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A connected-graph expansion of the anharmonic-oscillator propagator

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Abstract. Two series representations of the propagator associated with the quantum anharmonic-oscillator are developed. A closed form for the Dyson series expansion of the propagator is obtained by using a phase-space perturbation technique. For Abelian interactions the Dyson series can be rearranged into an exponentiated connected-graph series. This representation is structurally similar to the cluster expansions of propagators associated with perturbations of the kinetic-energy Hamiltonian. The connected-graph series is particularly useful for the development of semiclassical expansions such as the wKB expansion. The analytic structure in the physical parameters such as mass, time and Planck's constant is readily extracted from the connected-graph series because of the explicit closed-form formula for the series.

1. Introduction

In the study of time evolution of quantum systems much information can be found from an investigation of the propagator. This article presents two series representations of the anharmonic-oscillator propagator. The first series comes from a study of the time-evolution integral equation and the second is a connected-graph re-summation of the first. Similar expansions have been studied in detail [1, 2] for systems based upon perturbations of the kinetic-energy Hamiltonian and these expansions have proven facile in use for semiclassical and nonperturbative studies of the propagator [1, 3]. Such a program is possible for the anharmonic-oscillator propagator because of the marked parallels in structure with the kinetic-energy based formulas. These structural features of the propagator are, in fact, common to all propagators based upon perturbations of quadratic Hamiltonians [4].

The state of the quantum system at time t is specified by a wavefunction ψ_t in the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^d)$. The mapping $\psi_s \mapsto \psi_t$ of the initial state ψ_s to the final state ψ_t defines a unitary operator $U(t, s)$ and the time development of the quantum system is completely specified by $U(t, s)$. This operator solves the initial-valued Schrödinger equation

$$i\hbar \frac{d}{dt} U(t, s) = \hat{H}(t) U(t, s) \tag{1.1a}$$

$$U(s, s) = I \tag{1.1b}$$

where $\hat{H}(t)$ is the Hamiltonian and I denotes the identity operator.

The propagator is the integral kernel of $U(t, s)$ and it generates a pointwise representation of the state vector $\psi_t = U(t, s)\psi_s$ given by the formula

$$(U(t, s)\psi_s)(x) = \int_{\mathbb{R}^d} K(t, s, x, y)\psi_s(y) dy. \tag{1.2}$$

The boundary condition (1.1b) forces a delta-function boundary behaviour upon the propagator

$$\lim_{t \rightarrow s} K(t, s, x, y) = \delta(x - y). \quad (1.3)$$

The family of Hamiltonians under consideration are time-dependent perturbations of the harmonic-oscillator \hat{L}_0 ,

$$\hat{H}(t) = \hat{L}_0 + \hat{V}(t) \quad (1.4a)$$

$$\hat{L}_0 = \frac{1}{2m} \hat{p} \cdot \hat{p} + \frac{m\omega^2}{2} \hat{q} \cdot \hat{q}. \quad (1.4b)$$

A flat-space metric $g_{\mu\nu}$ is employed in the scalar product

$$x \cdot y = x_\mu y^\mu = g_{\mu\nu} x^\nu y^\mu. \quad (1.5)$$

Its signature, denoted by $\text{sign}(g)$, is the difference between the number of positive and the number of negative eigenvalues of g . The signature has magnitude $|\text{sign}(g)| \leq d$. When the magnitude equals d this corresponds to a description of the non-relativistic quantum harmonic-oscillator. If the magnitude of the signature is less than d then the theory corresponds to the relativistic scalar field theory of Schwinger and DeWitt [5-7].

The momentum and position operators, respectively \hat{p}_μ and \hat{q}_μ , satisfy the canonical commutation relations

$$[\hat{p}_\mu, \hat{p}^\nu] = 0 \quad (1.6a)$$

$$[\hat{q}_\mu, \hat{q}^\nu] = 0 \quad (1.6b)$$

$$[\hat{p}_\mu, \hat{q}^\nu] = -i\hbar \delta_\mu^\nu. \quad (1.6c)$$

The Schrödinger representation of this algebra describes the effect of these operators upon wavefunctions as multiplication and differential operators:

$$(\hat{p}_\mu \psi)(x) = -i\hbar \frac{\partial}{\partial x^\mu} \psi(x) \quad (1.7a)$$

$$(\hat{q}^\mu \psi)(x) = x^\mu \psi(x). \quad (1.7b)$$

The combination $\hat{p} \cdot \hat{p}$ of momentum operators appearing in \hat{L}_0 form a multiple of the D'Alembertian operator,

$$\hat{p} \cdot \hat{p} = -\hbar^2 \square. \quad (1.8)$$

The potential $\hat{V}(t)$ is defined by a smooth function (normal-ordered symbol) v on phase space. Let $\alpha = (\alpha_1, \dots, \alpha_d)$ denote a multi-index with length $|\alpha| = \alpha_1 + \dots + \alpha_d$. If the function v has a Taylor-series expansion

$$v(x, \hat{p}; t) = \sum_{|\alpha| \geq 0} c_\alpha(x, t) \hat{p}^\alpha \quad (1.9)$$

then the effect of $\hat{V}(t)$ on a wavefunction ψ is defined by

$$(\hat{V}(t)\psi)(x) = v(x, \hat{p}; t)\psi(x). \quad (1.10)$$

On occasion it will be useful to collect the phase space variables q and p into a single argument $z = (q, p)$ and write $v(q, p; t) = v(z; t)$.

The evolution problem for the unperturbed harmonic-oscillator is well understood. The family of operators that solve the Schrödinger equation are an exponentiation of \hat{L}_0 and form a one-parameter unitary group. Denoting the time difference between the initial and final times by $\Delta t = t - s$, the time evolution operator is

$$U_0(t, s) = e^{-i(\Delta t/\hbar)\hat{L}_0} \tag{1.11}$$

The harmonic-oscillator propagator is the integral kernel of this evolution operator and it has an explicit expression known as Mehler's formula [8]

$$K_0(t, s, x, y) = \left[\frac{m\omega}{2\pi\hbar \sin(\omega\Delta t)} \right]^{d/2} e^{-i(\pi/4)\text{sign}(g)} e^{(im\omega/2\hbar)[[x\cdot x + y\cdot y] \cot(\omega\Delta t) - 2x\cdot y \text{cosec}(\omega\Delta t)]} \tag{1.12}$$

The branch cut used in the definition of the square root function selects the argument of a complex number to lie in the interval $(-\pi, \pi]$. The classical harmonic-oscillator motion is caustic whenever $\omega\Delta t \rightarrow n\pi$ for some integer n . At these times, K_0 obeys the delta function condition

$$\lim_{\omega\Delta t \rightarrow n\pi} K_0(t, s, x, y) = e^{ind\pi/2} \delta((-1)^n x - y) \tag{1.13}$$

The boundary behaviour (1.3) of the full propagator is directly attributable to the $\Delta t \rightarrow 0$ behaviour of the harmonic-oscillator propagator. Notice that the $\sin(\omega\Delta t)$ in the normalizing factor in (1.12) changes sign as t moves through a caustic. This introduces an implicit phase factor that is a necessary feature of the harmonic-oscillator propagator. It ensures that the function K_0 defines an integral operator that is strongly continuous in t for all times, including the caustics.

The arguments presented in this article closely parallel the phase-space method of Barvinsky and Osborn [2]. The chief distinction lies in which free Hamiltonian is perturbed to obtain the full Hamiltonian. Barvinsky and Osborn use perturbations from the kinetic-energy Hamiltonian $\hat{H}_0 = \hat{p} \cdot \hat{p}/(2m)$ and their propagator expressions use the associated kinetic-energy propagator

$$\mathcal{K}_0(t, s, x, y) = \left[\frac{m}{2\pi\hbar|\Delta t|} \right]^{d/2} e^{-i(\pi/4)\text{sign}(\Delta t g)} e^{(im/2\hbar\Delta t)(x-y)\cdot(x-y)} \tag{1.14}$$

From a purely formal point of view, treating the full Hamiltonian as a perturbation of the harmonic-oscillator Hamiltonian is equivalent to treating it as a different perturbation of the kinetic-energy Hamiltonian. The two perturbations would differ from one another by the harmonic-oscillator potential. The equivalence of these formalisms at the kernel level is not as easily seen. One useful connection that can be easily exploited when comparing the harmonic-oscillator formulae against the kinetic-energy formulae in [2] is to treat the angular frequency parameter ω as a coupling constant. By taking the limit $\omega \rightarrow 0$, formulae based on the harmonic-oscillator propagator will converge to the corresponding kinetic energy based expressions. For example, the harmonic-oscillator and kinetic-energy propagators exhibit this property,

$$\lim_{\omega \rightarrow 0} K_0(t, s, x, y) = \mathcal{K}_0(t, s, x, y) \tag{1.15}$$

The reverse connection is not so easily made. Although the kinetic-energy and harmonic-oscillator representations of the propagator are formally equivalent there can be practical advantages to choosing one over the other. When studying anharmonic-oscillator systems, the harmonic -oscillator representation of the propagator is the more natural choice. For such a system, one would expect a more rapid convergence in the harmonic-oscillator representation of the propagator than in the kinetic-energy representation.

There are many structural features such as the appearance and placement of the Green functions in the propagator's formula that are common to the kinetic energy and harmonic-oscillator representations of the full propagator. These features have been shown to be common to all propagators based upon quadratic Hamiltonians in a recent work by Molzahn and Osborn [4]. In a sense, their results subsume the results in this article and in [2] but because of the generality of their Hamiltonians they do not give complete closed form expressions for the propagator. Specifically they do not give details about the time dependence of each unperturbed propagator because it differs for each possible quadratic Hamiltonian. The time dependence is left as an implicit function that can be found, in principal, once the Jacobi equations are solved. There is more detail to the formulae appearing in this article and in [2] because the propagators of the Hamiltonians \hat{L}_0 and \hat{H}_0 are explicitly known. This additional information is used to extract a complete closed form expression for the full propagator.

In section 2 the Dyson series analysis of the full propagator is carried out. To begin, the Schrödinger equation (1.1) is inverted into an operator-valued integral equation. Its iterative solution is known as the Dyson series [9] and the individual terms in the Dyson series are normal ordered through use of operator algebra. The resulting operator equation is then converted into the corresponding kernel equation. Here the explicit form (1.12) of the harmonic-oscillator propagator is exploited by allowing the evaluation of all derivatives acting upon it.

The constructive argument in section 2 finds a closed form for the Dyson series representation of the propagator. In section 3 the Dyson series formula is manipulated to produce an exponentiated connected-graph series representation. This is accomplished by first changing the domains of integration. It is necessary that the potentials be Abelian in order to make this change of domain. Next, certain combinatorial features appearing in the integrals are recognized. These combinatorics are essentially the same as those appearing in Mayer's cluster expansion of the partition function [10] and they yield the connected-graph formula for the propagator.

Concluding remarks are gathered in section 4.

2. The Dyson series expansion

The initial-valued Schrödinger problem (1.1) may be converted into the integral equation

$$U(t, s) = e^{-i(\Delta t/\hbar)\hat{L}_0} + \frac{1}{i\hbar} \int_s^t e^{-i(t-u)/\hbar)\hat{L}_0} \hat{V}(u) U(u, s) du. \quad (2.1)$$

The iterative solution of this produces the Dyson series. It converges in the operator norm topology if $\hat{V}(u)$ is bounded but for unbounded potentials the resulting series is usually asymptotic. The iteration of (2.1) produces an n -dimensional hyper-triangle domain of integration,

$$T_n^> = \{(u_1, \dots, u_n) \in [s, t]^n \mid s \leq u_n \leq \dots \leq u_1 \leq t\}. \quad (2.2)$$

Using the interaction-picture notation

$$\hat{V}_1(u) = e^{(iu/\hbar)\hat{L}_0} \hat{V}(u) e^{-(iu/\hbar)\hat{L}_0} \tag{2.3}$$

the Dyson series may be written as

$$U(t, s) = e^{-(i\Delta t/\hbar)\hat{L}_0} + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_{T_n^+} e^{-(it/\hbar)\hat{L}_0} \hat{V}_1(u_1) \hat{V}_1(u_2) \dots \hat{V}_1(u_n) e^{(is/\hbar)\hat{L}_0} d^n u. \tag{2.4}$$

The formula

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \dots \tag{2.5}$$

is used to explicitly evaluate $\hat{V}_1(u)$. From the algebra in (1.6) the harmonic-oscillator Hamiltonian satisfies the commutator relations

$$[\hat{L}_0, \hat{q}^\mu] = -\frac{i\hbar}{m} \hat{p}^\mu \tag{2.6a}$$

$$[\hat{L}_0, \hat{p}^\mu] = im\hbar\omega^2 \hat{q}^\mu. \tag{2.6b}$$

Combining this with formula (2.5) gives the relationship

$$e^{(iu/\hbar)\hat{L}_0} \hat{q}^\mu e^{-(iu/\hbar)\hat{L}_0} = \hat{q}^\mu \cos(\omega u) + \frac{1}{m\omega} \hat{p}^\mu \sin(\omega u) \tag{2.7a}$$

$$e^{(iu/\hbar)\hat{L}_0} \hat{p}^\mu e^{-(iu/\hbar)\hat{L}_0} = -m\omega \hat{q}^\mu \sin(\omega u) + \hat{p}^\mu \cos(\omega u). \tag{2.7b}$$

In turn, formulae (2.7a) and (2.7b) are used to evaluate the interaction potential with the result

$$\hat{V}_1(u) = v \left(\hat{q} \cos(\omega u) + \frac{1}{m\omega} \hat{p} \sin(\omega u), \hat{p} \cos(\omega u) - m\omega \hat{q} \sin(\omega u); u \right). \tag{2.8}$$

The next step is to commute the evolution operator $\exp\{-it\hat{L}_0/\hbar\}$ in (2.4) through each interaction potential until it can be combined with $\exp\{is\hat{L}_0/\hbar\}$. The calculation is similar to that used in obtaining (2.8) and for a single interaction potential the result is

$$e^{-(it/\hbar)\hat{L}_0} \hat{V}_1(u) = v(\hat{X}(u), \hat{P}(u); u) e^{-(it/\hbar)\hat{L}_0} \tag{2.9}$$

where

$$\hat{X}(u) = \hat{q} \cos(\omega(t - u)) - \frac{1}{m\omega} \hat{p} \sin(\omega(t - u)) \tag{2.10a}$$

$$\hat{P}(u) = \hat{p} \cos(\omega(t - u)) + m\omega \hat{q} \sin(\omega(t - u)). \tag{2.10b}$$

The Dyson series may now be written as

$$U(t, s) = e^{-(i\Delta t/\hbar)\hat{L}_0} + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_{T_n^+} v(\hat{X}(u_1), \hat{P}(u_1); u_1) \dots \times v(\hat{X}(u_n), \hat{P}(u_n); u_n) e^{-(i\Delta t/\hbar)\hat{L}_0} d^n u. \tag{2.11}$$

Equation (2.11) is an operator-valued equation and it implies a corresponding equation for the kernel of $U(t, s)$. The conversion to the kernel equation is made by replacing both $U(t, s)$ and $\exp\{-i\Delta t \hat{L}_0/\hbar\}$ by their respective kernels $K(t, s, x, y)$ and $K_0(t, s, x, y)$. The \hat{q} 's appearing in the arguments of the potentials are replaced by x and momentum operators \hat{p} in the arguments of the potentials act as partial derivatives on the x -variable. These derivatives act both on the x -dependence in the potentials and in the free propagator. The free propagator and momentum operator satisfy the commutation relation

$$[\hat{p}_\mu, K_0(t, s, x, y)] = K_0(t, s, x, y)(m\omega x_\mu \cot(\omega\Delta t) - m\omega y_\mu \operatorname{cosec}(\omega\Delta t)) \quad (2.12)$$

and this can be used to commute K_0 through the product of potentials. On commuting K_0 to the extreme left, the full propagator can be written as a product of the free propagator with the configuration function

$$K(t, s, x, y) = K_0(t, s, x, y)F(t, s, x, y). \quad (2.13)$$

The configuration function is given by

$$F(t, s, x, y) = 1 + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_{T_n^2} v(\hat{\mathcal{X}}(u_1), \hat{\mathcal{P}}(u_1); u_1) \dots v(\hat{\mathcal{X}}(u_n), \hat{\mathcal{P}}(u_n); u_n) 1 \, d^n u \quad (2.14)$$

where

$$\hat{\mathcal{X}}(u) = q_c(u) - \frac{1}{m\omega} \hat{p} \sin(\omega(t-u)) \quad (2.15a)$$

$$\hat{\mathcal{P}}(u) = p_c(u) + \hat{p} \cos(\omega(t-u)). \quad (2.15b)$$

The quantities q_c and p_c are

$$q_c(u) = x \frac{\sin(\omega(u-s))}{\sin(\omega\Delta t)} + y \frac{\sin(\omega(t-u))}{\sin(\omega\Delta t)} \quad (2.16a)$$

$$p_c(u) = m\omega x \frac{\cos(\omega(u-s))}{\sin(\omega\Delta t)} - m\omega y \frac{\cos(\omega(t-u))}{\sin(\omega\Delta t)}. \quad (2.16b)$$

They represent the classical path and momentum of the harmonic oscillator obeying the two-point boundary condition $q(s) = y$ and $q(t) = x$. There are caustics in the classical motion at the times $\omega\Delta t = n\pi$ where n is integer. The two-point boundary problem at these times will have a solution only if $x = y$ for even n or $x = -y$ for odd n .

As quantum operators $\hat{\mathcal{X}}(u)$ and $\hat{\mathcal{P}}(u')$ satisfy the commutation relationships

$$[\hat{\mathcal{P}}_\mu(u), \hat{\mathcal{X}}^\nu(u')] = -i\hbar \delta_\mu^\nu \cos(\omega(u-u')) \quad (2.17a)$$

$$[\hat{\mathcal{X}}_\mu(u), \hat{\mathcal{X}}^\nu(u')] = -\frac{i\hbar}{m\omega} \delta_\mu^\nu \sin(\omega(u-u')) \quad (2.17b)$$

$$[\hat{\mathcal{P}}_\mu(u), \hat{\mathcal{P}}^\nu(u')] = -i\hbar m\omega \delta_\mu^\nu \sin(\omega(u-u')). \quad (2.17c)$$

From this algebra, we see that for equal times $u = u'$, $\hat{\mathcal{X}}(u)$ and $\hat{\mathcal{P}}(u)$ form a canonical pair of position and momentum operators.

The 1 appearing after the product of the potentials in (2.14) is thought of as a function of x upon which the \hat{p} 's act. The momentum operators will also act upon the x -dependence in the potentials appearing to their right and we wish to evaluate these derivatives. This

can be accomplished by the normal ordering of these operators with the method of external sources. Effectively, $\hat{\mathcal{X}}(u)$ and $\hat{\mathcal{P}}(u)$ are separated from the arguments of the potentials and transferred into the arguments of exponentials. These exponential operators are then placed into normal order. Let I_k, J_k ($1 \leq k \leq n$) denote pairs of d -dimensional vectors. The product of potentials appearing in (2.14) satisfies

$$v(\hat{\mathcal{X}}(u_1), \hat{\mathcal{P}}(u_1); u_1) \dots v(\hat{\mathcal{X}}(u_n), \hat{\mathcal{P}}(u_n); u_n) 1 \\ = v(\nabla_{I_1}, \nabla_{J_1}; u_1) \dots v(\nabla_{I_n}, \nabla_{J_n}; u_n) e^{J_1 \cdot \hat{\mathcal{X}}(u_1)} e^{I_1 \cdot \hat{\mathcal{P}}(u_1)} \dots e^{J_n \cdot \hat{\mathcal{X}}(u_n)} e^{I_n \cdot \hat{\mathcal{P}}(u_n)} 1 \Big|_{I, J=0} \quad (2.18)$$

where the delimiter refers to setting each I_k and J_k to 0.

Before normal ordering the exponentials in (2.18) it is convenient to introduce some notation. There will appear in the normal-ordering procedure three Green functions. The first two Green functions, satisfy the one-dimensional equation

$$\left(\frac{\partial^2}{\partial u^2} + \omega^2 \right) g(u, u') = \delta(u - u') \quad (2.19)$$

on the interval $[s, t]$ but they are subject to different boundary conditions. Denoting these functions by g_1 and g_2 , they and their respective boundary conditions are

$$g_1(u, u') = \frac{\sin(\omega(u_{>} - t)) \sin(\omega(u_{<} - s))}{\omega \sin(\omega \Delta t)}; \quad (2.20a)$$

$$g_1(s, u') = g_1(t, u') = 0 \quad (2.20b)$$

$$g_2(u, u') = \frac{\cos(\omega(u_{>} - t)) \cos(\omega(u_{<} - s))}{\omega \sin(\omega \Delta t)} \quad (2.21a)$$

$$\frac{\partial g_2}{\partial u}(s, u') = \frac{\partial g_2}{\partial u}(t, u') = 0. \quad (2.21b)$$

Here $u_{>}$ and $u_{<}$ are the times $u_{>} = \max\{u, u'\}$ and $u_{<} = \min\{u, u'\}$. The derivatives $(\partial/\partial u)g_1 \equiv \dot{g}_1$ and $(\partial/\partial u)g_2 \equiv \dot{g}_2$ appear in the third Green function and are given by the formulae

$$\dot{g}_1(u, u') = -\dot{g}_2(u', u) = \begin{cases} \frac{\cos(\omega(u - t)) \sin(\omega(u' - s))}{\sin(\omega \Delta t)} & \text{if } u > u' \\ \frac{\cos(\omega(u - s)) \sin(\omega(u' - t))}{\sin(\omega \Delta t)} & \text{if } u < u'. \end{cases} \quad (2.22)$$

The third Green function is a $2d \times 2d$ matrix $\mathcal{D}(u, u')$ which is the fundamental solution to the Jacobi equation,

$$\mathcal{J} \left(\frac{\partial}{\partial u} \right) \mathcal{D}(u, u') = -\mathbf{J} \delta(u - u'). \quad (2.23)$$

Here \mathbf{J} denotes the $2d \times 2d$ symplectic matrix

$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} \quad (2.24)$$

and $\mathcal{J}(\partial/\partial u)$ is the Jacobi operator. Letting $1 \leq a, b \leq 2d$ denote the component indices, the matrix $\mathcal{D}(u, u')$ may be written in block form as

$$\mathcal{D}^{ab}(u, u') = \begin{pmatrix} \frac{1}{m}g_1(u, u')g^{ab} & -\dot{g}_2(u, u')\delta_{b-d}^a \\ \dot{g}_1(u, u')\delta_{a-d}^b & m\omega^2g_2(u, u')g_{a-d,b-d} \end{pmatrix}. \tag{2.25}$$

The Jacobi operator is obtained [11] from a first-order variation of Hamilton's equations of motion for the harmonic-oscillator. It forms a $2d \times 2d$ matrix which in block form is

$$\mathcal{J}_{ab}\left(\frac{\partial}{\partial u}\right) = \begin{pmatrix} \frac{\partial}{\partial u}\delta_b^a & -\frac{1}{m}g^{a,b-d} \\ m\omega^2g_{a-d,b} & \frac{\partial}{\partial u}\delta_{a-d}^{b-d} \end{pmatrix}. \tag{2.26}$$

An important property of $\mathcal{D}(u, u')$ is the symmetry relation

$$\mathcal{D}^{ab}(u, u') = \mathcal{D}^{ba}(u', u). \tag{2.27}$$

This relation is critical for showing the integrand in (2.14) is symmetric under any permutation of the times u_1, \dots, u_n . This invariance under permutations ultimately leads to the cluster expansion in section 3.

There is one more detail about the Green function $\mathcal{D}(u, u')$ that requires clarification. It is not presently defined for equal time arguments because $\dot{g}_1(u, u')$ and $\dot{g}_2(u, u')$ each have a jump of 1 across $u = u'$. Nevertheless there exist two situations where equal time arguments for $\mathcal{D}(u, u')$ arise and we shall distinguish between these situations by employing the notation $\mathcal{D}(u, u)$ and $\mathcal{D}(u+, u)$. The $u+$ refers to taking a limit $u + \epsilon$ as $\epsilon \downarrow 0$. For the first possibility the time arguments are the same variable, say $u = u' = u_j$. In this situation, we employ the definition (2.25) for $\mathcal{D}(u_j, u_j)$ but with the stipulation of using $\dot{g}_1(u_j-, u_j)$ and $\dot{g}_2(u_j+, u_j)$. The second possibility occurs with two distinct time variables, say $u = u_j$ and $u' = u_k$. Assuming that $u_j \geq u_k$, these can be numerically equal on the boundary $u_j = u_k$. The boundary is a set of measure zero and any definitions will be irrelevant, but using $\mathcal{D}(u_j, u_k) = \mathcal{D}(u_k+, u_k)$ for values on the boundary will reproduce the correct formula for the integrand.

The exponential operators in (2.18) may now be put into normal order. This is best carried out in stages. Those exponentials containing both x and \hat{p} in a sum must be split into a product of exponentials containing x and \hat{p} separately. The resulting exponential products are then normal ordered. The Baker-Campbell-Hausdorff (henceforth BCH) formula and an auxillary equation resulting from the BCH formula are used to normal order these. If A and B are operators that commute with their commutator then

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} \tag{2.28a}$$

$$e^A e^B = e^B e^A e^{[A,B]}. \tag{2.28b}$$

The BCH formula (2.28a) is used to separate those x 's and \hat{p} 's appearing together in the argument of an exponential operator and we obtain

$$e^{J_k \cdot \hat{\mathcal{X}}(u_k)} = e^{J_k \cdot q_c(u_k)} e^{(1/m\omega)J_k \cdot \hat{p} \sin(\omega(u_k-t))} e^{-(i\hbar/2m)g_1(u_k, u_k)J_k \cdot J_k} \tag{2.29a}$$

$$e^{J_k \cdot \hat{\mathcal{P}}(u_k)} = e^{J_k \cdot p_c(u_k)} e^{J_k \cdot \hat{p} \cos(\omega(u_k-t))} e^{-(i\hbar m\omega^2/2)g_2(u_k, u_k)J_k \cdot J_k}. \tag{2.29b}$$

Next the product $e^{J_k \cdot \hat{\mathcal{X}}(u_k)} e^{J_k \cdot \hat{\mathcal{P}}(u_k)}$ is normal ordered using the formula (2.28b),

$$e^{J_k \cdot \hat{\mathcal{X}}(u_k)} e^{J_k \cdot \hat{\mathcal{P}}(u_k)} = e^{-(i\hbar/2)\phi_k(u_k)} e^{J_k \cdot q_c(u_k) + J_k \cdot p_c(u_k)} e^{(1/m\omega)J_k \cdot \hat{p} \sin(\omega(u_k-t)) + J_k \cdot \hat{p} \cos(\omega(u_k-t))}. \tag{2.30}$$

The phase angle $\phi_k(u_k)$ in (2.30) is

$$\phi_k(u_k) = \mathcal{I}_{ka} \mathcal{D}^{ab}(u_k, u_k) \mathcal{I}_{kb}. \quad (2.31)$$

The vectors \mathcal{I}_k are $2d$ -dimensional vectors and in block form as a column vector its components are

$$\mathcal{I}_{ka} = \begin{pmatrix} J_{ka} \\ I_k^{a-d} \end{pmatrix}. \quad (2.32)$$

The summation convention of summing over repeated a 's and b 's is being employed in (2.31). The final step is to normal order the product over k of $e^{J_k \cdot \hat{\mathcal{X}}(u_k)} e^{I_k \cdot \hat{\mathcal{P}}(u_k)}$. This is again accomplished by using formula (2.28b) with the result

$$\begin{aligned} & e^{J_1 \cdot \hat{\mathcal{X}}(u_1)} e^{I_1 \cdot \hat{\mathcal{P}}(u_1)} \dots e^{J_n \cdot \hat{\mathcal{X}}(u_n)} e^{I_n \cdot \hat{\mathcal{P}}(u_n)} 1 \\ &= e^{-(i\hbar/2)\Psi_n} \left[\prod_{j=1}^n e^{J_j \cdot q_c(u_j) + I_j \cdot p_c(u_j)} \right] \left[\prod_{k=1}^n e^{(1/m\omega)J_k \cdot \hat{p} \sin(\omega(u_k - t)) + I_k \cdot \hat{p} \cos(\omega(t - u_k))} \right] 1. \end{aligned} \quad (2.33)$$

The phase angle Ψ_n may be written in the form

$$\Psi_n = \sum_{j,k=1}^n \mathcal{I}_{ja} \mathcal{D}^{ab}(u_j, u_k) \mathcal{I}_{kb}. \quad (2.34)$$

This completes the normal ordering of (2.18).

Those exponential operators in (2.33) containing the momentum operators in their arguments act upon the constant function 1 and when evaluated yield a value of 1. The gradients ∇_{J_k} and ∇_{I_k} appearing in the potentials in (2.18) can be partially evaluated using the commutative relation

$$\nabla_{J_k} e^{J_k \cdot q_c(u_k) + I_k \cdot p_c(u_k)} = e^{J_k \cdot q_c(u_k) + I_k \cdot p_c(u_k)} [\nabla_{J_k} + q_c(u_k)] \quad (2.35a)$$

$$\nabla_{I_k} e^{J_k \cdot q_c(u_k) + I_k \cdot p_c(u_k)} = e^{J_k \cdot q_c(u_k) + I_k \cdot p_c(u_k)} [\nabla_{I_k} + p_c(u_k)]. \quad (2.35b)$$

Collecting the normal-ordered results with these and substituting into (2.18) and then (2.14), the configuration function becomes

$$\begin{aligned} F(t, s, x, y) &= 1 + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_{T_n^*} v(q_c(u_1) + \nabla_{J_1}, p_c(u_1) + \nabla_{I_1}; u_1) \dots \\ &\quad \times v(q_c(u_n) + \nabla_{J_n}, p_c(u_n) + \nabla_{I_n}; u_n) e^{-(i\hbar/2)\Psi_n} \Big|_{I, J=0} d^n u. \end{aligned} \quad (2.36)$$

There remains a final manipulation on the Dyson series to prepare the expansion for the connected-graph representation in section 3. We first note that for any two smooth functions f and g ,

$$f(\nabla_z)g(z)|_{z=0} = g(\nabla_z)f(z)|_{z=0}. \quad (2.37)$$

Equation (2.37) may be verified by a Taylor series expansion. This formula will allow a reversal of roles from the potentials in (2.36) which act as operators on the exponentials to the exponentials which will act as operators on the potentials. For $1 \leq j, k \leq n$, introduce

$2d$ -dimensional phase-space gradients \mathbb{D}_j and let f be a function of n phase-space variables $z_k = (x_k, p_k)$. Then \mathbb{D}_j acts as a gradient on the j th argument,

$$\mathbb{D}_j f(z_1, \dots, z_n) = \nabla_{z_j} f(z_1, \dots, z_n). \quad (2.38)$$

In the application here f is the product of potentials and the effect of \mathbb{D}_j is

$$\mathbb{D}_j v(z_1; u_1) \dots v(z_n; u_n) = v(z_1; u_1) \dots (\nabla v)(z_j; u_j) \dots v(z_n; u_n). \quad (2.39)$$

By applying identity (2.37) to (2.36) the Dyson series representation of the configuration function becomes

$$F(t, s, x, y) = 1 + \sum_{n=1}^{\infty} (i\hbar)^{-n} \int_{T_n^>} e^{-(i\hbar/2) \sum_{j,k=1}^n \mathcal{D}^{ab}(u_j, u_k) \mathbb{D}_j a \mathbb{D}_k b} v(z_c(u_1); u_1) \dots v(z_c(u_n); u_n) d^n u \quad (2.40)$$

where $z_c(u)$ is the phase space variable $(q_c(u), p_c(u))$.

3. Connected-graph expansion

The connected-graph representation of the configuration function is a rearrangement of Dyson series into an exponentiated series. The Abelian nature of the potential is used to accomplish this. Specifically, the commutative property of the potential is necessary to change the time-ordered integrals over $T_n^>$ to unrestricted integrals over the hyper-cubes $[s, t]^n$. This feature is necessary in order to associate the individual terms of the Dyson series with connected graphs. Once the series has been reordered via a re-summation over graphs, the analytic behaviour of the propagator with respect to the physical parameters \hbar , m and Δt is easily extracted. These behaviours are very important for the various semiclassical expansion schemes. The small \hbar asymptotics give the WKB expansion; the large mass behaviour leads to a gauge invariant derivative expansion; and the Schwinger-Dewitt asymptotics comes from the small time behaviour.

To facilitate an understanding of the small time behaviour, a change of variables in the integrals in (2.40) must be made. Let $\xi \in [0, 1]$ be the scaled time coordinate related to the time u by

$$\xi = \frac{u - s}{\Delta t}. \quad (3.1)$$

Many functions will depend implicitly on the scaled time coordinates via the inverse relation expressing u as a function of ξ . To make the ξ dependence more explicit replace u by the the function $\xi^0 = u(\xi) = s + \xi \Delta t$. Then functions such as the classical path $q_c(u)$ and momentum $p_c(u)$ become

$$q_c(\xi^0) = x \frac{\sin(\omega \Delta t \xi)}{\sin(\omega \Delta t)} + y \frac{\sin(\omega \Delta t (1 - \xi))}{\sin(\omega \Delta t)} \quad (3.2a)$$

$$p_c(\xi^0) = m\omega x \frac{\cos(\omega \Delta t \xi)}{\sin(\omega \Delta t)} - m\omega y \frac{\cos(\omega \Delta t (1 - \xi))}{\sin(\omega \Delta t)}. \quad (3.2b)$$

The change of variables $u_j \rightarrow \xi_j$ changes the domain of integration from the hyper-triangle $T_n^>$ to the hyper-triangle

$$Q_n^> = \{(\xi_1, \dots, \xi_n) \in [0, 1]^n \mid 0 \leq \xi_n \leq \dots \leq \xi_1 \leq 1\}. \quad (3.3)$$

The n th-order differential becomes $d^n u = (\Delta t)^n d^n \xi$. After this change of variables the configuration function is

$$F(t, s, x, y) = \sum_{n=0}^{\infty} \frac{1}{n!} Z_n(t, s, x, y) \tag{3.4a}$$

$$Z_0(t, s, x, y) = 1 \tag{3.4b}$$

$$Z_n(t, s, x, y) = n! \left(\frac{\Delta t}{i\hbar} \right)^n \int_{Q^n} e^{-(i\hbar/2) \sum_{j,k=1}^n \mathcal{D}^{ab}(\xi_j^0, \xi_k^0) \mathbb{D}_{ja} \mathbb{D}_{kb}} \times v(z_c(\xi_1^0); \xi_1^0) \dots v(z_c(\xi_n^0); \xi_n^0) d^n \xi \quad n \geq 1. \tag{3.4c}$$

The integrand is invariant under permutations of the variables ξ_1, \dots, ξ_n because the potentials commute with themselves and because of the Green function's symmetry relation (2.27). As a result the integral over the hyper-triangle may be replaced by an integral over the hyper-cube $I^n = [0, 1]^n$ and a multiplicative factor of $1/n!$. Furthermore because the phase space gradients \mathbb{D}_j commute with themselves the exponential operator in (3.4c) may be split into a product of exponential operators. Consequently Z_n may be written as

$$Z_1(t, s, x, y) = \frac{\Delta t}{i\hbar} \int_I e^{-(i\hbar/2) \mathcal{D}^{ab}(\xi_1^0, \xi_1^0) \mathbb{D}_{1a} \mathbb{D}_{1b}} v(z_c(\xi_1^0); \xi_1^0) d\xi_1 \tag{3.5a}$$

$$Z_n(t, s, x, y) = \left(\frac{\Delta t}{i\hbar} \right)^n \int_{I^n} \left[\prod_{1 \leq j < k \leq n} e^{-i\hbar \mathcal{D}^{ab}(\xi_j^0, \xi_k^0) \mathbb{D}_{ja} \mathbb{D}_{kb}} \right] e^{-(i\hbar/2) \sum_{j=1}^n \mathcal{D}^{ab}(\xi_j^0, \xi_j^0) \mathbb{D}_{ja} \mathbb{D}_{jb}} \times v(z_c(\xi_1^0); \xi_1^0) \dots v(z_c(\xi_n^0); \xi_n^0) d^n \xi \quad n \geq 2. \tag{3.5b}$$

The configuration function series (3.4a) is ready to be reorganized into the exponentiated cluster series. This has become a standard exercise in the recent literature and details may be found in section 3 of [1]. Essentially, the linked-graph resummation argument parallels those for the cluster expansion of the partition function [10]. Of particular importance are the features of having an integration domain I^n and having the product over $1 \leq j < k \leq n$. The product over $j < k$ can be expanded into a sum whose terms are in one-to-one association with n -vertex graphs. The hyper-cube domain feature allows a factorization of integrals over I^n into products of integrals over lower-dimensional hyper-cubes. The result is series (3.4a) can be rearranged into a product of series solely involving connected graphs.

The relevant notation for the sum over graphs is as follows. A graph [12] is a pair, $C = (\bar{\ell}, E)$, consisting of a vertex set $\bar{\ell} = \{1, \dots, \ell\}$ and an edge set E . The elements $\alpha \in E$ are unordered pairs of distinct integers from $\bar{\ell}$. If each pair of vertices in a graph is joined by a path the graph is said to be connected. If between any two vertices there is at most one edge the graph is said to be simple. The term 'cluster' is synonymous with a connected simple graph. Let $C_{\bar{\ell}}$ denote the set of all clusters formed over a given index set $\bar{\ell}$ and define the sum

$$\sum_{\bar{\ell}} = \sum_{C \in C_{\bar{\ell}}} \left(\prod_{\alpha \in E} \sum_{h_{\alpha}=1}^{\infty} \right). \tag{3.6}$$

Let $r(E)$ be the sum over the summation indices h_{α} ,

$$r(E) = \begin{cases} 0 & \text{if } E = \emptyset \\ \sum_{\alpha \in E} h_{\alpha} & \text{otherwise} \end{cases} \tag{3.7}$$

The integer $r(E)$ satisfies $r(E) \geq \ell - 1$ and the equality in this relation is equivalent to having the minimally-connected graphs and each $h_\alpha = 1$. The minimally-connected graphs are also referred to as tree graphs. To each $\alpha \equiv (j, k) \in E$ one can associate a differential operator

$$\mathbb{B}_\alpha = \mathcal{D}^{ab}(\xi_j^0, \xi_k^0) \mathbb{D}_{ja} \mathbb{D}_{kb}. \tag{3.8}$$

There is a second type of differential operator that appears and it is defined by

$$\mathbb{A}_\ell = \sum_{j=1}^{\ell} \mathcal{D}^{ab}(\xi_j^0, \xi_j^0) \mathbb{D}_{ja} \mathbb{D}_{jb}. \tag{3.9}$$

Employing this notation, the configuration function can be rearranged into the exponentiated series

$$F(t, s, x, y) = \exp \left\{ \sum_{\ell=1}^{\infty} L_\ell(t, s, x, y) \right\}. \tag{3.10}$$

The functions $L_\ell(t, s, x, y)$ are called cluster integrals and are defined by

$$L_\ell(t, s, x, y) = \sum_{g_i} \sum_{n=0}^{\infty} \frac{(-1)^{r(E)+n} (i\hbar)^{r(E)+n-\ell} (\Delta t)^\ell}{2^n \ell! n!} \times \int_{I^\ell} \left[\prod_{\alpha \in E} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{h_\alpha!} \right] (\mathbb{A}_\ell)^n v(z_c(\xi_1^0); \xi_1^0) \dots v(z_c(\xi_\ell^0); \xi_\ell^0) d^\ell \xi. \tag{3.11}$$

The first three cluster integrals are relatively easy to write out. The formulae rapidly become more complicated as the number of vertices increases. For $\bar{\ell} = \{1\}$ there is but one possible graph, $C = (\{1\}, \emptyset)$. The cluster integral is

$$L_1(t, s, x, y) = -\frac{i\Delta t}{\hbar} \sum_{n=0}^{\infty} \frac{(-i\hbar/2)^n}{n!} \int_I (\mathbb{A}_1)^n v(z_c(\xi_1^0); \xi_1^0) d\xi_1. \tag{3.12}$$

For the vertex set $\bar{\ell} = \{1, 2\}$ the only possible connected graph is 1-2. Setting $\alpha = (1, 2)$ the cluster integral is

$$L_2(t, s, x, y) = \sum_{h_\alpha=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+n} (i\hbar)^{h_\alpha+n-2} (\Delta t)^2}{2^n 2! n!} \times \int_{I^2} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{h_\alpha!} (\mathbb{A}_2)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) d^2 \xi. \tag{3.13}$$

There are four graphs that contribute to the third cluster integral. Three of these are tree graphs, 1-2-3, 1-3-2 and 2-1-3 and the fourth is the complete graph 1-2-3-1. Denoting each of the possible edges by $\alpha = (1, 2)$, $\beta = (1, 3)$ and $\gamma = (2, 3)$ the third cluster integral is

$$L_3(t, s, x, y) = \sum_{h_\alpha=1}^{\infty} \sum_{h_\beta=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+h_\beta+n} (i\hbar)^{h_\alpha+h_\beta+n-3} (\Delta t)^3}{2^n 3! n!} \times \int_{I^3} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{h_\alpha!} \frac{(\mathbb{B}_\beta)^{h_\beta}}{h_\beta!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3 \xi$$

$$\begin{aligned}
 & + \sum_{h_\beta=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\beta+h_\gamma+n} (i\hbar)^{h_\beta+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\beta)^{h_\beta}}{h_\beta!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{h_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi \\
 & + \sum_{h_\alpha=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+h_\gamma+n} (i\hbar)^{h_\alpha+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{h_\alpha!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{h_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi \\
 & + \sum_{h_\alpha=1}^{\infty} \sum_{h_\beta=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+h_\beta+h_\gamma+n} (i\hbar)^{h_\alpha+h_\beta+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{h_\alpha!} \frac{(\mathbb{B}_\beta)^{h_\beta}}{h_\beta!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{h_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi.
 \end{aligned} \tag{3.14}$$

The formulae (3.10) and (3.11) are the second principal result of this work. They are exact in the sense that no approximations have been made by neglecting terms. The arguments leading up to these however are purely formal and this expression for the propagator is typically asymptotic. For many purposes, such as semiclassical expansions, the asymptotic nature of the cluster expansion suffices. For example, consider the small \hbar behaviour. This behaviour has been studied in detail [13] for representations of the propagator based upon the kinetic-energy propagator. The leading order behaviour of the argument of the exponential appearing in the propagator is $O(\hbar^{-1})$ and this term is associated with the tree graphs. The WKB expansion follows as a natural consequence of this leading order behaviour and the propagator in the limit $\hbar \rightarrow 0$ has the asymptotic behaviour

$$K(t, s, x, y) \sim \left[\frac{m}{2\pi\hbar|\Delta t|} \right]^{d/2} e^{-i(\pi/4)\text{sign}(\Delta t g)} e^{(i/\hbar)S(t,s,x,y)+O(\hbar^0)}. \tag{3.15}$$

The function $S(t, s, x, y)$ is the classical action. Structurally the \hbar dependence of the harmonic-oscillator-based formula for the propagator is similar to the kinetic-energy-based formula. From (3.11) one can read off the lowest order \hbar contribution which occurs when $r(E) = \ell - 1$ and $n = 0$. The tree graphs and setting each $h_\alpha = 1$ correspond to having $r(E) = \ell - 1$. In the limit $\hbar \rightarrow 0$ the propagator for the harmonic-oscillator-based formula behaves as

$$K(t, s, x, y) \sim \left[\frac{m\omega}{2\pi\hbar \sin(\omega\Delta t)} \right]^{d/2} e^{-i(\pi/4)\text{sign}(g)} e^{(i/\hbar)\tilde{S}(t,s,x,y)+O(\hbar^0)}. \tag{3.16}$$

The function $\tilde{S}(t, s, x, y)$ is

$$\tilde{S}(t, s, x, y) = \frac{m\omega}{2} [x \cdot x + y \cdot y] \cot(\omega\Delta t) - 2x \cdot y \text{cosec}(\omega\Delta t) + \tilde{T}(t, s, x, y) \tag{3.17}$$

and the function \tilde{T} is

$$\tilde{T}(t, s, x, y) = \sum_{\ell=1}^{\infty} \sum_{C \in \mathcal{T}_\ell} \frac{(-\Delta t)^\ell}{\ell!} \int_{I^\ell} \left[\prod_{\alpha \in E} \mathbb{B}_\alpha \right] v(z_c(\xi_1^0); \xi_1^0) \dots v(z_c(\xi_\ell^0); \xi_\ell^0) d^\ell \xi. \tag{3.18}$$

$$\begin{aligned}
 & + \sum_{h_\beta=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\beta+h_\gamma+n} (i\hbar)^{h_\beta+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\beta)^{h_\beta}}{\hbar_\beta!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{\hbar_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi \\
 & + \sum_{h_\alpha=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+h_\gamma+n} (i\hbar)^{h_\alpha+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{\hbar_\alpha!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{\hbar_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi \\
 & + \sum_{h_\alpha=1}^{\infty} \sum_{h_\beta=1}^{\infty} \sum_{h_\gamma=1}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{h_\alpha+h_\beta+h_\gamma+n} (i\hbar)^{h_\alpha+h_\beta+h_\gamma+n-3} (\Delta t)^3}{2^n 3! n!} \\
 & \times \int_{I^3} \frac{(\mathbb{B}_\alpha)^{h_\alpha}}{\hbar_\alpha!} \frac{(\mathbb{B}_\beta)^{h_\beta}}{\hbar_\beta!} \frac{(\mathbb{B}_\gamma)^{h_\gamma}}{\hbar_\gamma!} (\mathbb{A}_3)^n v(z_c(\xi_1^0); \xi_1^0) v(z_c(\xi_2^0); \xi_2^0) v(z_c(\xi_3^0); \xi_3^0) d^3\xi.
 \end{aligned} \tag{3.14}$$

The formulae (3.10) and (3.11) are the second principal result of this work. They are exact in the sense that no approximations have been made by neglecting terms. The arguments leading up to these however are purely formal and this expression for the propagator is typically asymptotic. For many purposes, such as semiclassical expansions, the asymptotic nature of the cluster expansion suffices. For example, consider the small \hbar behaviour. This behaviour has been studied in detail [13] for representations of the propagator based upon the kinetic-energy propagator. The leading order behaviour of the argument of the exponential appearing in the propagator is $O(\hbar^{-1})$ and this term is associated with the tree graphs. The WKB expansion follows as a natural consequence of this leading order behaviour and the propagator in the limit $\hbar \rightarrow 0$ has the asymptotic behaviour

$$K(t, s, x, y) \sim \left[\frac{m}{2\pi\hbar|\Delta t|} \right]^{d/2} e^{-i(\pi/4)\text{sign}(\Delta t g)} e^{(i/\hbar)S(t,s,x,y)+O(\hbar^0)}. \tag{3.15}$$

The function $S(t, s, x, y)$ is the classical action. Structurally the \hbar dependence of the harmonic-oscillator-based formula for the propagator is similar to the kinetic-energy-based formula. From (3.11) one can read off the lowest order \hbar contribution which occurs when $r(E) = \ell - 1$ and $n = 0$. The tree graphs and setting each $h_\alpha = 1$ correspond to having $r(E) = \ell - 1$. In the limit $\hbar \rightarrow 0$ the propagator for the harmonic-oscillator-based formula behaves as

$$K(t, s, x, y) \sim \left[\frac{m\omega}{2\pi\hbar \sin(\omega\Delta t)} \right]^{d/2} e^{-i(\pi/4)\text{sign}(g)} e^{(i/\hbar)\tilde{S}(t,s,x,y)+O(\hbar^0)}. \tag{3.16}$$

The function $\tilde{S}(t, s, x, y)$ is

$$\tilde{S}(t, s, x, y) = \frac{m\omega}{2} ([x \cdot x + y \cdot y] \cot(\omega\Delta t) - 2x \cdot y \text{cosec}(\omega\Delta t)) + \tilde{T}(t, s, x, y) \tag{3.17}$$

and the function \tilde{T} is

$$\tilde{T}(t, s, x, y) = \sum_{\ell=1}^{\infty} \sum_{C \in \mathcal{T}_\ell} \frac{(-\Delta t)^\ell}{\ell!} \int_{I^\ell} \left[\prod_{\alpha \in E} \mathbb{B}_\alpha \right] v(z_c(\xi_1^0); \xi_1^0) \dots v(z_c(\xi_\ell^0); \xi_\ell^0) d^\ell \xi. \tag{3.18}$$

Here the set $\mathcal{T}_{\bar{\ell}}$ is the set of all tree graphs formed from the index set $\bar{\ell}$. The details behind the expansion (3.17) remain to be investigated. It is likely that \bar{S} is indeed the classical action for the anharmonic-oscillator and the higher-order terms may be obtained as they have been done for the kinetic-energy-based propagator formula.

Mizrahi [14] has studied the WKB expansion of the quantum propagator for the one-dimensional oscillator perturbed by the anharmonic potential $\lambda x^4/4$, obtaining an expansion in the form

$$K(t, s, x, y) = \left(\frac{M(t, s, x, y)}{2\pi i\hbar} \right)^{1/2} e^{i(\hbar)S(t, s, x, y)} \{1 + \hbar K_1(t, s, x, y) + \hbar^2 K_2(t, s, x, y) + \dots\}. \quad (3.19)$$

Here $M(t, s, x, y)$ is the Van Vleck–Morette function, and the coefficient functions K_j are expressed in terms of path integrals. (The exponentiated \hbar series (3.16) may readily be arranged into the form of (3.19) by use of the cumulant formulas.) In deriving (3.19) Mizrahi utilizes exact expressions for the classical trajectories of the anharmonic-oscillator to find formulae for the Green function and propagator. By contrast, in the present work where the anharmonic potential $v(x, \hat{p}; t)$ is left arbitrary, these trajectories and Green functions cannot be written in closed form. Instead it is the classical trajectory and Green function of the harmonic-oscillator which arise.

4. Concluding remarks

The Dyson series representation (2.40) for the configuration function represents the first principal result of this article. It has the advantage over the connected graph expansion of being applicable to a broader class of potentials. For example, potentials with spin degrees of freedom are admissible to the Dyson series representation [15, 16] but not to the connected graph representation. They fail for the latter because these potentials do not commute with themselves in general. The commutative property was crucial for reorganizing the Dyson series into the connected graph series.

There is some overlap between the Dyson series and the semiclassical expansion techniques developed by Langouche *et al* [17–19]. Those authors describe the full propagator $K(t, s, x, y)$ with a phase-space functional integral and then carry out asymptotic expansions of the integral with respect to small deviations about the classical trajectory. The higher-order coefficients to their expansion may be described with one of the Green functions of the Jacobi operator for the associated classical problem.

The cluster expansion (3.10)–(3.11) of the configuration function is the second principal result of this article. In the sense that there have been no terms which have been neglected, this formula for F is exact. The derivation has been formal in that no conditions have been specified on the potentials to guarantee convergence of the series involved. The Dyson series itself is often only asymptotic and hence the connected-graph representation would be, at best, asymptotic. For the class of potentials consisting of Fourier transforms of complex measures of compact support it has been shown [15, 16, 20] that the Dyson series representation of the propagator converges pointwise for sufficiently small times or large mass. Nevertheless the corresponding connected-graph expansion was asymptotic.

In other applications a coupling constant expansion may be obtained from the cluster expansion by replacing the potential by $v \rightarrow \lambda v$. By inspection $L_\ell = O(\lambda^\ell)$ and the cluster representation for the configuration function is an exponentiated series in the coupling

constant λ . This could be used to develop non-perturbative expansions of the propagator. These expansions would be non-perturbative in the sense that any given term would have all powers of the coupling constant because the coupling constant is part of the argument of an exponential.

Although the Dyson series was key to obtaining the connected-graph expansion of the propagator there exist other avenues by which graphical methods may be utilized. Equation (3.10) has been obtained through a combination of the cluster methods with quantum transport equations [21]. The transport equation method is sufficiently general for applications of graph theory to transport equations outside of quantum mechanics. A functional integral method has been developed by Roekaerts *et al* [22–24] for studying exponentiated series expansions of the imaginary time propagator (heat kernel). However, the graphs they utilize are more complicated than clusters and their coefficients are not expressed in closed form.

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References

- [1] Molzahn F H and Osborn T A 1987 *J. Phys. A: Math. Gen.* **20** 3073
- [2] Barvinsky A O and Osborn T A 1992 A Phase-space technique for the perturbation expansion of Schrödinger propagators *Preprint* University of Manitoba MANIT-92-01
- [3] Papiez L, Osborn T A and Molzahn F H 1988 *J. Math. Phys.* **29** 642
- [4] Molzahn F H and Osborn T A 1994 A phase space fluctuation method for quantum dynamics *Ann. Phys., NY* in press
- [5] Schwinger J 1951 *Phys. Rev.* **82** 664
- [6] DeWitt B S 1965 *Dynamical Theory of Groups and Fields* (New York: Gordon and Breach)
- [7] DeWitt B S 1975 *Phys. Rep.* **19** 295
- [8] Simon B 1979 *Functional Integration and Quantum Physics* (New York: Academic)
- [9] Dyson F J 1949 *Phys. Rev.* **75** 1736
- [10] Pathria R K 1984 *Statistical Mechanics* (Oxford: Pergamon) ch 9
- [11] Choquet-Bruhat Y, DeWitt-Morette C and Dillard-Bleick M 1977 *Analysis, Manifolds and Physics* (Amsterdam: North-Holland)
- [12] Wilson R J 1975 *Introduction to Graph Theory* (New York: Academic) ch 2
- [13] Molzahn F H and Osborn T A 1986 *J. Math. Phys.* **27** 88
- [14] Mizrahi M M 1979 *J. Math. Phys.* **20** 844
- [15] Osborn T A, Corns R A and Fujiwara Y 1985 *J. Math. Phys.* **26** 453
- [16] Corns R A and Osborn T A 1990 *J. Math. Phys.* **31** 901
- [17] Langouche F, Roekaerts D and Tirapegui E 1982 *Functional Integration and Semiclassical Expansions* (Dordrecht: Reidel)
- [18] Langouche F, Roekaerts D and Tirapegui E 1981 *Phys. Rev. D* **23** 1290
- [19] Langouche F, Roekaerts D and Tirapegui E 1981 *Nuovo Cimento* **64** 357
- [20] Osborn T A, Papiez L and Corns R 1987 *J. Math. Phys.* **28** 103
- [21] Molzahn F H 1992 *J. Phys. A: Math. Gen.* **25** 4913
- [22] Tirapegui E, Langouche F and Roekaerts D 1983 *Phys. Rev. A* **27** 2649
- [23] Bollé D and Roekaerts D 1984 *Phys. Rev. A* **30** 2024
- [24] Bollé D and Roekaerts D 1986 *Phys. Rev. A* **31** 1667; 1986 *Phys. Rev. D* **33** 1427(E)