in atomic theory.[12] The pair of equations (3.17) and (3.38) illustrate a common feature of Green's functions, namely that the imaginary part of the Green's function has the physical interpretation of state density and so must be singularity free in the $\vec{x} = \vec{x}'$ limit. The real part of the Green's function has no direct physical interpretation and so the characteristic singularity $|\vec{x}-\vec{x}'|^{d-2}$ appears only in the real part of the function.

The definition of the classical Green's function, Eq. (3.35), provides us with an analytic function of z. This analyticity induces asymptotic expansions for both the momentum-summed classical Green's function and the classical state density $\tilde{e}(s,\vec{x})$,

$$\int\delta(H(\vec{p},\vec{x}) - s)\,\frac{d\vec{p}}{h^d} = \frac{1}{(4\pi q)^{d/2}\Gamma(d/2)}[s - v(\vec{x})]^{d/2-1}. \tag{3.39}$$

Furthermore,

$$\frac{d}{ds}\tilde{e}(s,\vec{x}) = \frac{1}{(4\pi q)^{d/2}\Gamma(d/2)}[s - v(\vec{x})]^{d/2-1}, \tag{3.40}$$

and has the asymptotic expansion

$$\frac{d}{ds}\tilde{e}(s,\vec{x}) \sim \frac{s^{d/2-1}}{(4\pi q)^{d/2}\Gamma(d/2)}\sum_{n=0}^{\infty}(-)^n\binom{d/2-1}{n}\frac{v(\vec{x})^n}{s^n}, \tag{3.41}$$

which should be compared with the quantum expression as given by Eq. (3.20). The classical limit is obtained from the correspondence

$$P_n(\vec{x},\vec{x};q)\to v(\vec{x})^n. \tag{3.42}$$

Specializing to the three-dimensional case, the classical regularized Green's function at point $\vec{x}$ and energy z is given by

$$\tilde{G}^R(z,\vec{x}) = [\tilde{G}(z,\vec{x}) - \tilde{G}_0(z,\vec{x})] \equiv \int\left(\frac{1}{\vec{p}^2/2m + v(\vec{x}) - z} - \frac{1}{\vec{p}^2/2m - z}\right)\frac{d\vec{p}}{h^3}, \tag{3.43}$$

which can be rewritten as an asymptotic expansion with the result

$$\tilde{G}^R(z,\vec{x}) \sim -\frac{i}{8\pi q^{3/2}}\sum_{n=1}^{\infty}a(n,0)\frac{v(\vec{x})^n}{z^{n-1/2}}, \tag{3.44}$$

where the coefficients $a(n,0)$ are defined by (3.9). Equation (3.44) is the classical counterpart of the quantal result as given by (3.10) from which it can be obtained by using (3.42). The series will converge for $|z| > |v(\vec{x})|$. Having established these exact classical results, we are in a position to examine the semiclassical limit.

The basic idea of a simple and smooth semiclassical limit resides in the definition of the configuration function F in Eq. (2.9). The complete classical limit of $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ as $h\to 0$ is very singular. In fact, as the formula (2.8) for $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ shows, this free-heat kernel has an essential singularity $h\to 0$. On the other hand, the function $F(\vec{x},\vec{x}';\beta,q)$ can be expected to have a smooth limit as $q\to 0$. In fact, if we set $q=0$ in the differential equation (2.14) for F, the solution is

$$F(\vec{x},\vec{x}';\beta,0)=\exp\left(-\beta\int_0^1 d\xi\, v(\vec{x}'+\xi(\vec{x}-\vec{x}'))\right). \tag{3.45}$$

This has the diagonal value

$$F(\vec{x},\vec{x};\beta,0)=e^{-\beta v(\vec{x})}. \tag{3.46}$$

This latter expression recovers the conventional classical partition function,[13]

$$Q_N^c(\Sigma)=\int_\Sigma d\vec{x}\langle\vec{x}|e^{-\beta H_0}|\vec{x}\rangle e^{-\beta v(\vec{x})}. \tag{3.47}$$

The simple factorization of the $h\to 0$ singularity structure in Eq. (2.9) allows us to define a semiclassical approximation by keeping h equal to its quantum value in $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ but at the same time using the smoothness of F in q to approximate it to a finite order in powers of q. This semiclassical approximation is then implemented through the functions P_n. Define the Mth-order semiclassical approximation for P_n by

$$P_n^{(M)}(\vec{x},\vec{x}';q)=\sum_{m=0}^{M} q^m D_{m,n}(\vec{x},\vec{x}'). \tag{3.48}$$

For $n<M+1$, $P_n^{(M)}=P_n$. Then the Mth order semiclassical configurational function is defined as

$$F^{(M)}(\vec{x},\vec{x}';\beta,q)=\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}P_n^{(M)}(\vec{x},\vec{x}';q). \tag{3.49}$$

The complete approximation for $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ to order M is then

$$\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle_{(M)}=\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle F^{(M)}(\vec{x},\vec{x}';\beta,q). \tag{3.50}$$

This form of a semiclassical approximation is suitable for practical calculations because $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$ is given by the explicit formula (2.8) and $F^{(M)}$ is determined from the functions P_n. Note that F has all the effects of the interaction $v(\vec{x})$ in it.

Through the Laplace transform, any approximation for $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ automatically engenders an approximation for the Green's function $\langle\vec{x}|G(z)|\vec{x}'\rangle$. Let us consider the diagonal case first. The Green's function equivalent of (3.50) is

$$\langle\vec{x}|G^R(z)|\vec{x}\rangle_{(M)}\sim\frac{-i}{8\pi q^{3/2}}\sum_{n=1}^{\infty}a(n,0)\frac{P_n^{(M)}(\vec{x},\vec{x};q)}{z^{n-1/2}}. \tag{3.51}$$

This is just (3.10) with $P_n^{(M)}$ replacing P_n. If $M=0$, then $P_n^{(0)}(\vec{x},\vec{x};q)=v(\vec{x})^n$ and we see that the classical series (3.44) is reproduced.

In fact, the semiclassical interpolating nature of P_n is evident in expansion (3.10). The P_n are just coefficients of $z^{-n+1/2}$. The q^0 part of P_n gives one the classical regularized Green's function $\tilde{G}^R$. The q^1 part of P_n gives the first semiclassical approximation, etc. The essential singularity aspect of the $h\to 0$ limit is not manifest, since the requirement that $\vec{x}=\vec{x}'$ removes the essential singularity from the matrix element $\langle\vec{x}|e^{-\beta H_0}|\vec{x}'\rangle$.

The situation is more complex for the general off-diagonal Green's function matrix element. The asymptotic expansion for the Mth-order approximation is

$$\langle\vec{x}|G^R(z)|\vec{x}'\rangle_{(M)}\sim\sum_{n=[d/2]}^{\infty}\frac{(-1)^n}{n!}P_n^{(M)}(\vec{x},\vec{x}';q)\left(\frac{\partial}{\partial z}\right)^n \times\langle\vec{x}|G_0(z)|\vec{x}'\rangle. \tag{3.52}$$

In particular, the zero-order approximation gives us the off-diagonal classical Green's function. Let $W(\vec{x},\vec{x}')$ be such that

$$W(\vec{x},\vec{x}')=\int_0^1 d\xi\, v(\vec{x}'+\xi(\vec{x}-\vec{x}'))=D_{0,1}(\vec{x},\vec{x}'). \tag{3.53}$$

Then, according to Eq. (3.45),

$$P_n^{(0)}(\vec{x},\vec{x}';q)=[W(\vec{x},\vec{x}')]^n. \tag{3.54}$$

Thus the zeroth-order approximation for $\langle\vec{x}|G(z)|\vec{x}'\rangle$ is given by

$$\langle\vec{x}|G(z)|\vec{x}'\rangle_{(0)}=\exp\left(-W(\vec{x},\vec{x}')\frac{\partial}{\partial z}\right)\langle\vec{x}|G_0(z)|\vec{x}'\rangle =\langle\vec{x}|G_0(z-W(\vec{x},\vec{x}'))|\vec{x}'\rangle, \tag{3.55}$$

where $\langle\vec{x}|G_0(z)|\vec{x}'\rangle$ is given by (3.1). The zeroth-order expansion $\langle\vec{x}|G(z)|\vec{x}'\rangle_{(0)}$ is seen to imbed the classical result (3.44) in a simple way. After regularization, when $\vec{x}=\vec{x}'$, then (3.55) collapses to the classical expansion (3.44).

The basic semiclassical approximation, Eq. (3.50) has several precursors[13-17] in the literature, particularly in the context of semiclassical approximation for virial coefficients. Generally, these earlier semiclassical approximations are efforts to derive the Wigner-Kirkwood expansion Eq. (1.4). Of particular note is the successful numerical calculation of Boyd, Larsen, and Kilpatrick[15] which shows, for a gas of the ^{4}He, the rate of convergence of the Wigner-Kirkwood expansion to the exact quantum results over a wide range of temperatures. After the renormalization of our expressions has been carried out (i.e., the summing to infinite order of the classical parts of P_n) we will demonstrate a close interrelationship to the formal representations of $F(\vec{x},\vec{x}';\beta,q)$ derived by Goldberger and Adams.[16] The exact kernel $\langle\vec{x}|e^{-\beta H}|\vec{x}'\rangle$ satisfies the semigroup property in the parameter β. The extent to which Wigner-Kirkwood approximations to $\langle \vec{x} | e^{-\beta H} | \vec{x}' \rangle$ will satisfy the semigroup property has been investigated by Baltin.[18]

IV. THE BORN SERIES AND THE FUNCTIONS P_n

The usefulness of the asymptotic expansion for the Green's functions and our semiclassical expansions depends on knowing explicit representations for the functions P_n and D_{nm}. In this section we will derive a closed integral representation for D_{nm}. The functions P_n are uniquely defined for all n by their recursion relation (2.19). Thus one can in principle construct P_n from this recursion relation. Following this procedure quickly leads to highly complicated integral forms, in which it is difficult to perceive the general structure of the functions P_n. One obvious drawback of the recursion relation (2.19) is its lack of symmetry. Although $P_n(\vec{x}, \vec{x}'; q)$ is symmetric under $\vec{x} \leftrightarrow \vec{x}'$, the differential operators in Eq. (2.19) act only on the left variable of P_n.

We will solve the problem of finding P_n another way. The Born series for $\langle \vec{x} | G(z) | \vec{x}' \rangle$ will be used, and an integral form for the Nth Born term will be derived. Then the terms in the Born series will be rearranged until the series assumes the form given by Eq. (2.4). Now, the coefficient of the term $(\partial/\partial z)^n \langle \vec{x} | G_0(z) | \vec{x}' \rangle$ should be $P_n(\vec{x}, \vec{x}'; q)$. We will verify that this is in fact correct by showing that the functions constructed in this manner satisfy the recursion relation (2.19).

The Born series, in a d-dimensional space, reads

$$\langle \vec{x} | G(z) | \vec{x}' \rangle = \sum_{N=0}^{\infty} (-1)^N B_N(\vec{x}, \vec{x}') . \tag{4.1}$$

The function B_N is the Nth Born term defined by

$$B_N(\vec{x}, \vec{x}') = \langle \vec{x} | G_0(z) [V G_0(z)]^N | \vec{x}' \rangle . \tag{4.2}$$

The Born series is basically an expansion in $V/|z|$ and can be expected to converge for large $|z|$. Convergence criteria for $d \geq 3$ may be found in Faris.[19]

It is shown in Appendix A that $B_N(\vec{x}, \vec{x}')$ can be represented as a parametric integral in the variable β. We use the following notation:

$$\int_{0 \leq \alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_N \leq 1} \cdots \int d\alpha_1 \ldots d\alpha_N = \int_A d^N \alpha , \tag{4.3}$$

$$\sum' = \sum_{j=1}^{N}, \qquad \sum'' = \sum_{1 \leq j < k \leq N}^{N} . \tag{4.4}$$

The integral representation of B_N takes the form

$$B_N(\vec{x}, \vec{x}') = \int_0^{\infty} d\beta (4\pi\beta q)^{-d/2} \beta^N \exp\left(z\beta - \frac{1}{4\beta q} (\vec{x} - \vec{x}')^2\right) \times \int_A d^N \alpha \exp\left[\beta q \left(\sum^{N\prime} \alpha_j (1-\alpha_j) \Delta_j + 2 \sum^{N\prime\prime} \alpha_j (1-\alpha_k) \vec{\nabla}_j \cdot \vec{\nabla}_k\right)\right] v((\alpha_1)) \ldots v((\alpha_N)) . \tag{4.5}$$

In Eq. (4.5) the variable (α_j) is

$$(\alpha_j) = (1-\alpha_j)\vec{x} + \alpha_j \vec{x}' . \tag{4.6}$$

The exponential of the Laplacian and gradient operators is defined by its series expansion. The notation $\vec{\nabla}_j$ or Δ_j means that these differential operators act only on the potential v with argument (α_j) in accordance with the formula

$$\Delta_j v((\alpha_i)) = \delta_{ji} (\Delta v)((\alpha_j)) . \tag{4.7}$$

The right-hand side of (4.7) is to be interpreted as letting Δ act on $v(\vec{x})$ then, after that putting $\vec{x} \to (\alpha_i)$.

The formula (4.5) is rather complicated, but is valid for all $d \geq 1$ and all $N > 0$. Note that the first portion of the integral in β is the integrand for $(\partial/\partial z)^N \langle \vec{x} | G_0(z) | \vec{x}' \rangle$. Further, the d dependence is trivial. It only appears in the factor $(4\pi\beta q)^{-d/2}$ and the definition of $\vec{x}$ and $\vec{\nabla}_x$. It is also evident that formula (4.5) requires that $v(\vec{x})$ be infinitely differentiable.

The second exponential in (4.5) should contain all the q dependence of $\langle \vec{x} | G(z) | \vec{x}' \rangle$ that does not appear in $(\partial/\partial z)^N \langle \vec{x} | G_0(z) | \vec{x}' \rangle$. Thus, let us define the mth-order term in q by

$$D_{m,N+m}(\vec{x}, \vec{x}') = \frac{(-1)^m (N+m)!}{m!} \int_A d^N \alpha \left(\sum^{N\prime} \alpha_j (1-\alpha_j) \Delta_j + 2 \sum^{N\prime\prime} \alpha_j (1-\alpha_k) \vec{\nabla}_j \cdot \vec{\nabla}_k\right)^m v((\alpha_1)) \ldots v((\alpha_N)) . \tag{4.8}$$

Note that $D_{m,N+m}(\vec{x}, \vec{x}')$ has no β dependence. Employing Eq. (4.8) in Eq. (4.5), let us write the Nth Born term as

$$B_N(\vec{x}, \vec{x}') = \sum_{m=0}^{\infty} \frac{(-q)^m}{(N+m)!} D_{m,N+m}(\vec{x}, \vec{x}') \left(\frac{\partial}{\partial z}\right)^{N+m} \langle \vec{x} | G_0(z) | \vec{x}' \rangle . \tag{4.9}$$

The last step is to construct $\langle\vec{x}|G(z)|\vec{x}'\rangle$ by the Born series (4.1) using expression (4.9) for B_N. The resultant series is summed over $N=0,\infty$ and then $m=0,\infty$. Change the summation indices by letting $N+m=n$. Then one obtains

$$\langle\vec{x}|G(z)|\vec{x}'\rangle \sim \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left(\sum_{m=0}^{n-1} q^m D_{m,n}(\vec{x},\vec{x}')\right)\left(\frac{\partial}{\partial z}\right)^n\langle\vec{x}|G_0(z)|\vec{x}'\rangle\,. \tag{4.10}$$

Formula (4.10) has the identical structure as the original asymptotic expansion (2.4). For a given analytic function of z, asymptotic expansions are unique; thus it is to be expected that the function within the square brackets is $P_n(\vec{x},\vec{x}';q)$. This expectation is not a rigorous mathematical conclusion, since in deriving expression (4.5), we have assumed it is permissible to interchange the order of integration. Also, in writing sum (4.10), we have changed the order of summation. Rather than making this formal proof rigorous, the simplest approach is just to verify that $D_{m,N+m}(\vec{x},\vec{x}')$ as defined by Eq. (4.8) satisfies the recursion relation (2.22).

Before proceeding to the proof, we should note that the symmetry with respect to the $\vec{x}\leftrightarrow\vec{x}'$ is implied by representation (4.8). In order to prove this, let $\vec{x}\leftrightarrow\vec{x}'$ and $\alpha_j\to 1-\alpha_j$ in the integral for $D_{m,N+m}$. Note that these two substitutions leave (α_j) unchanged, so that (4.8) now reads

$$D_{m,N+m}(\vec{x}',\vec{x}) = \frac{(-1)^m(N+m)!}{m!}\int_{0\le\alpha_N\le\cdots\alpha_1\le 1}\cdots\int d\alpha_1\cdots d\alpha_N\left(\sum_j\alpha_j(1-\alpha_j)\Delta_j + 2\sum_{j<k}(1-\alpha_j)\alpha_k\vec{\nabla}_j\cdot\vec{\nabla}_k\right)^m \times v((\alpha_1))\cdots v((\alpha_N))\,. \tag{4.11}$$

The restrictions in the domain of the α_j suggest that we make the replacement $\alpha_j\to\alpha_{N+1-j}$. Thus, the domain restriction is restored to the form it has in (4.8) Note the product of the potentials transforms into itself under this relabeling. Finally, consider the $\vec{\nabla}_j\cdot\vec{\nabla}_k$ term. Here, the effect of $\alpha_j\to\alpha_{N+1-j}$ is

$$\sum_{j<k}(1-\alpha_j)\alpha_k\vec{\nabla}_j\cdot\vec{\nabla}_k \to \sum_{N+1-j>N+1-k}(1-\alpha_{N+1-j})\alpha_{N+1-k}\vec{\nabla}_{N+1-j}\cdot\vec{\nabla}_{N+1-k}\,. \tag{4.12}$$

Set $j'=N+1-k$ and $k'=N+1-j$; then the right-hand part of (4.12) becomes

$$\sum_{j'<k'}(1-\alpha_{k'})\alpha_{j'}\vec{\nabla}_{k'}\cdot\vec{\nabla}_{j'}\,. \tag{4.13}$$

Except for the primes on the dummy summation indices, this sum is identical to that in Eq. (4.8). Thus we have shown

$$D_{m,N+m}(\vec{x},\vec{x}') = D_{m,N+m}(\vec{x}',\vec{x}) = \frac{(-1)^m(N+m)!}{m!}\int_A d^N\alpha\left(\sum^{N}{}'\,\alpha_j(1-\alpha_j)\Delta_j + 2\sum^{N}{}''\,\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)^m v([\alpha_1])\cdots v([\alpha_N])\,, \tag{4.14}$$

where $[\alpha]=\alpha\vec{x}+(1-\alpha)\vec{x}'$ according to the definition in Eq. (2.20).

To prove representation (4.8) satisfies the recursion relation (2.22) for $D_{n,m}$, we must show expression (4.8) or (4.14) satisfies

$$D_{m,N+m}(\vec{x},\vec{x}') = (N+m)\int_0^1 d\xi\,\xi^{N+m-1}v([\xi])D_{m,N+m-1}([\xi],\vec{x}') - (N+m)\int_0^1 d\xi\,\xi^{N+m-1}\Delta_y D_{m-1,N+m-1}(\vec{y},\vec{x}')\big|_{\vec{y}=[\xi]}\,. \tag{4.15}$$

Use expression (4.14) to compute the right-hand side of (4.15). In (4.14), we must make the substitution $\vec{x}\to[\xi]=\xi\vec{x}+(1-\xi)\vec{x}'$ and $[\alpha_i]=\alpha_i\vec{x}+(1-\alpha_i)\vec{x}'\to\xi\alpha_i\vec{x}+(1-\xi\alpha_i)\vec{x}'=[\xi\alpha_i]$. The two right-hand terms in (4.15) are, respectively,

$$\frac{(-1)^m(N+m)!}{m!}\int_0^1 d\xi\,\xi^{N+m-1}v([\xi])\int_A d^{N-1}\alpha\left(\sum^{N-1}{}'\alpha_j(1-\alpha_j)\Delta_j + 2\sum^{N-1}{}''\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)^m v([\xi\alpha_1])\cdots v([\xi\alpha_{N-1}])\,, \tag{4.16}$$

and

$$\frac{-(-1)^{m-1}(N+m)!}{(m-1)!}\int_0^1 d\xi\,\xi^{N+m-1}\Delta_y\int_A d^N\alpha\left(\sum^{N}{}'\alpha_j(1-\alpha_j)\Delta_j + 2\sum^{N}{}''\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)^{m-1} \times v(\alpha_1\vec{y}+(1-\alpha_1)\vec{x}')\cdots v(\alpha_N\vec{y}+(1-\alpha_N)\vec{x}')\big|_{\vec{y}=\xi\vec{x}+(1-\xi)\vec{x}'}\,. \tag{4.17}$$

These two terms are simplified by several variable substitutions. In the integral (4.16), let $\xi=\alpha_N$ and $\xi\alpha_j\to\alpha_j$. Then, (4.16) becomes

$$\frac{(-1)^m(N+m)!}{m!}\int_A d^N\alpha\left[\sum^{N}{}'\alpha_j\left(1-\frac{\alpha_j}{\alpha_N}\right)\Delta_j+2\sum^{N}{}''\alpha_j\left(1-\frac{\alpha_k}{\alpha_N}\right)\vec{\nabla}_j\cdot\vec{\nabla}_k\right]^m v([\alpha_1])\cdots v([\alpha_N]). \tag{4.18}$$

Note that we can extend the sums $\sum'$ and $\sum''$ from $N-1$ to N since the coefficient multiplying the Nth term is zero. For the same reason, the term $v([\xi])$ may be moved to the right of all the differential operators in $(\ )^m$. In the second term (4.17), the Laplacian operator Δ_y and the $d^N\alpha$ integration may be interchanged because the derivatives of $v(x)$ are bounded. The effect of Δ_y acting on the potentials is

$$\Delta_y v(\alpha_1\vec{y}+(1-\alpha_1)\vec{x}')\cdots v(\alpha_N\vec{y}+(1-\alpha_N)\vec{x}')=\sum_{j=1}^{N}\sum_{k=1}^{N}\alpha_j\alpha_k\vec{\nabla}_j\cdot\vec{\nabla}_k v(\alpha_1\vec{y}+(1-\alpha_1)\vec{x}')\cdots v(\alpha_N\vec{y}+(1-\alpha_N)\vec{x}'). \tag{4.19}$$

Let $\alpha_j\xi\to\alpha_j$ for $j=1$, N and let $\xi=\alpha_{N+1}$. Then (4.17) becomes

$$\frac{(-1)^m(N+m)!}{m!}\int_A d^N\alpha\, m\int_{\alpha_N}^{1}d\alpha_{N+1}\left[\sum^{N}{}'\alpha_j\left(1-\frac{\alpha_j}{\alpha_{N+1}}\right)\Delta_j+2\sum^{N}{}''\alpha_j\left(1-\frac{\alpha_k}{\alpha_{N+1}}\right)\vec{\nabla}_j\cdot\vec{\nabla}_k\right]^{m-1}$$
$$\times\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\alpha_j\alpha_k}{\alpha_{N+1}^2}\vec{\nabla}_j\cdot\vec{\nabla}_k v([\alpha_1])\cdots v([\alpha_N]). \tag{4.20}$$

Observe that in $v([\alpha_1])\cdots v([\alpha_N])$, there is no α_{N+1} dependence. Thus, with the help of the identity

$$\frac{d}{d\alpha_{N+1}}\left[\sum^{N}{}'\alpha_j\left(1-\frac{\alpha_j}{\alpha_{N+1}}\right)\Delta_j+2\sum^{N}{}''\alpha_j\left(1-\frac{\alpha_k}{\alpha_{N+1}}\right)\vec{\nabla}_j\cdot\vec{\nabla}_k\right]^m=m[\cdots]^{m-1}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\alpha_j\alpha_k}{\alpha_{N+1}^2}\vec{\nabla}_j\cdot\vec{\nabla}_k \tag{4.21}$$

the $d\alpha_{N+1}$ integral can be evaluated exactly giving us two terms. The term from the lower limit $\alpha_{N+1}=\alpha_N$ is the negative expression (4.18). Thus the entire right-hand side of (4.15) now reads

$$\frac{(-1)^m(N+m)!}{m!}\int_A d^N\alpha\left(\sum^{N}{}'\alpha_j(1-\alpha_j)\Delta_j+2\sum^{N}{}''\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)^m v([\alpha_1])\cdots v([\alpha_N]). \tag{4.22}$$

But, this is the formula for $D_{m,N+m}(\vec{x},\vec{x}')$. So we have established that expression (4.14) satisfies recursion relation (2.22).

Our exact representation (4.8) is a convenient starting point for the investigation of the general structure of the functions $D_{m,N+m}(\vec{x},\vec{x}')$. Recall that the value of m in $D_{m,N+m}(\vec{x},\vec{x}')$ gives the order in q of the contribution of $D_{m,N+m}$ to P_{N+m}. The index N is associated with the Nth Born term. The classical term is $m=0$. Expression (4.8) is just the $d^N\alpha$ integral over the product of potentials. Because of the symmetry of the integrand in $\alpha_1,\ldots,\alpha_N$ the integral gives

$$D_{0,N}(\vec{x},\vec{x}')=\left(\int_0^1 d\alpha\, v((\alpha))\right)^N=D_{0,1}(\vec{x},\vec{x}')^N. \tag{4.23}$$

Another simple result is that for the first Born-term-generated parts of $D_{m,N+m}$. Setting $N=1$ leads to

$$D_{m,1+m}(\vec{x},\vec{x}')=(-1)^m(m+1)\int_0^1 d\alpha[\alpha(1-\alpha)]^m(\Delta^m v)((\alpha)). \tag{4.24}$$

The diagonal case reduces to

$$D_{m,1+m}(\vec{x},\vec{x})=(-1)^m\frac{m!\,(m+1)!}{(2m+1)!}\Delta^m v(\vec{x}). \tag{4.25}$$

Consider next the semiclassical term. This term is defined by representation (4.8) with $m=1$, viz.,

$$D_{1,N+1}(\vec{x},\vec{x}')=-(N+1)!\int_A d^N\alpha\left(\sum^{N}{}'\alpha_j(1-\alpha_j)\Delta_j+2\sum^{N}{}''\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)v((\alpha_1))\cdots v((\alpha_N)). \tag{4.26}$$

Carrying out the integration over $d^N\alpha$ in accordance with domain restriction (4.3) leads us to

$$D_{1,N+1}(\vec{x},\vec{x}')=-N(N+1)\left(\int_0^1 d\alpha\,\alpha(1-\alpha)(\Delta v)((\alpha))\right)D_{0,1}(\vec{x},\vec{x}')^{N-1}$$
$$-2(N-1)N(N+1)\left(\int_{0\le\alpha_1\le\alpha_2\le1}\int d\alpha_1 d\alpha_2\,\alpha_1(1-\alpha_2)(\vec{\nabla}v)((\alpha_1))\cdot(\vec{\nabla}v)((\alpha_2))\right)D_{0,1}(\vec{x},\vec{x}')^{N-2}. \tag{4.27}$$

The diagonal case reduces to

$$D_{1,N+1}(\bar{x},\bar{x}) = -\frac{N(N+1)}{6}\,v(\bar{x})^{N-1}\Delta v(\bar{x}) - \frac{(N-1)N(N+1)}{12}\,v(\bar{x})^{N-2}[\bar{\nabla} v(\bar{x})]^2 . \qquad (4.28)$$

In this manner the functions $D_{m,N+m}$ and P_n may be systematically calculated. In Appendix B we quote the values for the first four off-diagonal P_n and the first six values for the diagonal case. From our experience so far, it would seem that beyond $n\sim 10$, the structure of the functions is sufficiently complicated that one would have to use a computer to determine them.

V. CONCLUSIONS

This paper has constructed the asymptotic expansion for the N-body Green's functions, in the case when the potential interactions are smooth functions. The asymptotic expansion is shown to be determined by the functions $P_n(\bar{x},\bar{x}';q)$. The resultant semiclassical expansion is a consequence of the Laplace transform of the matrix element representation of $e^{-\beta H}$, viz.,

$$\langle \bar{x}|e^{-\beta H}|\bar{x}'\rangle = \langle \bar{x}|e^{-\beta H_0}|\bar{x}'\rangle F(\bar{x},\bar{x}';\beta,q)\,, \qquad (5.1)$$

$$F(\bar{x},\bar{x}';\beta,q) \sim \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} P_n(\bar{x},\bar{x}';q)\,. \qquad (5.2)$$

The factorization in Eq. (5.1) allows one to define a smooth semiclassical limit. The essential singularity in the $q\to 0$ limit is restricted to the factor $\langle \bar{x}|e^{-\beta H_0}|\bar{x}'\rangle$. The configurational function, on the other hand, is continuous in the limit $q\to 0$. The semiclassical approximation that this factorization in Eq. (5.1) makes possible is to keep q equal to its quantum value in the function $\langle \bar{x}|e^{\beta H_0}|\bar{x}'\rangle$ while at the same time letting $F(\bar{x},\bar{x}';\beta,q)$ be approximated to any finite order in q.

In the course of our analysis, we have solved the recursion relations that define the $P_n(\bar{x},\bar{x}';q)$ and we quote in Appendix B the specific forms of these functions. The apparent advantages of our approach to semiclassical expansions are the following: It is valid for any space dimension (or number of particles), it is defined for both on- and off-diagonal matrix elements of the Green's functions, and [since the $P_n(\bar{x},\bar{x}';q)$ are computed] it is explicit. The expansion obtained in (5.1) and (5.2) has close links to the semiclassical expansions derived from the Feynman path-integral representation of quantum mechanics.[20-23] For example, the path-integral method has been used to compute semiclassical expansion for $\mathrm{Tr}\,e^{-\beta H}$. A $d\bar{x}$ integration of Eq. (5.1) after $\bar{x}'=\bar{x}$ also constructs this same trace. The semiclassical expansion, which comes from using formulas (B4)–(B6), is in agreement with that given by Yaglom.[22] One extensive application of semiclassical methods has been to determine the discrete spectra of a system with Hamiltonian H.[24] The usefulness of our Green's-function expansion (2.4) for this purpose is not clear and requires further study. Since the expansion (2.4) is built up from a high-energy asymptotic series for $\langle \bar{x}|G(z)|\bar{x}'\rangle$, it is not directly suitable for describing the bound-state poles in $\langle \bar{x}|G(z)|\bar{x}'\rangle$. Such poles always involve potential effects to infinite order and would not be described by any finite Mth order h truncation of the type given in Eq. (3.51).

There are two groups of problems intimately related to the expansions described here. The first is the semiclassical expansion of the few-body virial coefficients.[15] The direct part of the N-body virial coefficient is just the x integral over the diagonal matrix elements of the fully connected cluster that is associated with $e^{-\beta H_N}$. Note that since our expansion is valid off-diagonal, one can compute semiclassical expressions for exchange contributions to the higher virials. The second set of problems wherein the method described above is already in partial use is the statement and derivation of sum rules (or trace identities) in scattering theory. Using the theory of time delay, it is understood that the classical expansion Eq. (3.44) leads to sum rules in classical scattering.[25] The quantum asymptotic expansion (2.4) has been the basis for deriving trace identities in the 1D case.[26] In the 3D case, one can obtain the time-delay type of sum rules.[3,27] Recently, the diagonal form of Eq. (2.4) was used as the starting point for deriving an infinite class of sum rules that assume the form of the power-moment problem.[28]

APPENDIX A

In this appendix, we present a derivation of the integral form of the Nth Born term. The heat kernel Eq. (2.8) provides, through the Laplace transform, a representation of the free Green's function in d dimensions, viz.,

$$\langle \bar{x}|G_0(z)|\bar{x}'\rangle = \int_0^{\infty} d\beta\, e^{z\beta}(4\pi\beta q)^{-d/2} \exp\left(-\frac{(\bar{x}-\bar{x}')^2}{4\beta q}\right). \qquad (A1)$$

In terms of (A1), the Nth Born term is defined as

$$B_N(\bar{x},\bar{x}')=\int_0^\infty\cdots\int_0^\infty d\beta_1\cdots d\beta_{N+1}[(4\pi q)^{N+1}\beta_1\cdots\beta_{N+1}]^{-d/2}e^{z(\beta_1+\cdots+\beta_{N+1})}$$
$$\times\int\cdots\int dx_1\cdots dx_N v(\bar{x}_1)\cdots v(\bar{x}_N)\exp\left(-\frac{(\bar{x}-\bar{x}_1)^2}{4\beta_1 q}-\frac{(\bar{x}_1-\bar{x}_2)^2}{4\beta_2 q}-\cdots-\frac{(\bar{x}_N-\bar{x}')^2}{4\beta_{N+1}q}\right). \tag{A2}$$

Our derivation of Eq. (4.5) for $B_N(\bar{x},\bar{x}')$ proceeds by a succession of variable changes in (A2).

The first step is to define new variables by

$$\beta=\beta_1+\beta_2+\cdots+\beta_{N+1},\quad \beta_i\geq 0,$$
$$\alpha_i=(\beta_1+\beta_2+\cdots+\beta_i)/\beta,\quad 1\geq\alpha_i\geq 0,\quad i=1,N. \tag{A3}$$

Note $d\beta_1\cdots d\beta_{N+1}=\beta^N d\beta\, d\alpha_1\cdots d\alpha_N$. Furthermore, the domain for the α integration satisfies the constraint $0\leq\alpha_1\leq\alpha_2\leq\cdots\leq\alpha_N\leq 1$. The quantity in large parentheses in (A2) is proportional to

$$\frac{(\bar{x}-\bar{x}_1)^2}{\alpha_1-\alpha_0}+\frac{(\bar{x}_1-\bar{x}_2)^2}{\alpha_2-\alpha_1}+\cdots+\frac{(\bar{x}_{N-1}-\bar{x}_N)^2}{\alpha_N-\alpha_{N-1}}+\frac{(\bar{x}_N-\bar{x}')^2}{1-\alpha_N}, \tag{A4}$$

where $\alpha_0\equiv 0$. Expression (A4) can also be written

$$(\bar{x}-\bar{x}')^2+\sum_{k=1}^{N}\frac{(1-\alpha_{k-1})}{(\alpha_k-\alpha_{k-1})(1-\alpha_k)}\left(\bar{x}_k-\frac{(1-\alpha_k)\bar{x}_{k-1}+(\alpha_k-\alpha_{k-1})\bar{x}'}{1-\alpha_{k-1}}\right)^2. \tag{A5}$$

In (A5), $\bar{x}_0=\bar{x}$. Equality of (A4) and (A5) is established by induction. Assume the equality holds for N, then use of the algebraic identity

$$\frac{(\bar{x}_N-\bar{x}_{N+1})^2}{\alpha_{N+1}-\alpha_N}+\frac{(\bar{x}_{N+1}-\bar{x}')^2}{1-\alpha_{N+1}}=\frac{1}{1-\alpha_N}(\bar{x}_N-\bar{x}')^2+\frac{(1-\alpha_N)}{(\alpha_{N+1}-\alpha_N)(1-\alpha_{N+1})}\left(\bar{x}_{N+1}-\frac{(1-\alpha_{N+1})\bar{x}_N+(\alpha_{N+1}-\alpha_N)\bar{x}'}{1-\alpha_N}\right)^2, \tag{A6}$$

shows the equality of (A4), and (A5) holds for $N+1$. Thus the integral for B_N takes the form

$$B_N(\bar{x},\bar{x}')=\int_0^\infty d\beta\,\beta^N e^{z\beta}(4\pi\beta q)^{-d/2}\exp\left(-\frac{1}{4\beta q}(\bar{x}-\bar{x}')^2\right)\int_A d^N\alpha[(4\pi\beta q)^N\alpha_1(\alpha_2-\alpha_1)\cdots(\alpha_N-\alpha_{N-1})(1-\alpha_N)]^{-d/2}$$
$$\times\prod_{k=1}^{N}\int dx_k v(\bar{x}_k)\exp\left[-\frac{1}{4\beta q}\frac{(1-\alpha_{k-1})}{(\alpha_k-\alpha_{k-1})(1-\alpha_k)}\left(\bar{x}_k-\frac{(1-\alpha_k)\bar{x}_{k-1}+(\alpha_k-\alpha_{k-1})\bar{x}'}{1-\alpha_{k-1}}\right)^2\right], \tag{A7}$$

where (A7) uses convention (4.3) for the $d\alpha$ integrations. Here we see that the usefulness of expression (A5) is that it allows us to display in the integrand of (A7) the kernel for the function $(\partial/\partial z)^N\langle\bar{x}|G_0(z)|\bar{x}'\rangle$.

The second modification of (A2) is to shift the $\bar{x}_k$ variables in (A7) so that the exponential on the right-hand side is simplified. This variable shift is carried out by the successive substitutions

$$\bar{x}_1\to\bar{x}_1+(1-\alpha_1)\bar{x}+\alpha_1\bar{x}',$$
$$\bar{x}_2\to\bar{x}_2+\frac{(1+\alpha_2)\bar{x}_1+(\alpha_2-\alpha_1)\bar{x}'}{1-\alpha_1},$$
$$\cdots$$
$$\bar{x}_k\to\bar{x}_k+\frac{(1-\alpha_k)\bar{x}_{k-1}+(\alpha_k-\alpha_{k-1})\bar{x}'}{1-\alpha_{k-1}}.$$
$$\cdots \tag{A8}$$

The net result of this successive change of variables is the replacement

$$\bar{x}_k\to\bar{x}_k+\frac{1-\alpha_k}{1-\alpha_{k-1}}\bar{x}_{k-1}+\frac{1-\alpha_k}{1-\alpha_{k-2}}\bar{x}_{k-2}+\cdots+\frac{1-\alpha_k}{1-\alpha_1}\bar{x}_1+(1-\alpha_k)x+\alpha_k\bar{x}'. \tag{A9}$$

Thus the dx_k portion of B_N now reads

$$X\equiv\prod_{k=1}^{N}\int d\bar{x}_k\exp\left(-\frac{(1-\alpha_{k-1})}{4\beta q(\alpha_k-\alpha_{k-1})(1-\alpha_k)}\bar{x}_k^2\right)v\left(\bar{x}_k+\frac{1-\alpha_k}{1-\alpha_{k-1}}\bar{x}_{k-1}+\cdots+\frac{1-\alpha_k}{1-\alpha_1}\bar{x}_1+(1-\alpha_k)\bar{x}+\alpha_k\bar{x}'\right). \tag{A10}$$

Finally, let the variable y_k be

$$\vec{y}_k=\left(\frac{(1-\alpha_{k-1})}{4\beta q(\alpha_k-\alpha_{k-1})(1-\alpha_k)}\right)^{1/2}\vec{x}_k\,. \tag{A11}$$

With this substitution, (A10) becomes

$$X=(4\beta q)^{Nd/2}[\alpha_1(\alpha_2-\alpha_1)\cdots(\alpha_N-\alpha_{N-1})(1-\alpha_N)]^{d/2}Y\,, \tag{A12}$$

$$Y\equiv\int\cdots\int d\vec{y}_1\cdots d\vec{y}_N\exp[-(\vec{y}_1^{\,2}+\cdots+\vec{y}_N^{\,2})]\prod_{k=1}^{N}v(\vec{\gamma}_k+(\alpha_k))\,, \tag{A13}$$

where

$$\vec{\gamma}_k\equiv(4\beta q)^{1/2}(1-\alpha_k)\sum_{i=1}^{k}\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)^{1/2}\vec{y}_i\,, \tag{A14}$$

$$(\alpha_k)\equiv(1-\alpha_k)\vec{x}+\alpha_k\vec{x}'\,. \tag{A15}$$

Here it is seen that the multiplicative factor before the Y integral will cancel the similar factor in (A7).

The last modification of the B_N integral is to represent v by its Taylor series expansion and to execute the y_i integrations. The Taylor series in d dimensions for v is

$$v(\vec{\gamma}_k+(\alpha_k))=\sum_{n=0}^{\infty}\frac{1}{n!}(\vec{\gamma}_k\cdot\vec{\nabla}_k)^n v((\alpha_k))=[\exp(\vec{\gamma}_k\cdot\vec{\nabla}_k)]v_k\,. \tag{A16}$$

In (A16), the notation $\vec{\nabla}_k v((\alpha_k))$ means that $\vec{\nabla}_x$ acts on $v(\vec{x})$; then $\vec{x}$ is replaced by (α_k). For $v((\alpha_k))$ we often write v_k. Insert (A16) into (A13), then the product of all the potential terms is

$$\exp\left(\sum_{k=1}^{N}\vec{\gamma}_k\cdot\vec{\nabla}_k\right)v_1\cdots v_k=\exp\left[(4\beta q)^{1/2}\sum_{i=1}^{N}\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)^{1/2}\vec{y}_i\cdot\left(\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right)\right]v_1\cdots v_k\,. \tag{A17}$$

Consider now the integration over the variable $\vec{y}_i$ in Y. We see from (A17) that we have succeeded in factoring all the $\vec{y}_i$ dependence. Thus, each $\vec{y}_i$ integral may be carried out independently of the other $\vec{y}$ integrals. The total exponential dependence in the $\vec{y}_i$ variable is

$$\begin{aligned}S&\equiv-\left[\vec{y}_i^{\,2}-(4\beta q)^{1/2}\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)^{1/2}\vec{y}_i\cdot\left(\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right)\right]\\&=-\left[\vec{y}_i-(\beta q)^{1/2}\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)^{1/2}\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right]^2+\beta q\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)\left(\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right)^2.\end{aligned} \tag{A18}$$

Thus we have

$$\int dy_i\,e^{S}v_1\cdots v_N=\pi^{d/2}\exp\left[(\beta q)\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)\left(\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right)^2\right]v_1\cdots v_N\,. \tag{A19}$$

In obtaining (A19) we have used

$$\int d\vec{y}\,e^{-(\vec{y}+\vec{a})^2}=\pi^{d/2} \tag{A20}$$

for any constant vector $\vec{a}$. Multiplying all $\vec{y}_i$ integrals gives us Y. The resultant exponential operator is given by

$$\sum_{i=1}^{N}\left(\frac{1}{1-\alpha_i}-\frac{1}{1-\alpha_{i-1}}\right)\left(\sum_{k=i}^{N}(1-\alpha_k)\vec{\nabla}_k\right)^2=\sum_{j=1}^{N}(1-\alpha_j)\alpha_j\Delta_j+2\sum_{1\le j<k\le N}\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\,. \tag{A21}$$

So the complete expression for Y becomes

$$Y=\pi^{Nd/2}\exp\left[(\beta q)\left({\sum}'^{N}\alpha_j(1-\alpha_j)\Delta_j+2{\sum}''^{N}\alpha_j(1-\alpha_k)\vec{\nabla}_j\cdot\vec{\nabla}_k\right)\right]v_1\cdots v_N\,. \tag{A22}$$

This explicit formula for Y means that we have succeeded in doing all the $d\vec{x}_1\cdots d\vec{x}_N$ integrals in (A2). The result is just a differential operator on $v_1\cdots v_N$. The function Y depends only on β,q and $\vec{x},\vec{x}'$. If Y is combined with (A12), (A10), and (A7), then Eq. (4.5) for $B_N(\vec{x},\vec{x}')$ is obtained.

APPENDIX B

In this appendix we list the results of our determination of the functions $P_n(\vec{x},\vec{x}';q)$. These forms are important because any application of the semiclassical expression described in Sec. III will depend on the formulas quoted below. The off-diagonal results from $n=1$ to 4 are given as well as the diagonal values for $n=1$ to 6. $P_1(\vec{x},\vec{x}';q)$ is given by Eq. (2.23):

$$P_2(\vec{x},\vec{x}';q)=[P_1(\vec{x},\vec{x}';\, q)]^2-2q\int_0^1 d\alpha\,\alpha(1-\alpha)(\Delta v)((\alpha))\,. \tag{B1}$$

The factor (α) is that stated in Eq. (4.6). In this formula the first term on the right is the classical term, the last is the first Born-term contribution:

$$\begin{aligned}P_3(\vec{x},\vec{x}';q)=[P_1(\vec{x},\vec{x}';q)]^3-q\bigg(&6P_1(\vec{x},\vec{x}';q)\int_0^1 d\alpha\,\alpha(1-\alpha)(\Delta v)((\alpha))\\&+12\int_{0\leq\alpha_1\leq\alpha_2\leq1}\int d\alpha_1 d\alpha_2\,\alpha_1(1-\alpha_2)(\vec{\nabla}v)((\alpha_1))\cdot(\vec{\nabla}v)((\alpha_2))\bigg)\\&+3q^2\int_0^1 d\alpha[\alpha(1-\alpha)]^2(\Delta^2 v)((\alpha))\,.\end{aligned} \tag{B2}$$

The term proportional to q contains the cross term that is the product of the classical term and the first Born factor, plus a scalar formed of the dot product of gradients:

$$\begin{aligned}P_4(\vec{x},\vec{x}';q)=[P_1(\vec{x},\vec{x}';q)]^4-6q\bigg(&2[P_1(\vec{x},\vec{x}';q)]^2\int_0^1 d\alpha\,\alpha(1-\alpha)(\Delta v)((\alpha))\\&+8P_1(\vec{x},\vec{x}';q)\int_{0\leq\alpha_1\leq\alpha_2\leq1}\int d\alpha_1 d\alpha_2\,\alpha_1(1-\alpha_2)(\vec{\nabla}v)((\alpha_1))\cdot(\vec{\nabla}v)((\alpha_2))\bigg)\\&+12q^2\bigg[\bigg(\int_0^1 d\alpha\,\alpha(1-\alpha)(\Delta v)((\alpha))\bigg)^2+4\int_{0\leq\alpha_1\leq\alpha_2\leq1}\int d\alpha_1 d\alpha_2[\alpha_1(1-\alpha_2)]^2(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v((\alpha_1))v((\alpha_2))\\&+P_1(\vec{x},\vec{x}';q)\int_0^1 d\alpha[\alpha(1-\alpha)]^2(\Delta^2 v)((\alpha))\\&+4\int_{0\leq\alpha_1\leq\alpha_2\leq1}\int d\alpha_1 d\alpha_2\,\alpha_1(1-\alpha_2)(\vec{\nabla}_1\cdot\vec{\nabla}_2)\Big(\alpha_1(1-\alpha_1)(\Delta v)((\alpha_1))v((\alpha_2))+\alpha_2(1-\alpha_2)v((\alpha_1))(\Delta v)((\alpha_2))\Big)\bigg]\\&-4q^3\bigg(\int_0^1 d\alpha[\alpha(1-\alpha)]^3(\Delta^3 v)((\alpha))\bigg)\,.\end{aligned} \tag{B3}$$

Formula (B3) starts to show the complexity that is characteristic of the higher $P_n(\vec{x},\vec{x}';q)$. Clearly there is a rapidly increasing number of ways of forming scalars from the operators $\vec{\nabla}$ and Δ.

The diagonal values of $P_n(\vec{x},\vec{x}';q)$ are obtained by setting $\vec{x}=\vec{x}'$ in (B1)–(B3), etc. When the formulas quoted below are reduced to the $d=1$ case, it is seen that upon comparison with the formula of Ref. 1 they have substantially more terms. Since the invariant polynomials in the 1D case construct the constants of motion of the KdV equation by an $\vec{x}$ integration over the real line, all the total derivative terms in P_n are omitted in the formulas given in Ref. 1. We keep all terms contributing to $P_n(\vec{x},\vec{x}';q)$ since they are necessary for the asymptotic series (2.4):

$$P_1(\vec{x},\vec{x};q)=v(\vec{x}),\quad P_2(\vec{x},\vec{x};q)=v(\vec{x})^2-q\tfrac{1}{3}\Delta v(\vec{x})\,, \tag{B4}$$

$$P_3(\vec{x},\vec{x};q)=v(\vec{x})^3-q\{v(\vec{x})\Delta v(\vec{x})+\tfrac{1}{2}[\vec{\nabla}v(\vec{x})]^2\}+q^2\tfrac{1}{10}\Delta^2 v(\vec{x})\,, \tag{B5}$$

$$\begin{aligned}P_4(\vec{x},\vec{x};q)=v(\vec{x})^4&-q\{2v(\vec{x})^2\Delta v(\vec{x})+2v(\vec{x})[\vec{\nabla}v(\vec{x})]^2\}\\&+q^2\{\tfrac{2}{5}v(\vec{x})\Delta^2 v(\vec{x})+\tfrac{1}{3}[\Delta v(\vec{x})]^2+\tfrac{4}{15}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1(\vec{x})v_2(\vec{x})+\tfrac{4}{5}\vec{\nabla}v(\vec{x})\cdot\vec{\nabla}[\Delta v(\vec{x})]\}-q^3\tfrac{1}{35}\Delta^3 v(\vec{x})\,,\end{aligned} \tag{B6}$$

$$\begin{aligned}P_5(\vec{x},\vec{x};q)=v^5&-q\{\tfrac{10}{3}v^3\Delta v+5v^2(\vec{\nabla}v)^2\}\\&+q^2\{v^2\Delta^2 v+\tfrac{5}{3}v(\Delta v)^2+\tfrac{5}{3}\Delta v(\vec{\nabla}v)^2+\tfrac{4}{3}v(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1v_2+4v\vec{\nabla}v\cdot\vec{\nabla}(\Delta v)+2(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_2\cdot\vec{\nabla}_3)v_1v_2v_3\}\\&-q^3\{\tfrac{1}{7}v\Delta^3 v+\tfrac{1}{3}\Delta v\Delta^2 v+\tfrac{1}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^3 v_1v_2+\tfrac{4}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2\Delta v_1v_2+\tfrac{3}{7}\vec{\nabla}v\cdot\vec{\nabla}(\Delta^2 v)+\tfrac{17}{42}[\vec{\nabla}(\Delta v)]^2\}+q^4\tfrac{1}{126}\Delta^4 v\,,\end{aligned} \tag{B7}$$

$$
\begin{aligned}
P_6(\vec{x},\vec{x};q) = {} & v^6 - q\{5v^4\Delta v + 10v^3(\vec{\nabla}v)^2\} \\
& + q^2\{2v^3\Delta^2 v + 5v^2(\Delta v)^2 + 10v\Delta v(\vec{\nabla}v)^2 + 4v^2(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1 v_2 + 12v^2\vec{\nabla}v\cdot\vec{\nabla}(\Delta v) \\
& \quad + 12v(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_2\cdot\vec{\nabla}_3)v_1v_2v_3 + \tfrac{5}{2}[(\vec{\nabla}v)^2]^2\} \\
& - q^3\{\tfrac{3}{7}v^2\Delta^3 v + 2v\Delta v\Delta^2 v + \tfrac{5}{9}(\Delta v)^3 + \Delta^2 v(\vec{\nabla}v)^2 + \tfrac{4}{3}\Delta v(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1v_2 + 4\Delta v[\vec{\nabla}v\cdot\vec{\nabla}(\Delta v)] \\
& \quad + \tfrac{6}{7}v(\vec{\nabla}_1\cdot\vec{\nabla}_2)^3 v_1v_2 + \tfrac{24}{7}v(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2\Delta v_1 v_2 + \tfrac{18}{7}v[\vec{\nabla}v\cdot\vec{\nabla}(\Delta^2 v)] + \tfrac{17}{7}v[\vec{\nabla}(\Delta v)]^2 \\
& \quad + \tfrac{24}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2(\vec{\nabla}_2\cdot\vec{\nabla}_3)v_1v_2v_3 + \tfrac{34}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_2\cdot\vec{\nabla}_3)\Delta v_1v_2v_3 + \tfrac{18}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_2\cdot\vec{\nabla}_3)v_1\Delta v_2v_3 \\
& \quad + \tfrac{64}{63}(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_3)(\vec{\nabla}_2\cdot\vec{\nabla}_3)v_1v_2v_3\} \\
& + q^4[\tfrac{1}{21}v\Delta^4 v + \tfrac{1}{7}\Delta v\Delta^3 v + \tfrac{1}{10}(\Delta^2 v)^2 + \tfrac{8}{105}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^4 v_1v_2 + \tfrac{8}{21}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^3\Delta v_1v_2 + \tfrac{8}{21}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2(\Delta^2 v_1)v_2 \\
& \quad + \tfrac{13}{35}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2\Delta v_1\Delta v_2 + \tfrac{4}{21}\vec{\nabla}v\cdot\vec{\nabla}(\Delta^3 v) + \tfrac{11}{21}\vec{\nabla}(\Delta v)\cdot\vec{\nabla}(\Delta^2 v)] - q^5\tfrac{1}{462}\Delta^5 v\,.
\end{aligned} \tag{B8}
$$

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