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Connected graph representations of the quantum propagator and semiclassical expansions

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Abstract. The time evolution operator $U(t, s)$ of a spinless non-relativistic N-body quantum system in Euclidean space with real analytic time-dependent scalar interaction $\nu(x, \tau)$ is studied. A complete formal asymptotic expansion involving simple connected graphs is derived for the full coordinate, and mixed coordinate-momentum representation propagators. The derivation is based on Dyson's series for $U(t, s)$, and the combinatorics involved in the cluster expansion of the classical grand partition function. These results provide an efficient means of generating non-perturbative propagator expansions in the physical variables: mass m, Planck's constant h, time displacement $t-s$. The structural bridge between the WKB and Wigner-Kirkwood expansions is sketched for mixed representations of $U(t, s)$. In the heat equation context the graphical expansions are found for mixed representations of the density operator $e^{-\beta H}$. Finally, an explicit differential formula is obtained for Wigner's distribution function $f(x, p; \beta)$.

1. Introduction

In this paper we derive connected graph representations of the quantum time evolution operator. For the non-relativistic N-body problem, set in Euclidean space without boundaries and having interparticle interactions described by smooth bounded time-dependent scalar fields, the graphical solutions for the propagator are obtained in a variety of Dirac bases. Using these fundamental solutions of the Schrödinger evolution problem the two most interesting singular perturbation limits are investigated. In the limit of Planck's constant $h \to 0$ a restructuring of the connected graph representation is shown to yield the multi-dimensional WKB approximation complete with explicit formulae for all the higher-order coefficient functions. In a similar fashion the infinite mass limit, $m \to \infty$, leads to the generalised Wigner-Kirkwood expansion (valid for both time evolution kernels and heat kernels). The common features and universality of the connected graph representations of the propagators in different bases are described.

The time-dependent Hamiltonian operator $H(t)$ appropriate for this quantum system is defined by the differential expression

$$H\left(x, \frac{\hbar}{\mathrm{i}} \nabla_x, t\right) = -\frac{\hbar^2}{2m} \nabla_x^2 + \mu \nu(x, t). \tag{1.1}$$

Here m is the particle mass, $h = 2\pi\hbar$ is Planck's constant and the vector $x \in \mathbb{R}^d$ $(d = 3N)$ describes the system configuration. The real parameter μ is the coupling constant and

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$v:\mathbb{R}^{d+1}\to\mathbb{R}$ is the potential energy of the system accounting for all interparticle forces as well as the interaction with any external sources. The scalar field v is assumed to be a real analytic function of x. The presumption of a common mass m for all particles represents no loss of generality since a change of coordinates can always transform the kinetic energy operator into the form appearing in (1.1).

The dynamical evolution of this quantum system from an initial time s to a final time t is given by the operator-valued solution of

$$i\hbar\frac{\partial}{\partial t}U(t,s)=H(t)U(t,s) \tag{1.2}$$

obeying the initial condition $U(s,s)=I$ (the identity). The evolution operator $U(t,s)$ is a unitary operator mapping the Hilbert space of $L^2(\mathbb{R}^d)$ functions onto itself. The quantum propagators we shall study are the following Dirac matrix elements of the evolution operator: $\langle x|U(t,s)|y\rangle$, $\langle x|U(t,s)|k\rangle$, $\langle p|U(t,s)|y\rangle$ and $\langle p|U(t,s)|k\rangle$. Here x and y denote configuration variables, whereas p and k are momentum variables. The mathematical interpretation of these Dirac notations is that the above propagators are, respectively, the integral kernels of the operators U, US^{-1}, SU and SUS^{-1} (where $U=U(t,s)$ and S denotes the Fourier transform from spatial to momentum coordinates). We shall show that the first three of the above propagators have formal connected graph representations.

These representations may be written in the following algebraically factored form. Suppose $\Delta t=t-s$ is the time displacement; then we find that

$$\langle x|U(t,s)|y\rangle=(ih\Delta t/m)^{-d/2}\exp\left(\frac{i}{\hbar}\frac{m}{2\Delta t}(x-y)^2\right)F^{\circ}(x,t;y,s) \tag{1.3a}$$

$$\langle x|U(t,s)|k\rangle=h^{-d/2}\exp\left(\frac{i}{\hbar}\left(x\cdot k-\frac{k^2}{2m}\Delta t\right)\right)F^{*}(x,t;k,s) \tag{1.3b}$$

$$\langle p|U(t,s)|y\rangle=h^{-d/2}\exp\left(\frac{i}{\hbar}\left(-y\cdot p-\frac{p^2}{2m}\Delta t\right)\right)F^{\#}(p,t;y,s). \tag{1.3c}$$

The functions written to the left of F°, F^{*} and $F^{\#}$ are just the well known propagators for the free Hamiltonian H_0, defined by (1.1) with $\mu=0$. In addition to the variables displayed in F°, F^{*} and $F^{\#}$, these functions also depend parametrically on μ, $\hbar$ and m.

The connected graph representations of the propagators in (1.3) are most simply described as exponentiated coupling constant expansions

$$F^{\circ}(x,t;y,s)=\exp\sum_{n=1}^{\infty}\mu^n L_n^{\circ}(x,t;y,s) \tag{1.4a}$$

$$F^{*}(x,t;k,s)=\exp\sum_{n=1}^{\infty}\mu^n L_n^{*}(x,t;k,s) \tag{1.4b}$$

$$F^{\#}(p,t;y,s)=\exp\sum_{n=1}^{\infty}\mu^n L_n^{\#}(p,t;y,s). \tag{1.4c}$$

The coefficient functions L_n°, L_n^{*} and $L_n^{\#}$ (or generically $L_n^{\bullet}$) are independent of μ, but still depend on $\hbar$ and m. In the following the functions $L_n^{\bullet}$ will be explicitly determined by a type of connected graph sum.

It is useful to state at the outset two of the important geometrical objects that enter the formulae for $L_n^{\bullet}$. For given initial and final times (s and t) consider the classical

free evolution problem with one boundary condition imposed at each of these endpoints. The absence of forces means that the classical path in coordinate space must be a straight line. The three two-point boundary value problems associated with (1.3) and (1.4) have trajectories given by (where τ is the running time variable)

$$\rho_0^\circ(\tau) = y + \frac{\tau - s}{t - s}(x - y) \tag{1.5a}$$

$$\rho_0^*(\tau) = x + (\tau - t)u \qquad u = k/m \tag{1.5b}$$

$$\rho_0^\#(\tau) = y + (\tau - s)v \qquad v = p/m. \tag{1.5c}$$

In the first of these paths the initial position y and the final position x are the given boundary condition data. In the second path, (1.5b), the initial velocity u and the final position x are specified; and in the last path the initial position y and the final velocity v are given.

A second basic ingredient that appears in the connected graph formulae for $L_n^\bullet$ is a class of one-dimensional Green functions. Let us scale the time variable τ so that the linear paths in (1.5) are parametrised by the unit interval. To this end, define $\xi = (\tau - s)/(t - s)$, $\xi \in [0, 1] \equiv I$. Consider the Green function solutions of the unit interval equation,

$$\frac{d^2}{d\xi^2} g^\bullet(\xi, \xi') = \delta(\xi - \xi'). \tag{1.6}$$

For each of the three different two-point boundary conditions given above, there is a related solution of (1.6). In particular, the Green function and its companion boundary conditions are:

$$g^\circ(\xi, \xi') = \xi_<(\xi_< - 1) \qquad g^\circ(0, \xi') = 0 \qquad g^\circ(1, \xi') = 0 \tag{1.7a}$$

$$g^*(\xi, \xi') = \xi_> - 1 \qquad \frac{\partial g^*}{\partial \xi}(0, \xi') = 0 \qquad g^*(1, \xi') = 0 \tag{1.7b}$$

$$g^\#(\xi, \xi') = -\xi_> \qquad g^\#(0, \xi') = 0 \qquad \frac{\partial g^\#}{\partial \gamma}(1, \xi') = 0 \tag{1.7c}$$

where $\xi_> = \max\{\xi, \xi'\}$ and $\xi_< = \min\{\xi, \xi'\}$.

The final formula for $L_n^\bullet$ is expressed in terms of $\rho_0^\bullet$ and $g^\bullet$ together with certain differential operators and a connected graph summation process. Absent from the list of possible cases in (1.3)-(1.7) is the momentum representation propagator $\langle p|U(t, s)|k\rangle$. The special character of this propagator is readily apparent. The momenta k and p determine the initial and final velocities u and v. However for $u \neq v$ there is no free linear trajectory with these different endpoint velocities. Similarly there is no Green function solution of (1.6) with vanishing ξ derivative at both endpoints Finally $\langle p|U(t, s)|k\rangle$ is distribution valued (as is evident from the free problem) in contrast with the other propagators which are all ordinary functions if $t \neq s$.

The derivation of the connected graph representation of the propagator has two basic stages. The first involves restructuring the coupling constant expansion of $F^\bullet$ in such a way that the time-ordering restriction inherent in the original Dyson series expansion is removed. These results are described in § 2. The second stage, presented in § 3, shows how the coupling constant series can be exponentiated with a combinatorial enumeration that is implemented with the connected graph method. An emphasis is given to describing the common analytical and geometrical features of

expansions (1.4). These results extend those developed earlier by Fujiwara *et al* (1982) wherein the heat kernel $\langle x|e^{-\beta H}|y\rangle$ of the canonical density operator $e^{-\beta H}$ for inverse temperature $\beta > 0$ was represented as a connected graph sum. Our time evolution kernel representations reduce to those for the x, y heat kernel if the potential $v(x, t)$ is assumed to be static and $t - s$ is replaced with $\hbar\beta/i$.

The formulae for L_n^* have great utility because they may be used to generate expansions in the various physical parameters $\hbar$, m^{-1}, μ and Δt (or β) by summing over selective subclasses of the connected graphs. In § 4 the $\hbar \to 0$ limit of the graphical sum is described and in this fashion the connection between the graphical sum and the WKB expansion for the three propagators $\langle x|U(t, s)|y\rangle$, $\langle x|U(t, s)|k\rangle$ and $\langle p|U(t, s)|y\rangle$ is established. In addition it is indicated how the graphical solutions allow one to construct a corresponding explicit solution to the Hamilton-Jacobi equation. The large mass limit $m^{-1} \to 0$ is used to obtain the explicit form of the generalised Wigner-Kirkwood expansion. It is shown that the connected graph representation generates directly all the coefficient functions in the Wigner-Kirkwood expansion without the use of recurrence relations. As a final application we derive an explicit differential formula mapping the heat kernel into the Wigner function representation.

The derivations leading to the connected graph representations are exact in that no approximations are made. However our analysis is heuristic in nature and in particular it is assumed throughout that the various series expansions have meaning and are at least asymptotic. It is worth mentioning some rigorous results which are known in this direction for bounded smooth potentials. Osborn (1984) has proved the asymptotic nature of the $m \to \infty$ and $\Delta t \to 0$ expansions of the time evolution kernel, and of the $\hbar^2/2m \to 0$ and $\beta \to 0$ expansions of the heat kernel. The WKB approximation is similarly an $\hbar \to 0$ asymptotic expansion, as has been shown by Fujiwara (1980).

We also expect the exponentiated forms (1.4*a-c*) of the propagators only to be valid for sufficiently short time displacements Δt. Formulae (1.4*a-c*) for F^* are a consequence of a reorganisation of the coupling constant Dyson expansion for $U(t, s)$. If the potential $v(x, t)$ is smooth and uniformly bounded then both the operator-valued Dyson series (2.2) and the associated coupling constant expansion of F^* converge absolutely for all μ and t (Osborn and Fujiwara 1983). However exponentiating the coupling constant expansion of F^* requires changing the order of a multiple summation. This step will introduce a restriction on the allowed values of Δt. The short-time limitation of representation (1.4*a*) is further characterised at the end of § 4.1, by an examination of the time behaviour in the solvable model of a d-dimensional harmonic oscillator potential.

2. Symmetrised coupling constant expansions

In this section we investigate the coupling constant expansion of each of the three distinct Dirac matrix elements of the evolution operator: $\langle x|U(t, s)|y\rangle$, $\langle x|U(t, s)|k\rangle$ and $\langle p|U(t, s)|y\rangle$. A basic goal is to introduce a permutation invariance into the coupling constant expansion which allows one to remove the time-ordering restriction. We give in detail the arguments needed to obtain the symmetrised expansion for the propagator $\langle x|U(t, s)|k\rangle$ and then indicate the required modifications of the proof for the two additional cases. The momentum space propagator will be discussed at the end of § 3.

It is convenient to denote the free evolution generated by $H_0 = -(\hbar^2/2m)\nabla_x^2$ as

$$U_0(t, s) = \exp(-i\Delta t H_0/\hbar).$$

The operator-valued integral equation equivalent to Schrödinger's differential equation (1.2) with initial condition $U(s, s) = I$ is

$$U(t, s) = U_0(t, s) + \frac{1}{i\hbar}\int_s^t d\tau\, U_0(t, \tau) V(\tau) U(\tau, s). \tag{2.1}$$

Here $V(\tau)$ is the operator obtained by multiplication with the scalar potential $\mu\nu(x, \tau)$. A basic effect of the time dependence of the interaction $V(\tau)$ is to cause $U(t, s)$ to depend separately on t and s and not solely on the time displacement $\Delta t = t - s$.

Successive iteration of (2.1) yields the time-ordered Dyson expansion

$$\begin{aligned} U(t, s) = U_0(t, s) + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_s^t d\tau_1 \int_s^{\tau_1} d\tau_2 \ldots \int_s^{\tau_{n-1}} d\tau_n \\ \times \exp[-i(t-\tau_1)H_0/\hbar] V(\tau_1) \exp[-i(\tau_1-\tau_2)H_0/\hbar] V(\tau_2) \ldots \\ \times \exp[-i(\tau_{n-1}-\tau_n)H_0/\hbar] V(\tau_n) \exp[-i(\tau_n - s)H_0/\hbar]. \end{aligned} \tag{2.2}$$

The operator-valued series (2.2) is the common starting point of the derivations of all four representations of the propagator. Consider the case of $\langle x|U(t, s)|k\rangle$ first. Begin by scaling out the trivial dependence on Δt. This is implemented by the change of variables $\tau_j = t - \xi_j \Delta t$ for $j = 1 \sim n$. So (2.2) becomes

$$\begin{aligned} U(t, s) = \Bigg[I + \sum_{n=1}^{\infty} \left(\frac{\Delta t}{i\hbar}\right)^n \int_{Q_n^<} d^n\boldsymbol{\xi}\, [\exp(-i\xi_1 \Delta t H_0/\hbar) V(t - \xi_1 \Delta t) \\ \times \exp(i\xi_1 \Delta t H_0/\hbar)] \times \ldots \times [..n..] \Bigg] U_0(t, s). \end{aligned} \tag{2.3}$$

Two notations are introduced in (2.3). Let the n-tuple $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_n)$ be an arbitrary point in the unit n-cube I^n. The symbol $Q_n^<$ specifies the triangular region $Q_n^< = \{\boldsymbol{\xi} \in I^n | 0 \leqslant \xi_1 \leqslant \ldots \leqslant \xi_n \leqslant 1\}$. Furthermore, the notation $[..n..]$ is an abbreviation for the first small square bracket operator in (2.3) with index 1 replaced by n.

Taking the $\langle x|\ldots|k\rangle$ Dirac matrix element of (2.3) one finds

$$\begin{aligned} \langle x|U(t, s)|k\rangle = \Bigg\{ 1 + \sum_{n=1}^{\infty} \left(\frac{\mu \Delta t}{i\hbar}\right)^n \int_{Q_n^<} d^n\boldsymbol{\xi} [\exp(i\zeta_1 \Delta_x) \nu(x, t - \xi_1 \Delta t) \\ \times \exp(-i\zeta_1 \Delta_x)] \times \ldots \times [..n..] \Bigg\} \langle x|\exp(-i\Delta t H_0/\hbar)|k\rangle. \end{aligned} \tag{2.4}$$

Here $\zeta_j = (\hbar \Delta t/2m)\xi_j$, and the free propagator is

$$\langle x|\exp(-i\Delta t H_0/\hbar)|k\rangle = h^{-d/2} \exp\left(\frac{i}{\hbar}\left(x \cdot k - \frac{k^2}{2m}\Delta t\right)\right). \tag{2.5}$$

Inserting (2.5) into (2.4), the factors independent of x may be brought to the left of the differential operator $\{\ldots\}$ in (2.4). Consequently, the propagator admits the factorisation (1.3b) where

$$\begin{aligned} F^*(x, t; k, s) = \exp(-ix \cdot k/\hbar) \Bigg[1 + \sum_{n=1}^{\infty} \left(\frac{\mu \Delta t}{i\hbar}\right)^n \int_{Q_n^<} d^n\boldsymbol{\xi}\, [\exp(i\zeta_1 \Delta_x) \nu(x, t - \xi_1 \Delta t) \\ \times \exp(-i\zeta_1 \Delta_x)] \times \ldots \times [..n..] \Bigg] \exp(ix \cdot k/\hbar). \end{aligned} \tag{2.6}$$

The next step is to move the right-most plane wave in (2.6) to the left. This is accomplished by using the formula

$$\exp(\mathrm{i}\zeta\Delta_x)\nu(x,\tau)\exp(-\mathrm{i}\zeta\Delta_x)=\nu(x+2\mathrm{i}\zeta\nabla_x,\tau) \tag{2.7a}$$

in each of the n factors $[..j..]$ in (2.6). Following this by a repeated use of the identity (for $\phi\in C^\infty$)

$$\nu(x+2\mathrm{i}\zeta\nabla_x,\tau)\exp(\mathrm{i}x\cdot k/\hbar)\phi(x)=\exp(\mathrm{i}x\cdot k/\hbar)\nu(x-2\zeta k/\hbar+2\mathrm{i}\zeta\nabla_x,\tau)\phi(x) \tag{2.7b}$$

allows the plane wave to be moved to the left. Thus one obtains the analogue of the representation found by Goldberger and Adams (1952) for the present case

$$F^*(x,t;k,s)=1+\sum_{n=1}^{\infty}\left(\frac{\mu\Delta t}{\mathrm{i}\hbar}\right)^n\int_{Q_n^<}\mathrm{d}^n\boldsymbol{\xi}\,\nu(x-2\zeta_1k/\hbar+2\mathrm{i}\zeta_1\nabla_x,\,t-\xi_1\Delta t)$$
$$\times\ldots\times\nu(x-2\zeta_nk/\hbar+2\mathrm{i}\zeta_n\nabla_x,\,t-\xi_n\Delta t)1. \tag{2.8}$$

In spite of its relatively simple appearance formula (2.8) for F^* is very complicated due to the presence of the gradient as an argument in the product of potentials. A simple variant of (2.7a) allows the jth factor of ν in (2.8) to be replaced by

$$\exp(\mathrm{i}\zeta_j\Delta_x)\nu(x-2\zeta_jk/\hbar,\,t-\xi_j\Delta t)\exp(-\mathrm{i}\zeta_j\Delta_x). \tag{2.9}$$

In the $j=n$ factor, the right exponential may be omitted since it acts on the constant 1.

The next goal is to simplify the differential structure in (2.8) and to make the permutation dependence of the indices $j=1\sim n$ more evident. We start by reorganising the differential structure arising from the Laplacians in (2.9). In order to do this we define a differential operator $D_j(j=1\sim n)$ which acts as a spatial gradient on the $\mathbb{R}^d$-vector argument of the potential containing the index j. Specifically

$$D_j\nu(x_i,\tau_i)=\delta_{ij}(\nabla\nu)(x_i,\tau_i)$$

where δ_{ij} is the Kronecker delta symbol. A useful property of the operators $\{D_j\}$ is that they commute with each other. The gradient of a product of potentials takes the form ($l\leqslant n$)

$$\nabla_x\prod_{j=l}^{n}\nu(x-2\zeta_jk/\hbar,\tau_j)=\left(\sum_{j=l}^{n}D_j\right)\prod_{j=l}^{n}\nu(x-2\zeta_jk/\hbar,\tau_j).$$

Employing the operators D_j in (2.8) and (2.9) yields

$$F^*(x,t;k,s)=1+\sum_{n=1}^{\infty}\left(\frac{\mu\Delta t}{\mathrm{i}\hbar}\right)^n\int_{Q_n^<}\mathrm{d}^n\boldsymbol{\xi}\exp\left\{\sum_{l=1}^{n}\mathrm{i}\zeta_l\left[\left(\sum_{j=l}^{n}D_j\right)^2\right.\right.$$
$$\left.\left.-\left(\sum_{j=l+1}^{n}D_j\right)^2\right]\right\}\prod_{l=1}^{n}\nu(x-2\zeta_lk/\hbar,\,t-\xi_l\Delta t)$$
$$=1+\sum_{n=1}^{\infty}\left(\frac{\mu\Delta t}{\mathrm{i}\hbar}\right)^n\int_{Q_n^<}\mathrm{d}^n\boldsymbol{\xi}\exp\left(\sum_{l=1}^{n}\sum_{j=1}^{n}\mathrm{i}\zeta_{l\wedge j}D_l\cdot D_j\right)$$
$$\times\prod_{l=1}^{n}\nu(x-2\zeta_lk/\hbar,\,t-\xi_l\Delta t)$$

where $l\wedge j=\min\{l,j\}$ and $l\vee j=\max\{l,j\}$. Now make the change of variables $\xi_j'=1-\xi_{n+1-j}$ (for $j=1\sim n$) which gives, upon dropping the primes,

$$F^*(x,t;k,s)=1+\sum_{n=1}^{\infty}\left(\frac{\mu\Delta t}{\mathrm{i}\hbar}\right)^n\int_{Q_n^<}\mathrm{d}^n\boldsymbol{\xi}\exp\left(\frac{\hbar\Delta t}{2\mathrm{i}m}\sum_{l,j=1}^{n}(\xi_{l\vee j}-1)D_l\cdot D_j\right)\prod_{l=1}^{n}\nu(\xi_l^*). \tag{2.10}$$

The arguments of the potential ν are the spacetime linear paths in $\mathbb{R}^{d+1}$ parametrised by $\xi_l \in I$:

$$\xi_l^* = (x + (\xi_l - 1)\Delta t k/m,\ s + \xi_l \Delta t) \qquad l = 1 \sim n.$$

Clearly the spatial component of $\xi_l^* \in \mathbb{R}^d \times \mathbb{R}$ is just the free linear path $\rho_0^*(s + \xi_l \Delta t)$, whereas its time component varies from s to t.

Now observe that the ordering restriction $0 \leqslant \xi_1 \leqslant \ldots \leqslant \xi_n \leqslant 1$ in (2.10) allows one to replace $\xi_{l \vee j} - 1$ by the Green function $g^*(\xi_l, \xi_j)$ which has the advantage of being a symmetric function of its arguments for all $(\xi_l, \xi_j) \in I^2$. Thus (2.10) assumes the form

$$F^*(x, t; k, s) = \sum_{n=0}^{\infty} \frac{\mu^n}{n!} Z_n^*(x, t; k, s) \tag{2.11}$$

where $Z_0^* = 1$, and for $n \geqslant 1$

$$Z_n^*(x, t; k, s) = n! \int_{Q_n^<} \mathrm{d}^n \boldsymbol{\xi} \exp\left(\frac{\hbar \Delta t}{\mathrm{i}m} \sum_{1 \leqslant i < j \leqslant n} g^*(\xi_i, \xi_j) D_i \cdot D_j \right) \mathscr{F}_n^*(\boldsymbol{\xi}). \tag{2.12}$$

Here we used the symmetry of $g^*(\xi_i, \xi_j) D_i \cdot D_j$ under the interchange of i and j. If $n = 1$ the sum $\sum_{i<j} \equiv 0$. Furthermore the quantity $\mathscr{F}_n^*$ is defined by

$$\mathscr{F}_n^*(\boldsymbol{\xi}) = \prod_{l=1}^{n} f_l^*(x, t; k, s; \xi_l)$$

where

$$f_l^*(x, t; k, s; \xi_l) = \frac{\Delta t}{\mathrm{i}\hbar} \exp[(\hbar \Delta t / 2\mathrm{i}m) g^*(\xi_l, \xi_l) D_l^2] \nu(\xi_l^*).$$

The integrand of (2.12) is invariant under any permutation of $(\xi_1, \xi_2, \ldots, \xi_n) = \boldsymbol{\xi}$. Hence Z_n^* may be expressed as an integral over the unit cube I^n without the factor $n!$,

$$Z_n^*(x, t; k, s) = \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \prod_{1 \leqslant i < j \leqslant n} [1 + a_{ij}^*(\boldsymbol{\xi})] \mathscr{F}_n^*(\boldsymbol{\xi}) \tag{2.13}$$

where we have set

$$a_{ij}^*(\boldsymbol{\xi}) = -1 + \exp\left(\frac{\hbar \Delta t}{\mathrm{i}m} g^*(\xi_i, \xi_j) D_i \cdot D_j \right). \tag{2.14}$$

If $n = 1$ then $\Pi_{i<j} \equiv 1$. The subtraction of -1 in the definition of a_{ij}^* is natural in that it ensures that $a_{ij}^* \to 0$ formally as $\hbar \Delta t / m \to 0$. Representation (2.11)-(2.14) achieves a spacetime linear path averaged form of the Dyson expansion for F^* wherein the time-ordering restriction has been removed.

The derivation just given for $\langle x | U(t, s) | k \rangle$ applies with evident modifications to the propagator $\langle x | U(t, s) | y \rangle$. The analogous result for $F^\circ(x, t; y, s)$ can be expressed as

$$F^\circ(x, t; y, s) = \sum_{n=0}^{\infty} \frac{\mu^n}{n!} Z_n^\circ(x, t; y, s) \tag{2.15}$$

where

$$Z_n^\circ(x, t; y, s) = \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \prod_{1 \leqslant i < j \leqslant n} [1 + a_{ij}^\circ(\boldsymbol{\xi})] \mathscr{F}_n^\circ(\boldsymbol{\xi}). \tag{2.16}$$

The function $\mathscr{F}_n^\circ$ is the product of potentials and operators

$$\mathscr{F}_n^\circ(\boldsymbol{\xi}) = \prod_{l=1}^{n} \left(\frac{\Delta t}{\mathrm{i}\hbar} \exp[(\hbar \Delta t / 2\mathrm{i}m) g^\circ(\xi_l, \xi_l) D_l^2] \nu(\xi_l^\circ) \right) \tag{2.17}$$

where the appropriate spacetime path is

$$\xi_l^\circ = (y + \xi_l(x-y),\ s + \xi_l \Delta t) \qquad \xi_l \in I.$$

The operators a_{ij}° (coupling index i to j) are given by

$$a_{ij}^\circ(\boldsymbol{\xi}) = -1 + \exp\left(\frac{\hbar \Delta t}{\mathrm{i}m} g^\circ(\xi_i, \xi_j) D_i \cdot D_j \right) \tag{2.18}$$

where g° is the Green function defined in (1.7a). The derivation of the symmetrised coupling constant expansion (2.15)-(2.18) for $\langle x|U(t, s)|y\rangle$ is similar to the expansion for $\langle x|\mathrm{e}^{-\beta H}|y\rangle$ and one may consult Fujiwara *et al* (1982) for additional details.

A simple method for obtaining the symmetrised μ expansion associated with the propagator $\langle p|U(t, s)|y\rangle$ is to employ the relation

$$\langle p|U(t, s)|y\rangle = \overline{\langle y|U(s, t)|p\rangle}. \tag{2.19}$$

This is a consequence of the self-adjoint nature of the Hamiltonian (1.1). Using (2.19) to translate the results of the case $\langle x|U(t, s)|k\rangle$ so as to determine $F^{\#}$ gives

$$F^{\#}(p, t; y, s) = \sum_{n=0}^{\infty} \frac{\mu^n}{n!} Z_n^{\#}(p, t; y, s) \tag{2.20}$$

where

$$Z_n^{\#}(p, t; y, s) = \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \prod_{1 \le i < j \le n} [1 + a_{ij}^{\#}(\boldsymbol{\xi})] \mathscr{F}_n^{\#}(\boldsymbol{\xi}). \tag{2.21}$$

Here $\mathscr{F}_n^{\#}$ is the product

$$\mathscr{F}_n^{\#}(\boldsymbol{\xi}) = \prod_{l=1}^{n} \left(\frac{\Delta t}{\mathrm{i}\hbar} \exp[(\hbar \Delta t / 2\mathrm{i}m) g^{\#}(\xi_l, \xi_l) D_l^2] \nu(\xi_l^{\#}) \right) \tag{2.22}$$

where the spacetime path is

$$\xi_l^{\#} = (y + \xi_l \Delta t p/m,\ s + \xi_l \Delta t) \qquad \xi_l \in I.$$

The operators $a_{ij}^{\#}$ are found to be

$$a_{ij}^{\#}(\boldsymbol{\xi}) = -1 + \exp\left(\frac{\hbar \Delta t}{\mathrm{i}m} g^{\#}(\xi_i, \xi_j) D_i \cdot D_j \right). \tag{2.23}$$

It is of particular interest to note that in all three cases $\cdot = \circ$, $*$ and $\#$ lead to coupling constant coefficients $Z_n^{\cdot}$, equations (2.13), (2.16) and (2.21) that have the same operator-combinatoric structure.

3. Connected graph exponentiation

Certain common combinatorial features of the coupling constant expansions of F°, F^* and $F^{\#}$ are characterised in this section. We explain how these features enable one to exponentiate the μ-series expansion of $F^{\cdot}$ in terms of coefficient functions

defined by connected graphs. The underlying combinatorics is just that involved in the cluster expansion of the classical grand partition function (Hill 1956). The generic expansion function $Z_n^{\cdot}$ found in (2.13), (2.16) and (2.21) has the universal form

$$Z_n^{\cdot} = \int_{I^n} \mathrm{d}^n\boldsymbol{\xi} \prod_{1 \leqslant i < j \leqslant n} (1 + a_{ij}^{\cdot}(\boldsymbol{\xi})) \mathscr{F}_n^{\cdot}(\boldsymbol{\xi}) \tag{3.1}$$

and as in § 1 · may be $\circ$, $*$ or $\#$.

The critical properties of the operators $a_{ij}^{\cdot}(\boldsymbol{\xi})$ are:

(*a*) $a_{ij}^{\cdot}(\boldsymbol{\xi})$ depends only on ξ_i, ξ_j;

(*b*) $a_{ij}^{\cdot}(\boldsymbol{\xi}) = a_{ji}^{\cdot}(\boldsymbol{\xi})$, all i, j;

(*c*) the $\boldsymbol{\xi}$ integration region is the cartesian product $I^n = [0,1] \times \ldots \times [0,1]$ (n factors);

(*d*) the operators $a_{ij}^{\cdot}(\boldsymbol{\xi})$ commute for all i, j and for all $\boldsymbol{\xi} \in I^n$.

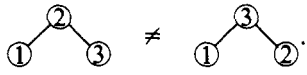
Recall first the following notation for graphs. The pair $G = (A, E)$ is called a *simple graph* if A (the vertex set) is a non-empty finite collection of distinct integers, and E (the edge set) consists of distinct unordered pairs

$$\alpha = \{i_\alpha, j_\alpha\} \qquad i_\alpha, j_\alpha \in A \qquad i_\alpha \neq j_\alpha.$$

Elements of the vertex and edge sets will be called vertices and links, respectively. The term simple emphasises that a pair of vertices may have at most one link between them and that a vertex may not be connected to itself by a link. The fact that a link is defined as an unordered pair means that links are not directed. For more details concerning this graph terminology see Wilson (1975).

A simple graph will be called a *cluster* if it is also connected, i.e. there is an unbroken pathway of links between every pair of vertices. There are many ways to form a cluster over a given vertex set A, if its cardinality $|A| \geqslant 3$. This arises because clusters may differ in structure, e.g.

or they may differ in labelling,



We denote by $\mathscr{C}(A)$ the set of all clusters formed on the vertex set A. The cluster concept is useful because we shall associate with each cluster $C = (A, E)$ the differential operator $\Pi_{\alpha \in E} a_\alpha^{\cdot}$. Furthermore, a given vertex set A induces a natural *cluster sum* S_A, defined as follows. The cluster sum S_A is the sum, with unit weighting, of the operators associated with all possible distinct clusters formed over A, that is

$$S_A \equiv \sum_{C \in \mathscr{C}(A)} \prod_{\alpha \in E} a_\alpha^{\cdot}.$$

For example if $A = \{1, 2, 3\}$ then

$$S_A = a_{12}^{\cdot} a_{23}^{\cdot} + a_{13}^{\cdot} a_{23}^{\cdot} + a_{12}^{\cdot} a_{13}^{\cdot} + a_{12}^{\cdot} a_{13}^{\cdot} a_{23}^{\cdot}.$$

In the case where $|A| = 2$, such as $A = \{1, 2\}$, there is only one cluster, so $S_A = a_{12}^{\cdot}$. If $|A| = 1$ then S_A is defined as unity.

A partition of the set $1 \sim n = \{1, \ldots, n\}$ into non-empty disjoint subsets A_λ is called a *decomposition* $\mathscr{D} = \{A_\lambda\}$ of $1 \sim n$. Specifically, it is required that $A_\lambda \neq \varnothing$, $A_\lambda \cap A_{\lambda'} = \varnothing$

($\lambda \neq \lambda'$) and $1 \sim n = \bigcup_\lambda A_\lambda$. Associated with each decomposition $\mathscr{D} = \{A_\lambda\}$ of $1 \sim n$ is a *cluster product*

$$P(\mathscr{D}) \equiv \prod_\lambda S_{A_\lambda}.$$

We now describe the structure of Z_n^* using this graph terminology. The basic combinatorial feature of (3.1) is the product over a_{ij}^*. Thus

$$\prod_{1 \leq i < j \leq n} (1 + a_{ij}^*) = 1 + \sum_{i<j} a_{ij}^* + \sum_{\substack{i<j,k<l \\ ij \neq kl}} a_{ij}^* a_{kl}^* + \ldots + (a_{12}^* a_{13}^* \ldots a_{n-1,n}^*). \tag{3.2}$$

Each term of (3.2) may be associated with an n-vertex simple graph $G = (1 \sim n, E)$ where a link $\{i, j\}$ occurs in the edge set E if and only if ij is a subscript of one of the factors a^* in the term. Property (b) implies that the link is not directed. There is at most one link between any two vertices since each pair i, j occurs only once in the product (3.2). Conversely, each simple graph G represents a term in (3.2) because for each link $\{i, j\} \in E$ a factor a_{ij}^* can be selected from the left-hand side of (3.2) and for each pair $\{k, l\} \notin E$ the corresponding 1 from $(1 + a_{kl}^*)$ may be selected.

Every cluster product $P(\mathscr{D})$ represents a number of terms in (3.2). In particular, if $\mathscr{D} = \{A, A', \ldots, A''\}$ with associated vertex sets $A = \{i, \ldots, k\}$, $A' = \{i', \ldots, k'\}$, etc, then $P(\mathscr{D})$ contains all the terms of (3.2) such that the vertices $i, j, \ldots, k$ form a cluster, $i', j', \ldots, k'$ form a cluster, etc. By varying $\mathscr{D}$ over all allowed decompositions of $1 \sim n$ and summing the $P(\mathscr{D})$ one obtains precisely all the terms of (3.2), so

$$\prod_{1 \leq i < j \leq n} (1 + a_{ij}^*) = \sum_{\mathscr{D}} P(\mathscr{D}). \tag{3.3}$$

In order to understand the complete relationship between simple graphs and the integrals in (3.1) observe that the operator (3.3) is to be applied to the product of functions $\Pi_{i=1}^n f_i^*$, and then integrated over $\int_{I^n} \mathrm{d}^n \boldsymbol{\xi}$. Properties (a)-(d) show that this integral factors into a product over its component clusters. Note that the functions f_i^* are to be associated with the vertices i and a_{ij}^* with the link between i and j. Thus with each cluster $C = (A, E)$, $A = \{i, j, \ldots, k\}$, we identify the integral

$$\int_{I^A} \mathrm{d}\xi_i \, \mathrm{d}\xi_j \ldots \mathrm{d}\xi_k \left(\prod_{\alpha \in E} a_\alpha^* \right) \prod_{l \in A} f_l^*.$$

Based on the vertex set $1 \sim j$ obtained by relabelling the integration variables above, one defines the *cluster integral of order j* by

$$L_j^* \equiv \frac{1}{j!} \int_{I^j} \mathrm{d}^j \boldsymbol{\xi} \, S_{\{1,\ldots,j\}} \prod_{j=1}^{l} f_l^*. \tag{3.4}$$

This notation lets us write for each decomposition $\mathscr{D} = \{A, A', \ldots, A''\}$ of $1 \sim n$

$$\begin{aligned} \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \, P(\mathscr{D}) \prod_{i=1}^{n} f_i^* &= \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \, S_A S_{A'} \ldots S_{A''} \prod_{i=1}^{n} f_i^* \\ &= \prod_{A_\lambda \in \mathscr{D}} |A_\lambda|! \, L_{|A_\lambda|}^* = (1! L_1^*)^{m_1} (2! L_2^*)^{m_2} \ldots (n! L_n^*)^{m_n} \end{aligned} \tag{3.5}$$

where $m_j \equiv m_j(\mathscr{D}) \geq 0$ is the number of connected subsets of cardinality j in $\mathscr{D}$. Obviously decomposition $\mathscr{D}$ satisfies the constraint

$$\sum_{j=1}^{n} j m_j = n. \tag{3.6}$$

Taken together equations (3.1), (3.3) and (3.5) give

$$Z_n^* = \sum_{\mathscr{D}} \prod_{j=1}^{n} (j! L_j^*)^{m_j(\mathscr{D})}. \tag{3.7}$$

For a given set $\boldsymbol{m} = (m_1, m_2, \ldots, m_n)$ obeying constraint (3.6) there are a variety of decompositions $\mathscr{D}$ all satisfying $\boldsymbol{m}(\mathscr{D}) = \boldsymbol{m}$, and their contributions to Z_n^* will be the same (since their corresponding integrals are identical). So (3.7) may be recast as

$$Z_n^* = \sum_{\boldsymbol{m}}^{(n)} N(\boldsymbol{m}) \prod_{j=1}^{n} (j! L_j^*)^{m_j}$$

where the superscript (n) on the sum means the allowed values of $\boldsymbol{m}$ are subject to constraint (3.6). Here $N(\boldsymbol{m})$ is the number of decompositions $\mathscr{D}$ of $1 \sim n$ consistent with a given $\boldsymbol{m}$. The determination of $N(\boldsymbol{m})$ is the counting problem of placing n objects into boxes, with m_j boxes each holding j objects. The number of ways to do this is $n!$ divided by $\Pi_{j=1}^{n} (j!)^{m_j} m_j!$. With this value for $N(\boldsymbol{m})$, Z_n^* takes the form

$$Z_n^* = \sum_{\boldsymbol{m}}^{(n)} n! \prod_{j=1}^{n} \frac{(L_j^*)^{m_j}}{m_j!} \qquad n \geq 1 \tag{3.8}$$

and Z_0^* is 1.

In order to complete the coupling constant exponentiation of F^* recall that (2.11), (2.15) and (2.20) have the common structure

$$F^* = \sum_{n=0}^{\infty} \frac{\mu^n}{n!} Z_n^*. \tag{3.9}$$

Substituting (3.8) into (3.9) yields

$$F^* = \sum_{n=0}^{\infty} \sum_{\boldsymbol{m}}^{(n)} \prod_{j=1}^{n} \frac{(\mu^j L_j^*)^{m_j}}{m_j!}$$

where $\Sigma^{(0)} = 1$. The double summation here can be reinterpreted as the sum over all $m_j (j \geq 1)$ without the restriction (3.6). Thus, provided one may interchange the order of summation over n and $\boldsymbol{m}$, it follows that

$$F^* = \exp\left(\sum_{j=1}^{\infty} \mu^j L_j^* \right). \tag{3.10}$$

The final form of interest for F^* is obtained by expanding the operators L_j^* in the physical parameter $\hbar/m$. Recall that from (2.14), (2.18) and (2.23) we have for link $\{i, j\}$ the associated series

$$\begin{aligned} a_{ij}^*(\boldsymbol{\xi}) &= -1 + \exp\left(\frac{\hbar \Delta t}{\mathrm{i}m} g^*(\xi_i, \xi_j) D_i \cdot D_j \right) \\ &= \sum_{l_{ij}=1}^{\infty} \frac{1}{l_{ij}!} \left(\frac{\hbar \Delta t}{\mathrm{i}m} \right)^{l_{ij}} [g^*(\xi_i, \xi_j)(D_i \cdot D_j)]^{l_{ij}}. \end{aligned} \tag{3.11}$$

Using expansion (3.11) for every link in the edge sets which occur in $S_{\{1,\dots,j\}}$ of the cluster integral (3.4) lets us write L_j as a sum in which the analytic dependence on $\hbar$, m and Δt is made explicit.

We first define the auxiliary quantities

$$b^{\cdot}_{\alpha}(\boldsymbol{\xi}) = g^{\cdot}(\xi_{i_\alpha}, \xi_{j_\alpha}) D_{i_\alpha} \cdot D_{j_\alpha}$$

$$c^{\cdot}_{j}(\boldsymbol{\xi}) = \sum_{i=1}^{j} g^{\cdot}(\xi_i, \xi_i) D_i \cdot D_i$$

$$r = \sum_{\alpha \in E} l_\alpha$$

where $\alpha = \{i_\alpha, j_\alpha\}$ is a member of some edge set E. Furthermore we introduce a summation convention $\mathscr{G}_j$. Write each cluster $C \in \mathscr{C}(1 \sim j)$ as $C = (1 \sim j, E)$. The sum $\mathscr{G}_j$ is defined as

$$\sum_{\mathscr{G}_j} = \sum_{C \in \mathscr{C}(1\sim j)} \left(\prod_{\alpha \in E} \sum_{l_\alpha = 1}^{\infty} \right).$$

Then (3.4) becomes

$$L^{\cdot}_{j} = \sum_{\mathscr{G}_j} \sum_{n=0}^{\infty} \hbar^{n+r-j} m^{-n-r} (\Delta t/\mathrm{i})^{j+n+r} (j!\, n!\, 2^n)^{-1} \times \int_{I^j} \mathrm{d}^j \boldsymbol{\xi} \left(\prod_{\alpha \in E} (l_\alpha !)^{-1} (b^{\cdot}_{\alpha}(\boldsymbol{\xi}))^{l_\alpha} \right) c^{\cdot}_{j}(\boldsymbol{\xi})^n \prod_{i=1}^{j} \nu(\xi^{\cdot}_i). \tag{3.12}$$

If $j = 1$ then $r = 0$ and the empty product $\Pi_{\alpha \in E}$ is 1. Of course expansion (3.12) of the cluster integral $L^{\cdot}_j$ is valid for any of the three Dirac representations investigated in § 2, i.e. $\cdot = \circ, *, \#$. In addition, note that the integrals over domain I^j in (3.12) are functions which are independent of the physical parameters μ and $\hbar$. If $\cdot = \circ$ they are free of m; if also ν is time independent they are free of t, s. Formula (3.12) is the principal result of this paper.

The Δt behaviour of $L^{\cdot}_j$ is explicitly displayed in (3.12). Since $r \geqslant j-1$, it is seen that $L^{\cdot}_j$ obeys the order estimate

$$L^{\cdot}_j = \mathrm{O}((\Delta t)^{2j-1} (m)^{-(j-1)}) \qquad j \geqslant 1.$$

Of course there is a time dependence in the spacetime path $\xi^{\cdot}_i$. However this appears only in the argument of ν and will not affect the estimate for $L^{\cdot}_j$. Because $L^{\cdot}_j$ decreases as $(\Delta t)^{2j-1}$ we can expect that the interchange of summation that leads to (3.10) is valid if Δt is sufficiently small.

We conclude this section with a discussion of the momentum space propagator $\langle p|U(t,s)|k\rangle$. In seeking an exponentiated coupling constant expansion of $\langle p|U(t,s)|k\rangle$ the first step is to obtain a symmetrised version of the Dyson series (2.2) in the Dirac basis $\langle p|\dots|k\rangle$. Proceeding as in § 2, it is found that

$$\langle p|U(t,s)|k\rangle = \exp(-\mathrm{i}\Delta t p^2/2m\hbar) \left[\delta(p-k) + \sum_{n=1}^{\infty} \left(\frac{\mu \Delta t}{\mathrm{i}\hbar} \right)^n B_n(p, t; k, s) \right] \tag{3.13}$$

where

$$B_n = h^{-d} \int \mathrm{d}y \exp[-\mathrm{i}(p-k)\cdot y/\hbar] \left(\frac{1}{n!} \int_{I^n} \mathrm{d}^n \boldsymbol{\xi} \int \mathrm{d}p_1 \dots \int \mathrm{d}p_n \times \prod_{1 \leqslant i < j \leqslant n} [1 + a^{\times}_{ij}(\boldsymbol{\xi}, p_i, p_j)] \prod_{l=1}^{n} f^{\times}_{l}(\xi_l, p_l, y) \right). \tag{3.14}$$

The functions $a_{ij}^{\times}$ and $f_l^{\times}$ are given by

$$a_{ij}^{\times}(\xi, p_i, p_j) = -1 + \exp\left(\frac{i\Delta t}{m\hbar} g^{\#}(\xi_i, \xi_j) p_i \cdot p_j\right)$$

$$f_l^{\times}(\xi_l, p_l, y) = \exp\left(iy \cdot p_l/\hbar + \frac{i\Delta t}{m\hbar} \xi_l p_l \cdot (p - \tfrac{1}{2}p_l)\right) \hat{\nu}(p_l, s + \xi_l \Delta t)$$

where $\hat{\nu}$ is the Fourier transform of ν, $\mu\hat{\nu}(p-p', \tau) = \langle p|V(\tau)|p'\rangle$. In formula (3.14) for B_n the integration over variables $p_1, \ldots, p_n$ comes from introducing complete sets of momentum states in evaluating the operator product of the original Dyson series. The y integral comes from replacing an overall momentum conserving delta function $\delta(p - k - \Sigma_{l=1}^{n} p_l)$ by its Fourier integral equivalent.

If one interchanges the n-summation with y integration then

$$\langle p|U(t, s)|k\rangle = \exp(-i\Delta t p^2/2m\hbar) h^{-d} \int dy \exp[-i(p-k) \cdot y/\hbar]$$

$$\times \left\{ \sum_{n=0}^{\infty} \left(\frac{\mu\Delta t}{i\hbar}\right)^n \frac{1}{n!} \int_{I^n} d^n\xi \int dp_1 \ldots \right.$$

$$\left. \times \int dp_n \prod_{1 \leq i < j \leq n} [1 + a_{ij}^{\times}] \prod_{l=1}^{n} f_l^{\times} \right\}. \tag{3.15}$$

From the preceding analysis in this section it is evident that we can obtain for each value of y a connected graph exponential representation of the quantity inside the curly brackets of (3.15). However the usefulness of this graphical exponentiation is diminished by the necessity of integrating over all configurations y. In fact the exponentiation of (3.15) leads to the same result one obtains in passing from $\langle p|U(t, s)|y\rangle$ to $\langle p|U(t, s)|k\rangle$ by Fourier transforming, namely

$$\langle p|U(t, s)|k\rangle = \int dy \langle p|U(t, s)|y\rangle\langle y|k\rangle$$

$$= h^{-d} \int dy \exp \frac{-i}{\hbar}\left((p-k) \cdot y + \frac{p^2}{2m}\Delta t\right) F^{\#}(p, t; y, s)$$

$$= h^{-d} \exp(-i\Delta t p^2/2m\hbar) \int dy$$

$$\times \exp\left(\frac{-i}{\hbar}(p-k) \cdot y + \sum_{j=1}^{\infty} \mu^j L_j^{\#}(p, t; y, s)\right). \tag{3.16}$$

Thus graphically exponentiating (3.15) has not yielded a result that is independent of the graph representation (3.10) with $\cdot = \#$.

This conclusion is in marked contrast with the behaviour of the previous three cases $\cdot = \circ$, $*$ and $\#$. Observe that in (1.3) each representation is in the form of an algebraically factored product of $F^{\cdot}$ times the free propagator. If one attempts to pass from the coordinate to a mixed representation in (1.3) one cannot proceed easily via a Fourier transform, since the Fourier transform of an algebraic product is a convolution, and not another algebraic product.

4. Applications

The graphically exponentiated coupling constant series (3.10) and (3.12) provides us with an exact solution of the Schrödinger time-evolution problem in the three bases $\cdot = \circ, *, \#$. However the formulae (3.12) for the coefficients $L^{\cdot}$ are far too complicated to be explicitly summed for an arbitrary smooth potential $v(x, t)$. For example the number of different connected graphs with cardinality 4, 5, 6 and 7 is respectively 38, 728, 26 204 and 1866 256 (Harary and Palmer 1973). Only for exceptionally simple interactions such as the d-dimensional harmonic oscillator is it possible to carry out the sum (3.10) in closed form.

In spite of the difficulties mentioned in the preceding paragraph, expansions (3.10)-(3.12) do have a useful range of applications. Their utility arises from two features. The first is that all of the analytic dependence on the physical parameters μ, $\hbar$ and m is stated explicitly in (3.12). The second is that many applications do not require the computation of all the cluster integrals in $L_j^{\cdot}$, but rather a smaller subset of graphs.

We sketch in this section two particular applications of representation (3.10). For the mixed propagator $\langle x|U(t, s)|k\rangle$ we establish how one may extract the higher-order WKB approximation from (3.10). In a second application, it is assumed that the potential is static and we derive the form of the Wigner-Kirkwood expansion for the mixed representation heat kernel $\langle x|e^{-\beta H}|k\rangle$. In these examples, we have chosen to discuss the mixed kernel representations since they are not often discussed in the literature. Similar applications are valid for the more familiar x, y coordinate kernels. The final topic of the section concerns the map from the Dirac basis of the density operator $e^{-\beta H}$ to the phase space basis found in the Wigner distribution. In this way we can extend the various asymptotic expansions for small $\hbar$, m^{-1}, μ or Δt to the Wigner-Weyl representation.

4.1. Comparisons with WKB

Consider the form assumed by the small Δt WKB approximation for $\langle x|U(t, s)|k\rangle$. From the partial differential equation (PDE) perspective $\langle x|U(t, s)|k\rangle$ is the fundamental solution of the time-dependent Schrödinger equation

$$\left(-i\hbar\frac{\partial}{\partial t}-\frac{\hbar^2}{2m}\Delta_x+\mu v(x, t)\right)\langle x|U(t, s)|k\rangle=0 \tag{4.1}$$

subject to the non-singular initial condition

$$\langle x|U(t, s)|k\rangle \to h^{-d/2}\, e^{ix\cdot k/\hbar} \tag{4.2}$$

as $t \to s$. The WKB approximation for $\langle x|U(t, s)|k\rangle$ is obtained from the ansatz

$$\langle x|U(t, s)|k\rangle = h^{-d/2}\exp[(i/\hbar)S^*(x, t; k, s)+\Lambda^*(x, t; k, s)] \tag{4.3}$$

where S^* is independent of $\hbar$ and real-valued, while the complex-valued $\Lambda^* = O(\hbar^0)$ as $\hbar \to 0$, and $\Lambda^* \to 0$ as $t \to s$. Ansatz (4.3) is essentially a statement of the analytic form that $\langle x|U(t, s)|k\rangle$ takes in the neighbourhood of $\hbar = 0$ for sufficiently small time displacements (Fujiwara 1980).

Substituting (4.3) into (4.1) and equating to zero the lowest-order coefficient of $\hbar$ leads to the usual requirement that S^* solve the Hamilton-Jacobi equation,

$$\partial_1 S^*(x, t; k, s) + \frac{1}{2m} |\nabla_1 S^*(x, t; k, s)|^2 + \mu\nu(x, t) = 0. \tag{4.4}$$

The notations ∂_i and ∇_i will denote the time derivative and the $\mathbb{R}^d$ gradient, respectively, of the ith spacetime argument of a function. The initial condition (4.2) leads to the requirement

$$S^*(x, t; k, s) \to x \cdot k \qquad t \to s. \tag{4.5}$$

It can be shown (Molzahn 1986) that the appropriate solution of (4.4) and (4.5) is given by the Legendre transformation of the classical action

$$S^*(x, t; k, s) = k \cdot q^*(s) + \int_s^t \mathrm{d}\tau\, L(q^*(\tau), \dot{q}^*(\tau), \tau) \tag{4.6}$$

where $L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - \mu\nu(x, t)$ is the Lagrangian of the physical system (1.1) and $q^* = q^*(\,\cdot\,; x, t; u, s)$ is the classical path that obeys Newton's equation together with the two-point boundary condition

$$\dot{q}^*(s) = u = k/m \qquad q^*(t) = x.$$

Our formalism assumes that a unique path q^* exists given any u, x and a sufficiently small Δt, for smooth bounded potentials $\nu(x, t)$.

Given S^*, the higher-order WKB approximation determines Λ^* in terms of an ascending series expansion in $\hbar$, namely

$$\Lambda^*(x, t; k, s) = \sum_{p=1}^{\infty} (\mathrm{i}\hbar)^{p-1} \Lambda_p^*(x, t; k, s). \tag{4.7}$$

The Λ_p^* are $\hbar$ independent and must satisfy

$$\Lambda_p^*(x, s; k, s) = 0 \tag{4.8}$$

in order that $\Lambda^* \to 0$ as $t - s \to 0$. Differential equations for Λ_p^* are determined by substituting (4.3) and (4.7) into Schrödinger's equation (4.1) and equating the coefficients of common powers of $\hbar$. In this way one obtains the recursive set of PDE for Λ_p^* ($p \geqslant 1$):

$$\partial_1 \Lambda_p^* + \frac{1}{m} \nabla_1 S^* \cdot \nabla_1 \Lambda_p^* = \frac{1}{2m} \left(\Delta_1 \Lambda_{p-1}^* + \sum_{n=1}^{p-1} \nabla_1 \Lambda_{p-n}^* \cdot \nabla_1 \Lambda_n^* \right). \tag{4.9}$$

Here $\Lambda_0^* \equiv S^*|_{\mu=0} - S^*$ and if $p = 1$ the sum is absent. The non-interacting S^* is easily found from (4.6) to be

$$S^*(x, t; k, s)|_{\mu=0} = k \cdot x - \frac{\Delta t}{2m} k^2.$$

Explicit solutions of (4.9) for Λ_p^* may be constructed if the WKB-transport method (Birkhoff 1933, Maslov and Fedoriuk 1981) is employed. First replace x, t in (4.9) by $q^*(\tau)$, τ. Next, with the aid of Jacobi's theorem (Gelfand and Fomin 1963), it may be shown that $\nabla_1 S^* = m\dot{q}^*$. Thus the left-hand side of (4.9) equals the total derivative $\mathrm{d}S^*(q^*(\tau), \tau; k, s)/\mathrm{d}\tau$. Then integrating over $\tau \in (s, t)$ subject to condition (4.8) yields

$$\Lambda_p^*(x, t; k, s) = \frac{1}{2m} \int_s^t \mathrm{d}\tau \left(\Delta_1 \Lambda_{p-1}^* + \sum_{n=1}^{p-1} \nabla_1 \Lambda_{p-n}^* \cdot \nabla_1 \Lambda_n^* \right)(q^*(\tau), \tau; k, s). \tag{4.10}$$

Equations (4.10) provide integral recursion relations determining all Λ_p^*. Note that Λ_0^* is known (given q^*) and that the right-hand side of (4.10) only contains Λ_n^* for $n < p$.

Having completed a summary of the higher-order WKB approximation of the propagator $\langle x|U(t,s)|k\rangle$, let us compare it with the connected graph expansion of § 3. The WKB formula can be written

$$\langle x|U(t,s)|k\rangle = h^{-d/2}\exp\frac{\mathrm{i}}{\hbar}\left(k\cdot x - \frac{k^2}{2m}\Delta t\right)\exp\left(\sum_{p=0}^{\infty}(\mathrm{i}\hbar)^{p-1}\Lambda_p^*(x,t;k,s)\right). \tag{4.11}$$

The first two factors on the right-hand side of (4.11) are just the free propagator, so the second exponential may be identified with $F^*(x,t;k,s)$. Thus (3.10) and (4.11) taken together are consistent if

$$\sum_{p=0}^{\infty}(\mathrm{i}\hbar)^{p-1}\Lambda_p^*(x,t;k,s) = \sum_{j=1}^{\infty}\mu^j L_j^*(x,t;k,s). \tag{4.12}$$

A first application of (4.12) is obtained by observing that formula (3.12) with $\cdot = *$ allows L_j^* to be expressed as a Laurent series in $\hbar$ with lowest power $\hbar^{-1}$. The coefficients in this series naturally involve subclasses of graphs from $\mathscr{C}(1\sim j)$. Putting (3.12) into (4.12) and comparing powers of $\hbar$ then yields *graphical formulae* for the quantities Λ_p^* (which were determined above using *classical mechanics*).

For example consider the subclass of graphs that determines S^*. The portions of L_j^* having $\hbar$ dependence $\hbar^{-1}$ are those terms in expansion (3.12) with $n+r-j=-1$. Since $r \geqslant j-1$ on a j-vertex edge set, the condition $n+r-j=-1$ requires $n=0$ and $r=j-1$. This latter equality implies the condition that the class of j-vertex connected graphs are tree graphs (the minimally connected family of graphs on the vertex set $1\sim j$). Thus it turns out that S^* may be expressed as a sum over tree graphs and this sum provides a constructive series solution S^* to the Hamilton-Jacobi equation. We will not pursue this application in detail, but remark that in Molzahn and Osborn (1986) similar reasoning applied to the x, y case yielded a rigorous explicit description of the classical action $S(x,t;y,s)$ for a suitable class of potentials.

Let us continue to investigate the structural consistency between the graphical and classical mechanical representations of Λ_p^*, $p \geqslant 1$. If we replace $k = mu$, then the linear path ξ^* carries no mass dependence. Using formula (3.12) with $\cdot = *$, it is seen that (4.12) implies

$$\Lambda_p^*(x,t;mu,s) = \sum_{l=p}^{\infty} m^{-l}G_p^{*l}(x,t;u,s). \tag{4.13}$$

The coefficients G_p^{*l} are mass independent and are determined by the subclass of graphs defined by $n+r-j=p-1$, and $n+r=l$.

A second derivation of expansion (4.13) that is independent of the consistency condition (4.12) is the following. Consider the behaviour in m of Λ_p^* that is implied by (4.10). The mass dependence of Λ_p^* arises from two mechanisms. The first is the explicit mass dependence in (4.10). The second is the implicit mass dependence found in q^*. Expand q^* in the form

$$q^*(\tau) = \sum_{j=0}^{\infty} m^{-j}\rho_j^*(\tau) \tag{4.14}$$

where coefficients $\rho_j^*:[s,t]\to\mathbb{R}^d$ are mass independent. The leading term ρ_0^* is the free path (1.5b) which satisfies the same boundary conditions as q^*.

The higher terms $\rho_j^*(j \geq 1)$ have zero initial velocity and zero final configuration. They may be determined recursively using the one-dimensional Green function $g^*(\xi, \xi')$, equation (1.7*b*). For example one obtains

$$\rho_1^*(s+\xi\Delta t) = -(\Delta t)^2 \mu \int_0^1 d\xi_1\, g^*(\xi, \xi_1) \nabla \nu(\xi_1^*). \tag{4.15}$$

If we write (4.14) in the form $q^* = \rho_0^* + \eta^*$, then a short calculation shows that (4.6) can be written in terms of Λ_0^* and η^* (rather than S^* and q^*)

$$\Lambda_0^*(x, t; mu, s) = \mu \int_s^t d\tau [-\tfrac{1}{2}\eta^*(\tau) \cdot \nabla \nu(q^*(\tau), \tau) + \nu(q^*(\tau), \tau)]. \tag{4.16}$$

Upon inserting $\eta^* = \Sigma_{j=1}^{\infty} m^{-j} \rho_j^*$ into (4.16) it is straightforward to find the m^{-1} expansion of Λ_0^*. If the τ integral in (4.16) is scaled to the unit interval by setting $\tau = s + \xi \Delta t$, and if formulae like (4.15) are used for ρ_j^*, then it is found that the resulting m^{-1} expansion agrees with the graphical formula (4.13) (with $p = 0$) term by term. In particular, notice that the mass-free spacetime argument becomes $\xi^* = (\rho_0^*(\tau), \tau)$. Similarly, an m^{-1} expansion of (4.10) based on (4.14) allows a term by term verification of the graphical series (4.13) for Λ_p^*, $p \geq 1$.

A discussion similar to the above may also be given for $\langle p|U(t, s)|y\rangle$. In this case, one should begin with the 'backward' Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial s} - \frac{\hbar^2}{2m} \Delta_y + \mu \nu(y, s)\right) \langle p|U(t, s)|y\rangle = 0$$

and then derive the associated higher-order WKB expansion using the transport method. The relevant classical path is $q^{\#}(\,\cdot\,; p, t; y, s)$ which in the free-motion or infinite mass limits reduces to $\rho_0^{\#}$ of (1.5*c*). The associated Green function is $g^{\#}(\xi, \xi')$ given by (1.7*c*).

In summary, we have demonstrated that for mixed representation propagators for the Hamiltonian system (1.1), the mutual consistency and structural connection between the higher-order WKB and the graphical representations is realised by a large mass expansion. This is the joint result of a large-mass expansion of the relevant classical path (q^* or $q^{\#}$) and the transport recurrence identities for the WKB correction terms (Λ_p^* or $\Lambda_p^{\#}$).

The geometrical origin of the averages over the linear paths ξ^* and $\xi^{\#}$ in (3.12) lies in the $m \to \infty$ expansion of q^* about the linear trajectory ρ_0^*. The weight factors g^* and $g^{\#}$ appearing in operators b_α^* and c_j^* in (3.12) arise as Green functions for the boundary conditions that define the acceptable solutions of Newton's equation in each case (see also Osborn and Molzahn (1986)).

Notice that our derivation of (4.12) relied on the fact that the right-hand side of equation (4.3) has only one term. For larger Δt, there may exist many classical paths q^* satisfying the two-point boundary conditions. Then (4.3) would be replaced by a sum of similar terms (one for each path) having relative phases determined by the Maslov index of the path. That equation (4.11) is not in the form of such a sum is consistent with its validity only within some limited region of small Δt.

The small Δt restriction implicit in our analysis can be further clarified by examining the behaviour of a solvable model. Consider the d-dimensional harmonic oscillator defined by the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \nabla_x^2 + \mu x^2.$$

Setting $\gamma = (2\mu/m)^{1/2}$ the function $F^{\circ}(x, t; y, s)$ defined by (1.3a) assumes the well known closed form

$$F^{\circ}(x, t; y, s) = \left(\frac{\gamma\Delta t}{\sin \gamma\Delta t}\right)^{d/2} \exp\left(\frac{im}{2\hbar\Delta t}[(x^2+y^2)(\gamma\Delta t \cot \gamma\Delta t - 1) - 2x \cdot y(\gamma\Delta t \operatorname{cosec} \gamma\Delta t - 1)]\right).$$

The exponentiated coupling constant expansion (1.4a) with $L_n^{\circ}(x, t; y, s)$ given by (3.12) with $\cdot = \circ$ should also construct this same function $F^{\circ}(x, t; y, s)$. The analysis of the cluster integral $L_j^{\circ}(x, t; y, s)$ is particularly simple in this case since most cluster integrals turn out to be zero. Because the harmonic oscillator potential supports only two derivatives with respect to x, the non-vanishing clusters of order j must be such that each vertex has a maximum of two links attached to it. As a consequence only two non-isomorphic types of clusters contribute to L_j°. If the vertices are arranged in a circle, then one possibility is a j-sided polygon—with each side corresponding to a link. The second distinct class of graphs is obtained if one of the links in the polygon is removed. In Fujiwara *et al* (1982) the values of all these graphs for the harmonic oscillator are computed and the series (1.4a) is shown to converge (uniformly in x and y) to the expression above for $F^{\circ}(x, t; y, s)$ provided that the time displacement satisfies

$$|\Delta t| < \pi/\gamma.$$

Now consider the location of the first caustic as one increases Δt for fixed x and y. The Van Vleck determinant for the harmonic oscillator is easily computed in terms of the action S

$$\det\left(-\frac{\partial^2 S}{\partial x\, \partial y}\right) = \left(\frac{(2m\mu)^{1/2}}{\sin \gamma\Delta t}\right)^{d}.$$

The classical evolution problem encounters multiple trajectories whenever this determinant is infinite. This occurs if $\gamma\Delta t = \pm n\pi$ ($n = 1, 2, 3, \ldots$). Thus it is seen that the caustic point for $n = \pm 1$ lies on the boundary of the radius of convergence of series (1.4a). As this example illustrates, one cannot expect to obtain the large Δt behaviour of the quantum system from expansion (1.4a). This limitation also excludes the possibility of determining the Maslov index for classical paths associated with the quantum solution (1.4a). In addition bound-state energies are $\Delta t = \infty$ properties of the system and also are not determined by expansion (1.4a).

4.2. Mixed representation of $e^{-\beta H}$

The generalised Wigner-Kirkwood expansion for evolution kernels is understood to be (Osborn 1984, Osborn and Molzahn 1986) the large mass expansion of $F^{\cdot}$ for $\cdot = \circ$, $*$ and $\#$. The conventional Wigner-Kirkwood expansions for kernels of the canonical density operator $e^{-\beta H}$ (Wigner 1932, Kirkwood 1933, Fujiwara *et al* 1982, Bollé and Roekaerts 1985) result if v is assumed to be static and one makes the formal analytic continuation defined by $\Delta t = \hbar\beta/i$ where β is the inverse temperature. Graphical expansions for $\langle x|e^{-\beta H}|y\rangle$ are discussed in detail in Fujiwara *et al* (1982) so we confine our discussion to the cases $\cdot = *$ and $\#$.

Write the x, k mixed representation of $e^{-\beta H}$ as

$$\langle x|e^{-\beta H}|k\rangle = \langle x|k\rangle\, e^{-\beta k^2/2m} F^{*}(x, k; \beta, q, \hbar)$$

where $q = \hbar^2/2m$. The expansion (3.10)-(3.12) becomes

$$\log F^*(x, k; \beta, q, \hbar) = \sum_{j=1}^{\infty} \mu^j \sum_{\mathcal{G}_j} \sum_{n=0}^{\infty} (-\beta)^{j+n+r} q^{n+r} \frac{2^r}{j!\,n!}$$
$$\times \int_{I^j} \mathrm{d}^j \boldsymbol{\xi} \left(\prod_{\alpha \in E} (l_\alpha!)^{-1} (b_\alpha^*)^{l_\alpha} \right) c_j^{*n} \prod_{l=1}^{j} \nu(\xi_l^*). \tag{4.17}$$

Some comments about (4.17) are necessary. The argument of the potentials is now just the spatial part of ξ_l^*, but because of the replacement of Δt it becomes

$$\xi_l^* = x + \frac{2\mathrm{i}}{\hbar} \beta q k (1 - \xi_l). \tag{4.18}$$

Notice that (4.18) is a complex vector. Nevertheless (4.17) is meaningful because of the assumed real-analytic (Fleming 1977) nature of ν. Finally, observe that F^* in (4.17) has an explicit dependence on $\hbar$ (i.e. other than that found in q) which arises because of the $\hbar$ dependence of (4.18). This $\hbar$ dependence may be traced back to the $\hbar$-dependent Fourier transform relating $|y\rangle$ to $|k\rangle$, and the fact that $\langle x|\mathrm{e}^{-\beta H}|y\rangle$ depends on $\hbar$ only via the factor q.

Often one desires to expand F^* in powers of $\hbar$, β or m^{-1}. In these cases it is clear that a Taylor expansion of $\nu(\xi_l^*)$ about $\nu(x)$ must be made in each of the j factors of ν in (4.17). (Such a complication is not present for $F^\circ(x, y; \beta, q)$.) Doing this, one obtains the formal result

$$\log F^*(x, k; \beta, q, \hbar)$$
$$= \sum_{j=1}^{\infty} \mu^j \sum_{\mathcal{G}_j} \sum_{n=0}^{\infty} (-\beta)^{j+n+r} m^{-n-r} \hbar^{2r+n} \frac{\mathrm{i}^n}{j!\,n!}$$
$$\times \int_{I^j} \mathrm{d}^j \boldsymbol{\xi} \left(\prod_{\alpha \in E} (l_\alpha!)^{-1} b_\alpha^{*l_\alpha} \right) \left[\sum_{l=1}^{j} (\xi_l - 1) D_l \cdot \left(\frac{\hbar}{2\mathrm{i}} D_l + k \right) \right]^n$$
$$\times \prod_{l=1}^{j} \nu(x_l) \Big|_{x_l = x}. \tag{4.19}$$

In (4.19), it is understood that, after D_l acts on $\nu(x_l)$, then x_l is set equal to x.

One use of (4.19) is the following. Several authors (Uhlenbeck and Beth 1936, Jennings *et al* 1975) found it convenient to study the function $w(x, k; \beta)$ defined by

$$\langle x|\mathrm{e}^{-\beta H}|k\rangle = h^{-d/2}\, \mathrm{e}^{\mathrm{i}x \cdot k/\hbar}\, \mathrm{e}^{-\beta H_c(k,x)} w(x, k; \beta)$$

where $H_c = k^2/2m + \mu\nu(x)$ is the classical Hamiltonian. It is evident that

$$w(x, k; \beta) = \mathrm{e}^{\beta\mu\nu(x)} F^*(x, k; \beta, q, \hbar).$$

The $j = 1$, $n = 0$ term in (4.19) shows that F^* contains a compensating factor $\mathrm{e}^{-\beta\mu\nu(x)}$, so it becomes possible to use the graphical representation (4.19) to write down expansions of w such as

$$w(x, k; \beta) = 1 + \hbar w_1(x, k; \beta) + \hbar^2 w_2(x, k; \beta) + \ldots.$$

In particular, formulae for the coefficients w_i result directly from (4.19). Thus the need to determine w_i by solving the tedious differential recurrence relations they obey is eliminated.

4.3. Wigner distribution function

The third and last of our applications concerns Wigner functions. The widely studied Wigner method in quantum statistical mechanics (de Groot and Suttorp 1972) is based on an integral transform which maps quantum operators A into functions $A_w(x, p)$ of classical phase space variables. The linear transform, introduced by Weyl (1927) has the explicit form

$$A_w(x, p) = \int \mathrm{d}y\, \mathrm{e}^{\mathrm{i}p\cdot y/\hbar}\langle x-\tfrac{1}{2}y|A|x+\tfrac{1}{2}y\rangle. \tag{4.20}$$

Of fundamental interest in the method is Wigner's distribution function f for a canonical ensemble having inverse temperature β,

$$f(x, p; \beta) = (h^d \operatorname{Tr} \mathrm{e}^{-\beta H})^{-1}(\mathrm{e}^{-\beta H})_w(x, p). \tag{4.21}$$

It readily follows from definition (4.20) that the Hilbert space trace Tr of A is given by the phase space integral of $A_w(x, p)$. Thus the partition function which is the normalising denominator in (4.21) takes the form

$$\operatorname{Tr} \mathrm{e}^{-\beta H} = h^{-d} \int\int \mathrm{d}x\, \mathrm{d}p(\mathrm{e}^{-\beta H})_w(x, p)$$

so it will be sufficient to consider the Weyl transform of $\mathrm{e}^{-\beta H}$.

Since $(\mathrm{e}^{-\beta H})_w$ is determined by the heat kernel, which in turn is determined by the configuration function F°, it is of interest to find a simple formula expressing $(\mathrm{e}^{-\beta H})_w$ in terms of F°.

Taking $A = \mathrm{e}^{-\beta H}$ in (4.20) and using (1.3a) with $\Delta t = \hbar\beta/\mathrm{i}$ gives

$$(\mathrm{e}^{-\beta H})_w(x, p) = \int \mathrm{d}y \exp(\mathrm{i}p\cdot y/\hbar)(4\pi\beta q)^{-d/2} \exp(-y^2/4\beta q) F^\circ\left(x-\frac{y}{2}, x+\frac{y}{2}\right) \tag{4.22}$$

where we omit writing β, q in the argument list of F° for brevity. Next, employ the identity

$$\begin{aligned}
&\exp(\mathrm{i}p\cdot y/\hbar) F^\circ\left(x-\frac{y}{2}, x+\frac{y}{2}\right) \\
&\quad = \exp(\mathrm{i}p\cdot y/\hbar) \exp\left(-\frac{y}{2}\cdot\nabla_1\right) \exp\left(\frac{y}{2}\cdot\nabla_2\right) F^\circ(x, x) \\
&\quad = \exp\left(\frac{\mathrm{i}\hbar}{2}\nabla_p\cdot(\nabla_1-\nabla_2)\right) \exp(\mathrm{i}p\cdot y/\hbar) F^\circ(x, x).
\end{aligned}$$

The notation used here is equivalent to writing $\nabla_1 = \nabla_{x_1}$, $\nabla_2 = \nabla_{x_2}$ then letting these gradients act on $F^\circ(x_1, x_2)$ and finally setting $x_1 = x_2 = x$. Placing the above expression in (4.20) and taking the derivatives outside the $\mathrm{d}y$ integral gives

$$\begin{aligned}
(\mathrm{e}^{-\beta H})_w(x, p) &= (4\pi\beta q)^{-d/2} \exp\left(\frac{\mathrm{i}\hbar}{2}\nabla_p\cdot(\nabla_1-\nabla_2)\right) \\
&\quad \times\left(F^\circ(x, x)\int \mathrm{d}y \exp(-y^2/4\beta q) \exp(\mathrm{i}p\cdot y/\hbar)\right) \\
&= \exp\left(\frac{\mathrm{i}\hbar}{2}\nabla_p\cdot(\nabla_1-\nabla_2)\right)[F^\circ(x, x) \exp(-\beta p^2/2m)].
\end{aligned}$$

The Gaussian may be brought to the left of the differential operator by using the identity

$$\exp(a\cdot\nabla_p)\exp(-\beta p^2/2m)=\exp(-\beta p^2/2m)\exp(-\beta p\cdot a/m)\exp(-\beta a^2/2m)$$

where $a=(i\hbar/2)(\nabla_1-\nabla_2)$. This provides us with

$$\begin{aligned}[\exp(-\beta H)]_w(x,p)&=\exp(-\beta p^2/2m)\exp\left(-\frac{i\hbar}{2m}\beta p\cdot(\nabla_1-\nabla_2)\right)\\&\quad\times\exp\left(\frac{\hbar^2\beta}{8m}(\nabla_1-\nabla_2)^2\right)F^\circ(x,x)\\&=\exp(-\beta p^2/2m)\exp\left(\frac{i\hbar}{2m}\beta p\cdot(\nabla_1-\nabla_2)\right)\exp\left(\frac{\hbar^2\beta}{8m}(\nabla_1-\nabla_2)^2\right)F^\circ(x,x).\end{aligned}$$

The second step used the symmetry $F^\circ(x_1,x_2)=F^\circ(x_2,x_1)$, which is a consequence of the Hermiticity and reality of the Hamiltonian (1.1). Taking the average of these two forms brings us to the desired formula

$$\begin{aligned}[\exp(-\beta H)]_w(x,p)&=\exp(-\beta p^2/2m)\left[\cos\left(\frac{\hbar\beta}{2m}p\cdot(\nabla_1-\nabla_2)\right)\exp\left(\frac{\hbar^2\beta}{8m}(\nabla_1-\nabla_2)^2\right)F^\circ\right](x,x).\end{aligned}\tag{4.23}$$

Formula (4.23) shows that the map from $F^\circ\to[\exp(-\beta H)]_w$ can be implemented by straightforward differentiation. Furthermore formula (4.23) allows one to transfer the series expansion of F° in $\hbar^2$, β or m^{-1} into corresponding series expansions for $[\exp(-\beta H)]_w(x,p)$. This mapping has a practical utility since the various series expansions of F° are known in great detail (Fujiwara *et al* 1982, Osborn 1984). Note that as $\hbar\to 0$ (or $m\to\infty$) the limiting value of the factor $\{\ \}$ is $\exp(-\beta\mu\nu(x))$, thus the series expansions generated by (4.23) have as their leading term the expression $\exp(-\beta H_c(x,p))$. Such expansions, derived using recursive methods to determine the coefficient functions, are found in Imre *et al* (1967) and Nienhuis (1970).

Formulae similar to (4.23) exist which map the mixed representation Dirac matrix element of $\exp(-\beta H)$ into $[\exp(-\beta H)]_w$. Let the functions F^* and $F^\#$ defined in (1.3*b*) and (1.3*c*) be extended to the heat kernel form by the substitution $\Delta t\to\hbar\beta/i$. Proceeding analogously to the derivation of (4.23) we find

$$\begin{aligned}[\exp(-\beta H)]_w(x,p)&=\exp\left(\frac{i\hbar}{2}\nabla_p\cdot\nabla_x\right)[\exp(-\beta p^2/2m)F^*(x,p)]\\&=\exp\left(-\frac{i\hbar}{2}\nabla_p\cdot\nabla_x\right)[\exp(-\beta p^2/2m)F^\#(p,x)].\end{aligned}$$

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