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Exponential cluster solutions to quantum transport equations

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Abstract. Connected graph methods are used to solve the transport equation arising in a semiclassical representation of the Schrödinger propagator $K(t,s,x,y)$. For a spinless quantum system whose Hamiltonian is a smooth position- and momentum-dependent perturbation of the Laplacian in $\mathbb{R}^d$, exponential cluster expansions for K are obtained. These formally exact solutions to the time-dependent Schrödinger equation employ explicit graphically-determined derivatives of the Hamiltonian's symbol, integrated along geodesics. For the special case of particles interacting with external electromagnetic fields, the propagator's gauge invariant derivative expansion coefficients are determined in closed form in terms of the Lorentz force. A tree graph formula for Hamilton's principal function is extracted from this result.

1. Introduction

In this paper, exponential connected graph representations of the quantum propagator $K(t,s,x,y)$ are obtained for Hamiltonians containing an arbitrary position- and momentum-dependent potential term. This includes the case of systems interacting with time-dependent external electromagnetic fields, and extends previous results [1–3] which assumed only position-dependent potentials $v(x,t)$. A new method of derivation is employed, which directly integrates the transport equation [4, 5] obtained after a suitable leading-order approximation for K has been factored out. The results efficiently provide explicit formulae for the coefficients of non-perturbative formal asymptotic propagator expansions.

The specific type of quantum transport equation to be studied has the form

$$\frac{\partial F}{\partial t}(t,x)+\frac{x-y}{t-s}\cdot\nabla_x F(t,x)=\frac{1}{\mathrm{i}\hbar}\tilde{H}\left(t,x,\frac{\hbar}{\mathrm{i}}\nabla_x\right)F(t,x) \qquad (1.1)$$

for which a smooth solution $F:\mathbb{R}\times\mathbb{R}^d\to\mathbb{C}$ is sought, subject to a suitable initial condition. The quantity $\tilde{H}(t,x,(\hbar/\mathrm{i})\nabla_x)$ represents an arbitrary linear partial differential operator, $2\pi\hbar$ is Planck's constant, and $s\in\mathbb{R}$, $y\in\mathbb{R}^d$ appear as parameters.

Transport equations of the form (1.1) can arise in quantum mechanics in the following basic way. Let $U(t,s)$ be the unitary operator-valued solution of the Schrödinger initial value problem

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t,s)=H(t)U(t,s) \qquad (1.2a)$$

$$U(s,s)=\mathrm{Id} \qquad (1.2b)$$

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describing quantum time evolution in the Hilbert space $L^2(\mathbb{R}^d)$. Let $K(t,s,x,y) \equiv \langle x|U(t,s)|y\rangle$ denote the integral kernel of $U(t,s)$ which is also called the propagator. For a wide variety of quantum systems, the physical Hamiltonian operator $H(t)$ arises in the form

$$H(t) = H_0 + V(t) \qquad H_0 = -\tfrac{1}{2}\epsilon\hbar^2\Box. \tag{1.3}$$

The 'free Hamiltonian' H_0 is some constant multiple of the Laplace–Beltrami operator $\Box$ on (flat) $\mathbb{R}^d$, while $V(t)$ is a possibly t-dependent 'perturbation'.

When the Hamiltonian has the decomposition (1.3), one natural option is to seek a corresponding factored form for the propagator:

$$K(t,s,x,y) = K_0(t,s,x,y)F(t,s,x,y). \tag{1.4}$$

Here K_0 represents the free propagator corresponding to H_0. Since K_0 has a well-known closed form (see (3.5*b*)), the quantity of interest then becomes the so-called 'configuration function' $F(t,s,x,y)$. If (1.4) is substituted into (1.2*a*) one finds that a transport equation of the type (1.1) is obeyed by F. The operator $\tilde{H}$ in (1.1) will be called the 'ersatz Hamiltonian'; it is generally different from the physical Hamiltonian $H(t)$. An initial condition for F is similarly induced from (1.2*b*). The initial time s and configuration y, upon which F depends parametrically, are seen to originate in the Cauchy initial condition for Schrödinger's equation.

If the right-hand side of (1.1) were not to contain derivatives of F, then (1.1) would appear as a first-order quasi-linear partial differential equation (PDE). An elementary technique—the method of characteristics [6, 7]—is available to solve such a PDE. This method maintains much usefulness for transport equation (1.1) because, upon introduction of the characteristic curves

$$t(\tau) = \tau \qquad x(\tau) = y + (\tau - s)\frac{x-y}{t-s} \tag{1.5}$$

the left-hand side of (1.1) assumes the form of the total derivative $\mathrm{d}F(\tau, x(\tau)\mathrm{d}\tau$. After integration from s to t an integro-differential equation is obtained for F,

$$F(t,x) = F(s,y) + \frac{1}{\mathrm{i}\hbar}\int_s^t \mathrm{d}\tau\, \tilde{H}\left(\tau, x(\tau), \frac{\hbar}{\mathrm{i}}\nabla\right) F(\tau, x(\tau)). \tag{1.6}$$

In section 2, the formal iterative solution of (1.6) is carried out in full. It should be emphasized that the solution thus obtained is not simply an infinite series of time-ordered N-dimensional integrals, with integrands containing N factors of $\tilde{H}$. Such a result, while correct, would be a perturbative expansion in $\tilde{H}$ that is difficult to compute with in general and of limited practical value. The analysis to be presented is carried well beyond that stage. It is shown that the configuration function F admits an exponential representation

$$F(t,s,x,y) = \exp\left\{\sum_{j=1}^{\infty} L_j(t,s,x,y)\right\} \tag{1.7}$$

in which the coefficient functions $L_j(t,s,x,y)$ are determined in closed form by a summation over simple connected graphs (clusters) on j vertices. Each summand is a parametric integral of derivatives of a product of j symbols of the operator $\tilde{H}$. This symbol $\tilde{H}(t,x,p)$ is a function of both the configuration x and a momentum variable p, and the graph-determined derivative structure employs differentiation with respect to both of these 'classical phase space' variables.

These results are valid for an ersatz Hamiltonian of a general form. In section 3, as a first application, they are specialized to the case of a quantum system with external electromagnetic fields, i.e. interactions described by arbitrary smooth time-dependent vector and scalar potentials, $a(x,t)$ and $v(x,t)$. In this case it is possible to base the calculation upon a gauge-invariant transport equation, which results when the propagator's $\mathrm{U}(1)$ gauge dependence is factored out in addition to the free propagator.

The result is a gauge-covariant exponential cluster expansion for the propagator. This extends to systems with electromagnetic fields; there are kindred results in the literature [1–3] that deal only with scalar potentials. Somewhat remarkably, the results for the general problem, as presented in section 3, are in many ways structurally simpler and more convenient than previous cluster expansions. One of these features is whether the L_j are automatically the coefficients of a gauge invariant derivative expansion [8, 9]. Furthermore, since the metric for $\mathbb{R}^d$ defining $\Box$ may have an indefinite signature, the results also apply to the Schwinger–DeWitt equation [10–12] of special-relativistic scalar field theory.

A second application of the cluster method for transport equations is made in section 4. There, Hamiltonians of the form (1.3) are considered for a general perturbing operator $V(t)$. Corresponding to the propagator factorization (1.4), the ersatz Hamiltonian $\tilde{H}$ retains terms arising both from H_0 and $V(t)$. It is shown that the cluster expansion can be 'resummed' by computing explicitly all the effects of the H_0-originating part of $\tilde{H}$. The result is again an exponentiated expansion like (1.7), but with the coefficients L_j now defined using products of the symbol of perturbation $V(t)$. The derivative structure associated with the clusters is modified by the resummation. This result not only provides a *non-perturbative (infinite order in $V(t)$)* cluster expansion, but also proves consistency of the present methods with the recent results of Barvinsky and Osborn [13].

Conclusions, comparison with the literature, and remarks concerning possible generalizations of this work, and its expected range of utility, are collected in section 5. The appendix proves a general integrand-symmetry theorem, which plays an essential role in deriving the exponential representation (1.7), as well as a useful role in simplifying the formulae for the coefficients L_j.

The detailed calculations in this paper are 'exact' in the sense that no approximation, such as neglecting certain terms, occurs. However, no attempt is made to justify the results in a mathematically rigorous fashion. It is assumed the formal series expansions are at least asymptotic, with validity for sufficiently short time displacements. They are intended to reveal the analytic and combinatorial structure present in the propagator. Different methods [14, 15] from those employed here would be needed to determine rigorous asymptotic error bounds and domains of validity.

2. Cluster method for a general transport equation

In this section a relatively generic transport equation is analysed. An exponential cluster representation is derived for the equation's solution. This result provides the basis for the more specific applications which will follow in sections 3 and 4. Accordingly, only interpretive remarks of a more general nature will be made about the cluster solution here.

Consider the linear transport PDE

$$\partial F(t,s,x,y) + \frac{x-y}{t-s} \cdot \nabla F = \frac{1}{\mathrm{i}\hbar} \tilde{H}\left(t,s,x,y,\frac{\hbar}{\mathrm{i}}\nabla\right) F \qquad (2.1a)$$

for the smooth function $F(\cdot,s,\cdot,y) : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$, which is subject to the initial condition

$$F(s,s,y,y) = 1 \qquad (2.1b)$$

for some fixed initial time $s \in \mathbb{R}$ and coordinate $y \in \mathbb{R}^d$, upon which F depends parametrically. In (2.1a) ∂F is the partial derivative of F with respect to its first scalar ('time') argument, and similarly ∇ denotes differentiation of F with respect to its first $\mathbb{R}^d$-vector ('spatial') argument. The ersatz Hamiltonian $\tilde{H}$ in (2.1a) is allowed to be a general formal partial differential operator,

$$\tilde{H}\left(t,s,x,y,\frac{\hbar}{\mathrm{i}}\nabla\right) = \sum_{\alpha\in\mathbb{W}^d} a_\alpha(t,s,x,y)\left(\frac{\hbar}{\mathrm{i}}\nabla\right)^\alpha \qquad (2.2a)$$

where $\mathbb{W}^d$ is the usual space of d-component multi-indices ($\mathbb{W}$ denotes the non-negative integers). Our derivations will assume that the complex coefficients $a_\alpha(t,s,x,y)$ are smooth functions of x. In (2.2a) $\tilde{H}$ is, for convenience and without loss of generality, assumed to be written in 'normal-ordered' form. That is, all gradient operators stand to the right of the x-dependence in a_α. Associated with this form of presenting $\tilde{H}$ is its symbol [16]

$$\tilde{H}(t,s,x,y,p) \equiv \sum_{\alpha\in\mathbb{W}^d} a_\alpha(t,s,x,y)p^\alpha \qquad (2.2b)$$

a function of the phase space variables $(x,p) \in \mathbb{R}^d \times (\mathbb{R}^d)^*$, the * indicating the dual space. In (2.2) the multi-index summation need not be finite: the powers p^α may be replaced by (suitably analytic) functions of p, whereby $\tilde{H}$ becomes a pseudodifferential operator. In what follows, however, the partial differential operator notation will be employed because this provides the most succinct way of expressing the results.

The method of formal solution for transport problem (2.1), which results in an exponential cluster formula for F, has a number of basic stages. First, a variable substitution based on the method of characteristics is employed to turn (2.1a) into an ODE, which integrates into an integral equation for F. This integral equation is then iterated to produce an infinite series of time-ordered integrals. By introducing appropriately symmetric integrands, the time-ordering restrictions may be removed. In this form the series can be exponentiated by graph-combinatorial techniques which yield the desired cluster expansion.

Proceeding now with the first of these steps, introduce the characteristic curve $q : \mathbb{R} \to \mathbb{R}^d$,

$$q(\tau) = q(\tau;Q) \equiv y + (\tau - s)\frac{x-y}{t-s}. \qquad (2.3)$$

Here Q is an abbreviation for the standard argument list (t, s, x, y). Evidently q is the linear path running from y to x during the time interval $[s, t]$,

$$q(s) = y \qquad q(t) = x \tag{2.4}$$

with constant velocity $\dot{q}(\tau) = (x - y)/(t - s)$. Accordingly, if throughout (2.1*a*) t is replaced with τ and subsequently x with $q(\tau)$, one obtains the ODE along q:

$$\frac{\mathrm{d}}{\mathrm{d}\tau} F(\tau, s, q(\tau), y) = \frac{1}{\mathrm{i}\hbar} \tilde{H} \left(\tau, s, q(\tau), y, \frac{\hbar}{\mathrm{i}} \nabla\right) F(\tau, s, q(\tau), y).$$

Integration of this equation, subject to (2.1*b*) and observing (2.4), results in the basic integral equation (1.6) obeyed by F. It is useful to display this equation after the integration variable $\tau \in [s, t]$ has been scaled to the unit interval by the variable change $\tau = \xi^0 \equiv s + \xi\Delta t$, where $\Delta t \equiv t - s$ and $\xi \in [0, 1]$. The integral equation then reads

$$F(Q) = 1 + \frac{\Delta t}{\mathrm{i}\hbar} \int_0^1 \mathrm{d}\xi \tilde{H} \left(\xi^0, s, \gamma\xi, y, \frac{\hbar}{\mathrm{i}} \nabla\right) F(\xi^0, s, \gamma\xi, y). \tag{2.5}$$

Here $\gamma\xi$ denotes the unit-interval parametrized geodesic from y to x in $\mathbb{R}^d$ which arises from (2.3),

$$\gamma\xi \equiv \gamma(\xi; x, y) \equiv q(\xi^0) = y + \xi(x - y). \tag{2.6}$$

Observe that $\xi^0 = \gamma(\xi; t, s)$, in $\mathbb{R}^1$.

The next stage of derivation, in which (2.5) is iterated, is perhaps the most delicate, and novel, stage. It is crucial to keep a careful account of where the derivatives ∇ in (2.5) act after successive iterations are performed. As is evident from (2.5), a formula representing an arbitrary spatial derivative of F, evaluated on the spacetime geodesic path $(\xi^0, \gamma\xi)$, is required. Begin by computing such a derivative at (t, x), by differentiating (2.5) with respect to x. For any multi-index $\alpha \in \mathbb{W}^d$ one has

$$\nabla^\alpha F(Q) = \delta_{\alpha,0} + \frac{\Delta t}{\mathrm{i}\hbar} \int_0^1 \mathrm{d}\lambda \nabla_x^\alpha \left\{ \tilde{H} \left(\lambda^0, s, \gamma\lambda, y, \frac{\hbar}{\mathrm{i}} \nabla\right) F(\lambda^0, s, \gamma\lambda, y) \right\}$$

where $\delta_{\alpha,0}$ is the Kronecker delta. Notice that the x-dependence of the $\{\cdots\}$ integrand here arises only through $\gamma(\lambda; x, y)$, given as in (2.6).

Let D be the differential operator acting on the first spatial argument of $\tilde{H}$, just as ∇ does on F. Then the chain and product rules imply

$$\nabla^\alpha F(Q) = \delta_{\alpha,0} + \frac{\Delta t}{\mathrm{i}\hbar} \int_0^1 \mathrm{d}\lambda \lambda^{|\alpha|} (D + \nabla)^\alpha \tilde{H} \left(\lambda^0, s, \gamma\lambda, y, \frac{\hbar}{\mathrm{i}} \nabla\right) F(\lambda^0, s, \gamma\lambda, y). \tag{2.7}$$

The required formula is obtained once (2.7) is evaluated on the geodesic by replacing $t \to \xi^0$ and $x \to \gamma\xi$. In doing this, the following geodesic composition laws are used

$$\gamma\lambda\Big|_{x=\gamma\xi} = \gamma(\lambda; \gamma\xi, y) = \gamma(\lambda\xi; x, y) = \gamma(\lambda\xi) \qquad \lambda^0\Big|_{t=\xi^0} = (\lambda\xi)^0.$$

They follow at once from (2.6). Also note that the Δt factor outside the integral in (2.7) becomes replaced by $\xi\Delta t$. A final change of integration variable from λ to $\beta = \lambda\xi$ results in

$$\nabla^\alpha F(\xi^0, s, \gamma\xi, y) = \delta_{\alpha,0} + \frac{\Delta t}{\mathrm{i}\hbar}\int_0^\xi \mathrm{d}\beta \left(\frac{\beta}{\xi}\right)^{|\alpha|} (D+\nabla)^\alpha \times \tilde{H}\left(\beta^0, s, \gamma\beta, y, \frac{\hbar}{\mathrm{i}}\nabla\right) F(\beta^0, s, \gamma\beta, y). \tag{2.8}$$

Let us iterate once by inserting (2.8) into (2.5). In doing so it is convenient to introduce the abbreviations $[\xi] = (\xi^0, s, \gamma\xi, y)$ and $[\xi, p] = ([\xi], p)$ for the geodesic-evaluated argument lists which occur. The first iterate of (2.5) in this notation is then

$$F(Q) = 1 + \frac{\Delta t}{\mathrm{i}\hbar}\int_0^d \xi \tilde{H}[\xi, 0] + \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^2 \int_0^1 \mathrm{d}\xi_1 \int_0^{\xi_1} \mathrm{d}\xi_2 \times \tilde{H}\left[\xi_1, \frac{\hbar}{\mathrm{i}}\frac{\xi_2}{\xi_1}(D_2+\nabla)\right] \tilde{H}\left[\xi_2, \frac{\hbar}{\mathrm{i}}\nabla\right] F[\xi_2]. \tag{2.9}$$

Notice how the part of the iteration which replaces F with the constant 1 eliminates the derivative in $\tilde{H}$, as in the single-integral term. In the double-integral term of (2.9), the subscript 2 on D_2 indicates that this gradient acts only on $\tilde{H}({\xi^0}_2, s, \cdot, y, (\hbar/\mathrm{i}))$.

The pattern of computation needed to obtain an arbitrary iterate emerges if one considers replacing $F[\xi_2]$ in (2.9) by using (2.8) again. Then the double-integral term of (2.9) splits into two new terms. The first is again the double-integral term with F set to 1 and hence both ∇ set to 0. The second new term is the ordered triple-integral

$$\left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^3 \int_0^1 \mathrm{d}\xi_1 \int_0^{\xi_1} \mathrm{d}\xi_2 \int_0^{\xi_2} \mathrm{d}\xi_3 \tilde{H}\left[\xi_1, \frac{\hbar}{\mathrm{i}}\frac{\xi_2}{\xi_1}\left(D_2 + \frac{\xi_3}{\xi_2}(D_3+\nabla)\right)\right] \times \tilde{H}\left[\xi_2, \frac{\hbar}{\mathrm{i}}\frac{\xi_3}{\xi_2}(D_3+\nabla)\right] \tilde{H}\left[\xi_3, \frac{\hbar}{\mathrm{i}}\nabla\right] F[\xi_3].$$

It arises after the ∇ operators appearing in (2.9) are replaced by $(\xi_3/\xi_2)(D_3+\nabla)$ due to (2.8). Notice, in the $\tilde{H}[\xi_1, \cdot]$ symbol, how the ξ_2 factors multiplying D_3 cancel; this kind of behaviour will be seen later to be critical in allowing the cluster method to work.

It should now be evident how an arbitrary iterate is formed. In stating this general result, it is helpful to use the following notation for the N-dimensional hyper-triangular domains which form the time-ordered integration regions,

$$Q_N^{>} \equiv \{\xi \in [0,1]^N | 1 \geqslant \xi_1 \geqslant \xi_2 \geqslant \cdots \geqslant \xi_N \geqslant 0\}. \tag{2.10}$$

The infinite series obtained by repeated iteration of (2.5) as described above is then

$$F(Q) = \sum_{N=0}^\infty \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \int_{Q_N^{>}} \mathrm{d}\xi \prod_{j=1}^N \tilde{H}\left[\xi_j, \frac{\hbar}{\mathrm{i}} \sum_{l=j+1}^N \frac{\xi_l}{\xi_j} D_l\right]. \tag{2.11}$$

Here the product is implicitly ordered so that factors appear from left to right with increasing index $j = 1, 2, \ldots, N$. The gradient D_l acts on the lth factor

$\tilde{H}(\xi^0{}_l, s, \cdot, y, p)$ only. The $N = 0$ term in (2.11) is defined to be 1, and similarly in the $j = N$ factor, one takes $\sum_{l=N+1}^{N} \equiv 0$. While the discussion leading to (2.11) has relied on inspecting the first few iterates, an inductive argument can be used to establish the same result.

In order to continue with the formal analysis of (2.11), assume that the symbol $\tilde{H}$ is an entire function of p admitting a (global) Taylor series representation in the form

$$\tilde{H}(Q,p) = \mathrm{e}^{p\cdot\hat{D}}\tilde{H}(Q,0)$$

where $\hat{D}$ is the gradient on the momentum argument, $[\hat{D}\tilde{H}](Q,p) = \nabla_p \tilde{H}(Q,p)$. If similarly $\hat{D}_j$ is the momentum gradient acting on the factor $\tilde{H}[\xi_j, \cdot]$ in (2.11), then this Taylor 'shift' formula allows all the differential operators to be gathered into an exponential factor, away from the symbols upon which they act,

$$F(Q) = \sum_{N=0}^{\infty}\left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \int_{Q_N^>} \mathrm{d}\xi \exp\left\{\frac{\hbar}{\mathrm{i}}\sum_{j=1}^{N-1}\sum_{l=j+1}^{N}\frac{\xi_l}{\xi_j} D_l\cdot\hat{D}_j\right\}\prod_{k=1}^{N}\tilde{H}[\xi_k, 0]. \qquad (2.12)$$

Notice that the ξ-dependent function ξ_l/ξ_j which 'couples' the operator D_l to $\hat{D}_j$ only depends on those indices, l and j. This is a consequence of the type of cancellation observed for ξ_2 earlier. Also, the fact that D_l does not couple to $\hat{D}_l$ (i.e. spatial derivatives do not act on their own symbol in (2.11)) is a consequence of choosing to write the ersatz Hamiltonian in normal-ordered form at the outset in (2.2*a*).

The final preparatory step that remains to be taken with (2.12) is to convert the ordered ξ-integral into a simple iterated integral over the unit N-cube. This is facilitated by introducing an appropriate symmetrized extension of the integrand. To this end, notice that the derivative coupling $(\xi_l/\xi_j)D_l\cdot\hat{D}_j$ only occurs with $j < l$. But since $\xi \in Q_N^>$, the inequality $j < l$ implies $\xi_j \geqslant \xi_l$. Thus, for almost all $\xi \in Q_N^>$, one may substitute

$$\begin{aligned}\frac{\xi_l}{\xi_j}D_l\cdot\hat{D}_j &= \Theta(j<l)\frac{\xi_l}{\xi_j}D_l\cdot\hat{D}_j + \Theta(j>l)\frac{\xi_j}{\xi_l}D_j\cdot\hat{D}_l \\ &= \Theta(\xi_j>\xi_l)\frac{\xi_l}{\xi_j}D_l\cdot\hat{D}_j + \Theta(\xi_l>\xi_j)\frac{\xi_j}{\xi_l}D_j\cdot\hat{D}_l \\ &\equiv S_{j,l}(\xi). \end{aligned} \qquad (2.13)$$

Here $\Theta(P)$ is the Heaviside function with value 1 if the proposition P is true, and value 0 if P is false. The 'link operator' $S_{j,l}(\xi)$, defined by (2.13) for all $j, l = 1, 2, \ldots, N$ and $\xi \in [0,1]^N$, is a symmetric function of j, l which vanishes when $j = l$,

$$S_{j,l}(\xi) = S_{l,j}(\xi) \qquad S_{j,j}(\xi) = 0. \qquad (2.14)$$

When (2.13) is used within the integrand of (2.12), it may be shown (see the appendix) that the resulting integrand is a symmetric function of $\xi \in I^N$, $I \equiv [0,1]$.

Consequently, the ξ integration may be carried out over all of I^N with a compensating factor of $1/N!$. The final 'pre-cluster' form of the result is therefore

$$F(Q) = \sum_{N=0}^{\infty} \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \frac{1}{N!} \int_{I^N} \mathrm{d}^N\xi \left[\prod_{1\leqslant j<l\leqslant N} \exp\left(\frac{\hbar}{\mathrm{i}} S_{j,l}(\xi)\right)\right] \prod_{k=1}^{N} \tilde{H}[\xi_k, 0]. \tag{2.15}$$

In the form presented by (2.15), the representation of F is now ready for standard cluster exponentiation methods to be applied. A careful exposition of this method is found in section 3 of [2]; also, compare (2.15) above with (2.11)–(2.14) of that reference. The structure of (2.15) is similar to that found in the cluster expansion of the classical grand partition function in statistical mechanics [17]. The product $\prod_{j<l}$ is analogous to a product of $\mathrm{e}^{-v_{jl}/kT}$ over pairs (j,l) of particles interacting via potential v_{jl}. The interval I plays the role of the configuration space for each statistical particle. Thus, (2.15) may be restructured by a graph combinatorial argument parallel to that given in [2]. The result is an exponential representation,

$$F(Q) = \exp\left\{\sum_{j=1}^{\infty} L_j(Q)\right\} \tag{2.16}$$

in which the coefficient functions L_j are determined by a graphical summation as follows.

Let $\mathcal{C}_j$ denote the set of all simple connected graphs [18] (or 'clusters') which may be formed on the vertex set $\overline{\jmath} \equiv \{1, 2, \ldots, j\}$. Thus $C \in \mathcal{C}_j$ means $C = (\overline{\jmath}, E)$, where the edge set E of C consists of distinct unordered pairs β of distinct integers in $\overline{\jmath}$, linking a connected graph. Define a graphical summation by

$$\sum_{\mathcal{G}_j} \equiv \sum_{C\in\mathcal{C}_j} \left(\prod_{\beta\in E} \sum_{l_\beta=1}^{\infty}\right) \tag{2.17}$$

that is a sum over all j-vertex clusters accompanied by a sum over a link integer $l_\beta \geqslant 1$ for each edge $\beta \in E$. Let r denote the sum of the link integers: $r = \sum_{\beta\in E} l_\beta$ (or $r = 0$ if $E = \varnothing$). The sums $\sum_{l_\beta\geqslant 1}$ in (2.17) originate in a power series representation of the quantity $-1 + \exp((\hbar/\mathrm{i}) S_\beta(\xi))$, where the link operator $S_{k,l}(\xi)$ associated with a link $\beta = \{k, l\}$ is denoted $S_\beta(\xi)$ (unambiguously so, due to the symmetry (2.14)). With this notation, the cluster sum formula for coefficient L_j is

$$L_j(Q) = \sum_{\mathcal{G}_j} \Delta t^j \hbar^{r-j} \mathrm{i}^{-r-j} \frac{1}{j!} \int_{I^j} \mathrm{d}^j\xi \left(\prod_{\beta\in E} (l_\beta!)^{-1} S_\beta(\xi)^{l_\beta}\right) \prod_{k=1}^{j} \tilde{H}[\xi_k, 0]. \tag{2.18}$$

It is possible to make one further practical simplification to (2.18). If the cluster sum $\sum_{\mathcal{G}}$ is taken inside the ξ integral then one can show (again see the appendix) that the resulting integrand is a symmetric function of ξ. Hence the integral may be recast into ordered form; i.e. (2.18) is valid with, for example, the replacement

$$\frac{1}{j!} \int_{I^j} \mathrm{d}^j\xi \to \int_{Q_j^>} \mathrm{d}^j\xi. \tag{2.19}$$

Such a form is more suitable for actual L_j coefficient calculation, because in an ordered region such as $Q_j^>$ the selection of maximum and minimum components of ξ is trivial and so the formula (2.13) for $S_\beta(\xi)$ reduces to a single term.

The exponential cluster representation (2.16)–(2.18) of the solution to the transport problem (2.1) is the main result of this section. It provides an exact formal expression for F in terms of parametric integrals, along geodesics, of the symbol $\tilde{H}$ and its derivatives. The symbols represent vertices of connected graphs, whose edges carry simple differential operators coupling pairs of symbols. Notice that the graphs describing this derivative structure contain no loops, i.e. link operators of the form $S_{j,j}(\xi)$ do not appear. This feature at first appears remarkably simple, because previous graphical propagator expansions [1–3] have always contained such loop contributions. In section 4 it will be seen how these two varieties of graph expansion are indeed consistent.

3. Gauge-covariant electromagnetic propagator

This section applies the results of section 2 to the specific case of the Schrödinger time evolution kernel (propagator) of a quantum system with electromagnetic fields. The cluster representation for this problem is found to have a number of beneficial features, which are discussed in detail. These features include: (i) the ability to represent the expansion coefficients in manifestly gauge-invariant form; (ii) a significant simplification in the graphical summation—caused in part by collapse of the infinite link integer sums to their first two terms; and (iii) the automatic organization of expansion (2.16) as a gauge-invariant derivative [8, 9] expansion. Explicit formulae for the first two coefficients L_1 and L_2 are considered. By examining the $\hbar$-dependence of the propagator and its WKB representation, a new tree graph formula for Hamilton's principal function with electromagnetic fields is extracted.

The quantum mechanical system to be studied here consists of spinless particles with a (collective) configuration space $\mathbb{R}^d$ having coordinate x. The particles' interaction with external electromagnetic and other forces is described by time-dependent covector and scalar fields $a(x,t)$ and $v(x,t)$. It is supposed $\mathbb{R}^d$ is supplied with a flat semi-Riemannian metric tensor, whose components in the given coordinates are g_{ij}. Thus $\mathbf{g} = [g_{ij}]$ is a symmetric x-independent non-singular $d \times d$ real matrix. Its inverse is denoted by $\mathbf{g}^{-1} = [g^{ij}]$, as is customary. The quantum evolution is governed by the time-dependent Schrödinger equation (cf (1.2a))

$$\mathrm{i}\hbar\frac{\partial}{\partial t}K(t,s,x,y) = H\left(t,x,\frac{\hbar}{\mathrm{i}}\nabla\right)K \tag{3.1}$$

where the physical Hamiltonian is the partial differential operator

$$H\left(t,x,\frac{\hbar}{\mathrm{i}}\nabla\right) = \frac{\epsilon}{2}\left\langle\frac{\hbar}{\mathrm{i}}\nabla - a(x,t)\right\rangle^2 + v(x,t) \tag{3.2}$$

dependent upon a scaling parameter $\epsilon > 0$. The angle-bracket notation $\langle,\rangle$ and $\langle\ \rangle^2$ will be used to denote scalar products involving either the metric matrix or its inverse. Thus for vectors $u, v \in \mathbb{R}^d$, $\langle uv\rangle \equiv u \cdot \mathbf{g}v = u^i g_{ij} v^j$, while for covectors $\omega, \lambda \in (\mathbb{R}^d)^*$ the notation means $\langle\omega\lambda\rangle \equiv \omega \cdot \mathbf{g}^{-1}\lambda = \omega_i g^{ij}\lambda_j$. The square $\langle\ \rangle^2$

is used for either inner product when both arguments are the same. In (3.2) for example, $((\hbar/\mathrm{i})\nabla - a)^2 = ((\hbar/\mathrm{i}\nabla) - a)\cdot \mathbf{g}^{-1}(\hbar/\mathrm{i}\nabla - a)$.

The quantum system (3.1)–(3.2) actually encompasses two very different spheres of physical application. In the first case, the metric is strictly Riemannian (positive definite)—typically $\mathbf{g}$ is the unit matrix. Then the Schrödinger equation (3.1) describes non-relativistic particles of common mass ϵ^{-1} subject to external electromagnetic fields. In the second application, the metric is indefinite, for example Minkowskian. Then (3.1) becomes the hyperbolic Schwinger–DeWitt equation [10–12] for a special-relativistic scalar field if one chooses a and v to be t-independent and $\epsilon = 2$. In this second case, t is a non-physical evolution parameter called the 'proper time' (the physical time is absorbed into x), and all electromagnetic effects are confined to the 4-vector potential $a(x)$. The treatment to follow will not distinguish between these two fields of application, although the language used will tend to be that appropriate to the non-relativistic case.

For the Schrödinger equation (3.1), let us seek to compute the fundamental solution (the propagator) defined by imposing the delta-function initial condition (cf (1.2*b*))

$$\lim_{t\to s} K(t,s,x,y) = \left|\det \mathbf{g}\right|^{-1/2}\delta(x-y) \qquad y\in\mathbb{R}^d \tag{3.3}$$

at some fixed time $s \in \mathbb{R}$. (The $\mathbf{g}$-dependent normalization in (3.3) is that appropriate in the L^2 Hilbert space defined by the natural volume measure $\mathrm{d}V = \left|\det\mathbf{g}\right|^{1/2}\mathrm{d}^d x$ of the semi-Riemannian manifold $\prec \mathbb{R}^d, \mathbf{g} \succ$.) In particular, we shall find a gauge-covariant representation for K which is a semiclassical asymptotic expansion as $\epsilon \downarrow 0$.

Recall the well-known $\mathrm{U}(1)$ gauge behaviour of the propagator. If $\Lambda : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ is the generator of a gauge transformation to new potentials $\bar a = a + \nabla\Lambda$, $\bar v = v - \partial\Lambda$, then the propagator $\bar K$ for the gauge-transformed Schrödinger equation is related to the original K by

$$\bar K(t,s,x,y) = \mathrm{e}^{-\Lambda(x,t)/\mathrm{i}\hbar} K(t,s,x,y)\mathrm{e}^{\Lambda(y,s)/\mathrm{i}\hbar}. \tag{3.4}$$

An ansatz for K which explicitly incorporates both the initial condition (3.3) and the gauge behaviour (3.4) is the factorization

$$K = K_0 \mathrm{e}^{J/\mathrm{i}\hbar} T \tag{3.5a}$$

where K_0 is the propagator for the free Hamiltonian $\frac{1}{2}\epsilon((\hbar/\mathrm{i})\nabla)^2 = -\frac{1}{2}\epsilon\hbar^2\Box$,

$$K_0(Q) \equiv \left|2\pi\epsilon\hbar\Delta t\right|^{-d/2} \exp(-\mathrm{i}(\pi/4)\mathrm{sign}(\Delta t\,\mathbf{g}) \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{\langle x-y\rangle^2}{2\epsilon\Delta t}\right\} \tag{3.5b}$$

and the gauge-phase function J is defined by the following path average of the potential fields

$$J(Q) \equiv \int_0^1 \mathrm{d}\xi[\Delta t v(\gamma\xi,\xi^0) - (x-y)\cdot a(\gamma\xi,\xi^0)] \tag{3.5c}$$

along the geodesic $\gamma(\xi; x, y)$ of (2.6). In (3.5*b*), the sign denotes the signature of a matrix (the number of positive minus the number of negative eigenvalues).

The salient features of the three factors in (3.5a) are as follows. The function K_0 is obviously gauge-invariant, and obeys the delta-function condition (3.3) on its own. The gauge factor $e^{J/i\hbar}$ has the value 1 when $t = s$ and $x = y$, and as a simple calculation shows, it completely provides the gauge behaviour (3.4) of the propagator. Therefore the residual factor T should (i) be gauge-invariant and (ii) satisfy the initial condition

$$T(s, s, y, y) = 1. \tag{3.6}$$

Function T is the quantity of interest, since it contains most of the information about the quantum effects of the physical forces acting.

It is the function T which (in the role of F) satisfies a transport equation of the type (2.1a). Thus (3.6) corresponds to (2.1b). The specific form of the transport equation obeyed by T is found by substituting (3.5a) into the Schrödinger equation (3.1). In this computation, a number of terms cancel, in part due to the transport PDE which J obeys

$$\partial J(Q) + \frac{x-y}{t-s} \cdot \nabla J = v(x,t) - \frac{1}{\Delta t}(x-y) \cdot a(x,t).$$

(For a proof of this identity, see lemma 2 of [8].) The consequent transport equation thus found to hold for T is

$$\partial T(Q) + \frac{x-y}{t-s} \cdot \nabla T = \frac{\epsilon}{i\hbar}\left(\frac{1}{2}\left\langle \frac{\hbar}{i}\nabla\right\rangle^2 - \left\langle A(Q), \frac{\hbar}{i}\nabla\right\rangle + \frac{1}{2}\left[\langle A^2\rangle + i\hbar\langle \nabla, A\rangle\right]\right) T. \tag{3.7}$$

The coefficient function $A(Q)$ appearing on the right-hand side of (3.7) is the gauge-invariant covector

$$A(Q) \equiv a(x,t) + \nabla J(Q) = -\Delta t \int_0^1 d\xi\, \xi \Omega(\xi) \tag{3.8}$$

where Ω is the classical Lorentz force

$$\Omega_j(\xi) = \Omega_j(\xi; Q) \equiv E_j(\gamma\xi, \xi^0) + F_{jk}(\gamma\xi, \xi^0)\frac{(x-y)^k}{\Delta t} \tag{3.9a}$$

expressed in terms of the 'electric' and 'magnetic' fields

$$E = -\nabla v - \partial a \qquad F_{jk} = \nabla_j a_k - \nabla_k a_j. \tag{3.9b}$$

The last equality in (3.8) follows by differentiating (3.5c) with respect to x and integrating one of the terms by parts. One might regard (3.7) as a gauge-invariant version of the Schrödinger equation in which free motion has also been factored out. T, like K, is not an element of Hilbert space.

The residual function T is determined as the solution to the transport problem (3.6)–(3.7), which is stated only with reference to gauge-invariant quantities. This implies the anticipated gauge-invariance of T. Clearly, the transport equation (3.7) takes on the form (2.1a) if the following ersatz Hamiltonian symbol is employed

$$\tilde{H}_{\hbar,\epsilon}(Q,p) \equiv \epsilon\left(\tfrac{1}{2}\langle p\rangle^2 - \langle A(Q), p\rangle + \tfrac{1}{2}[\langle A\rangle^2 + i\hbar\langle\nabla, A\rangle]\right). \tag{3.10}$$

This symbol has contributions arising from both the free Hamiltonian and from the potentials.

With this identification of $\tilde{H}$, the results (2.18)–(2.19) may be applied at once. In doing so, it is useful to extract the overall ϵ factor in $\tilde{H}$. That is, the fact that $\tilde{H}_{\hbar,\epsilon} = \epsilon \tilde{H}_{\hbar,1}$ and that L_j scales like j factors of $\tilde{H}$ leads to the exponential cluster representation for T:

$$T(Q) = \exp\left\{\sum_{j=1}^{\infty} L_j(Q)\right\} \tag{3.11a}$$

$$L_j(Q) = (\epsilon\Delta t)^j \sum_{\mathcal{G}_j} \frac{\hbar^{r-j}}{\mathrm{i}^{r+j}} \int_{Q_j^>} \mathrm{d}^j\xi \prod_{\beta\in E} (l_\beta!)^{-1} S_\beta(\xi)^{l_\beta} \prod_{k=1}^{j} \tilde{H}_{\hbar,1}[\xi_k, 0]. \tag{3.11b}$$

Combined with (3.5), equation (3.11) provides a gauge-covariant cluster expansion for the propagator of a quantum system with arbitrary smooth vector and scalar potentials. In a sense, this is the central result of this section, although its properties will be examined closely in what follows.

Notice that all the ϵ-dependence of L_j resides in the explicit factor ϵ^j, because the link operators S_β and the symbols $\tilde{H}_{\hbar,1}$ are ϵ-independent. (By contrast, $\tilde{H}_{\hbar,1}$ will generally contain further $\hbar$ and Δt dependence.) This means that (3.11*a*) is an exponentiated $\epsilon \downarrow 0$ formal asymptotic expansion. In the non-relativistic context, this is the large-mass limit responsible for the Wigner–Kirkwood semiclassical expansion [19, 20]. This type of propagator expansion has been studied in [20], and generalized to curved semi-Riemannian manifolds in [9]. However these references relied on recursive techniques for computing the ϵ^j coefficient functions. While such recursive techniques do have a wide range of applicability, nevertheless, within the flat-space setting considered here formula (3.11*b*) clearly is a more powerful closed-form solution, which provides each L_j without reference to previous coefficients.

In continuing to examine the properties of (3.11*b*), it is relevant to make a number of general observations concerning simplification and specialization of the graph structure. The cluster sum $\sum_{\mathcal{G}_j}$ in (3.11*b*) explicitly involves (cf (2.17)) summation over all simple connected graphs on j vertices. However, due to the special forms of the symbol $\tilde{H}_{\hbar,1}$ and link operator S_β, it will be seen that many of the terms in $\sum_{\mathcal{G}_j}$ actually do not contribute.

Clearly each symbol $\tilde{H}_{\hbar,1}[\xi_k, 0]$ is formally associated with a labelled vertex: k Because of the ordered integration region $Q_j^>$ chosen in (3.11*b*), the link operators in (2.13) reduce to a single term

$$S_\beta(\xi) = \frac{\xi_{\vee\beta}}{\xi_{\wedge\beta}} D_{\vee\beta} \cdot \widehat{D}_{\wedge\beta} \qquad \xi \in Q_j^>. \tag{3.12}$$

Here $\wedge\beta$ and $\vee\beta$ denote the minimum and maximum elements, respectively, of the unordered pair (edge) β. The formal expression on the right-hand side of (3.12) is not a symmetric function of $(\wedge\beta, \vee\beta)$. It should therefore be associated with a *directed edge*, or *arc*, denoted by $\longrightarrow$. Let us agree that the arrowed end of the arc represents the momentum gradient $\widehat{D}_{\wedge\beta}$, while the unadorned end of the arc represents the spatial gradient $D_{\vee\beta}$. Thus, arcs will always point from a vertex with larger label to one with smaller label, e.g.

$$2 \longrightarrow 1 \tag{3.13}$$

It is therefore seen that a *directed graph*, or *digraph* [18, 21], structure will be naturally imposed on top of each cluster.

Turn now to the implications of formula (3.10) for symbol $\tilde{H}_{\hbar,1}$ in the electromagnetic case. Evidently $\tilde{H}_{\hbar,1}$ is a quadratic function of p, whose leading term $\frac{1}{2}\langle p\rangle^2$ is free of x-dependence. Moreover, as formula (3.11*b*) shows, after all appropriate derivatives of the symbol are computed, variable p is set to 0. Consequently, each vertex (symbol) in a digraph supports *at most two* momentum gradients. One can distinguish vertices on this basis: a vertex k is said to be of type-n ($n \geqslant 0$) if its momentum-incidence is n, i.e. if exactly n of the edges β incident to k satisfy $\wedge\beta = k$. Figure 1 shows a digraph with three vertices of type-0 (no. 3, 5, 6), and single vertices of type-1 (no. 4), type-2 (no. 2) and type-3 (no. 1). The contribution of this digraph to L_6 will be 0 because of vertex no. 1.

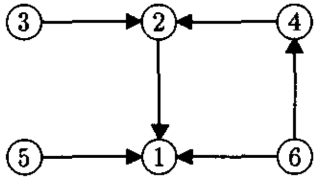

Figure 1. A simple digraph.

More specifically, the algebraic content of the various vertex types is as follows.

Type-0. Since a cluster is connected, type-0 vertices represent at least one spatial (D) derivative of $\frac{1}{2}[\langle A\rangle^2 + \mathrm{i}\hbar\langle\nabla, A\rangle]$ whenever there are edges (i.e. $j \geqslant 2$).

Type-1. These vertices support any number (including 0) of spatial derivatives of $-\mathbf{g}^{-1}A$.

Type-2. These vertices contribute only if they are *not* struck by spatial derivatives, because $\frac{1}{2}\langle p\rangle^2$ is x-independent. In this case, a type-2 vertex just leads to an inner product (metric contraction) of the spatial derivatives associated with the two vertices to which it is adjacent (cf figure 2).

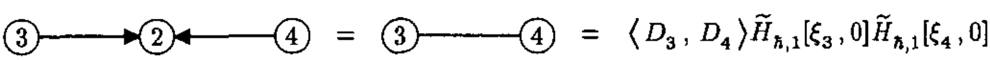

Figure 2. Contraction of a non-zero type-2 vertex.

Type-$n \geqslant 3$. Any digraph containing this type of vertex is ignorable in the sense that it contributes 0. As figure 1 shows, this type of vertex can occur after the edges of the underlying cluster are directed.

A very significant simplification is implied by these observations. Recall that the cluster sum $\sum_{\mathcal{G}_j}$ also entails infinite sums over a link integer $l_\beta \geqslant 1$ for each edge β in a cluster. The effects of these integers are confined to the expressions (cf (3.11*b*), (3.12))

$$\frac{1}{l_\beta!}\left(\frac{\xi_{\vee\beta}}{\xi_{\wedge\beta}} D_{\vee\beta} \cdot \widehat{D}_{\wedge\beta}\right)^{l_\beta}$$

which may be interpreted as yielding digraphs with multiple arcs from $\vee\beta$ to $\wedge\beta$. In this sense, if $l_\beta \geqslant 3$ vertex $\wedge\beta$ will be at least of type-3 and so that term will contribute 0. Thus each infinite link integer sum collapses to a finite sum, $\sum_{l_\beta=1}^{2}$. Moreover, the $l_\beta = 2$ contributions are trivial since vertex $\wedge\beta$ is then at least of type-2 (it could be of higher type due to edges other than β). It follows that formula (3.11*b*) for $L_j(Q)$ involves only a *finite* number of terms.

This discussion outlines the general restrictions and simplifications which are observed when computing the ϵ-expansion coefficients L_j. A brief illustrative example is to obtain explicit formulae for the first two coefficients.

For $j = 1$, the only cluster on one vertex is the trivial one with an empty edge set. Thus (3.11*b*) gives

$$L_1(Q) = \frac{\epsilon\Delta t}{\mathrm{i}\hbar}\int_0^1 \mathrm{d}\xi\,\tilde{H}_{\hbar,1}[\xi,0] = \frac{\epsilon\Delta t}{2}\int_0^1 \mathrm{d}\xi\left(\frac{1}{\mathrm{i}\hbar}\langle A\rangle^2 + \langle\nabla, A\rangle\right)[\xi]. \tag{3.14}$$

When $j = 2$ there is only one cluster; the associated digraph is the one displayed in (3.13). If $l \equiv l_{\{1,2\}}$ is the link integer, then from (3.11*b*)

$$L_2(Q) = (\epsilon\Delta t)^2\sum_{l=1}^{2}\frac{\hbar^{l-2}}{\mathrm{i}^{l+2}}\int_0^1 \mathrm{d}\xi_1\int_0^{\xi_1}\mathrm{d}\xi_2\frac{1}{l!}\left(\frac{\xi_2}{\xi_1}D_2\cdot\widehat{D}_1\right)^l\tilde{H}_{\hbar,1}[\xi_1,0]\tilde{H}_{\hbar,1}[\xi_2,0].$$

The required derivatives of $\tilde{H}_{\hbar,1}$ are readily computed from (3.10), and the resulting formula for L_2 is

$$\begin{aligned}L_2(Q) = (\epsilon\Delta t)^2\int_0^1 \mathrm{d}\xi\int_0^{\xi}\mathrm{d}\lambda\,&\left\{\frac{\lambda}{\xi}\frac{1}{\mathrm{i}\hbar}A^j[\lambda]\nabla^k A_j[\lambda]A_k[\xi] + \frac{\mathrm{i}\hbar\lambda^2}{4\xi^2}\Box\langle\nabla, A\rangle[\lambda]\right.\\ &\left.+\frac{\lambda}{2\xi}\langle A[\xi],\nabla\rangle\langle\nabla, A\rangle[\lambda] + \frac{1}{2}\frac{\lambda^2}{\xi^2}(\nabla^j A^k[\lambda]\nabla_j A_k[\lambda] + \langle A, \Box A\rangle[\lambda])\right\}.\end{aligned} \tag{3.15}$$

Formulae (3.14)–(3.15) express L_1 and L_2 in terms of the non-local gauge-invariant covector potential A, which is, in turn, a weighted integral average, (3.8), of the Lorentz force. If the appropriate derivatives of (3.8) are substituted into these formulae it is possible to simplify them further by explicitly performing some of the iterated integrals. The resulting expressions will not be displayed here because they may be found in [20], where they were computed recursively. The general structure which emerges is that each ϵ^j coefficient is a finite sum in ascending powers of $\hbar$,

$$\epsilon^{-j}L_j(Q) = \sum_{l=0}^{j}(\mathrm{i}\hbar)^{l-1}G_l^j(Q). \tag{3.16}$$

The author has verified that the G_l^1 and G_l^2 computed from (3.14)–(3.15) are in complete agreement with the corresponding formulae in section IV of [20]. This provides a good check on the present graphical method.

Another observation worth making concerns the behaviour of (3.11) for the free problem, where a and v, hence A, are all 0. In this case one must find that each

$L_j = 0$ so that $T = 1$. The way that this happens, however, is not entirely trivial because $\tilde{H} = \langle p \rangle^2/2 \neq 0$ when $A = 0$. If $j \geqslant 2$, at least one vertex (namely j) in each cluster will always be struck by a spatial gradient, implying $L_j = 0$. For $j = 1$ there are no arcs to carry a D, but (3.11b) requires setting $p = 0$ in $\tilde{H}$, so $L_1 = 0$ too.

As a final application of the cluster representation (3.11), a formula for Hamilton's principal function $S(t, s, x, y)$ will be extracted from it. This is done by comparing the cluster expansion with the WKB approximation [5, 22-24] of the quantum propagator. The short-time WKB ($\hbar \downarrow 0$) ansatz is

$$K(Q) \sim \left|2\pi\epsilon\hbar\Delta t\right|^{-d/2} \exp(-\mathrm{i}\tfrac{1}{4}\pi\,\mathrm{sign}\,(\Delta t\,\mathbf{g}))\exp\left\{\frac{\mathrm{i}}{\hbar}S(Q) + \mathcal{O}(\hbar^0)\right\} \tag{3.17}$$

where the principal function, or 'action', S is defined as the integral of the Lagrangian along the (assumed unique) classical interacting path from y, s to x, t.

Comparing (3.14) with (3.5) and (3.11) suggests that S should equal minus the coefficient of $(\mathrm{i}\hbar)^{-1}$ in the exponentiated part of the propagator. Thus the action has a free portion $\langle x - y \rangle^2/2\epsilon\Delta t$, a gauge-dependent term $-J(Q)$, and finally an infinite series of contributions coming from each L_j, specifically $-\epsilon^j G_0^j(Q)$ in the notation of (3.16).

Formulae (3.10) and (3.11b) make it easy to identify the latter contributions. Since a connected graph on j vertices must have at least $j-1$ links β, and each link integer $l_\beta \geqslant 1$, thus the sum of link integers $r \geqslant j - 1$. But $\tilde{H}_{\hbar,1}$ is a linear polynomial in $\hbar$, so (3.11b) implies that $\hbar^{-1}$ can only occur if $r = j - 1$. This happens if and only if: the cluster is a tree (minimally connected) graph, all $l_\beta = 1$, and $\hbar$ is set to 0 in the symbol. The consequent constructive series for the action is

$$S(Q) = \frac{\langle x - y \rangle^2}{2\epsilon\Delta t} - J(Q) + \sum_{j=1}^{\infty} \sum_{T \in \mathcal{T}_j} (-\epsilon\Delta t)^j \int_{Q_j^>} \mathrm{d}^j\xi \prod_{\beta \in E} S_\beta(\xi) \prod_{k=1}^{j} \tilde{H}_{0,1}[\xi_k, 0] \tag{3.18}$$

where $\mathcal{T}_j$ is the set of all tree graphs $T = (\daleth, E)$.

Of course the WKB comparison argument above only guarantees that (3.18) is a plausible conjecture. It remains to establish that the resulting series converges under suitable hypotheses, that it is a complete integral [25] of the Hamilton–Jacobi equation, etc. This more complete analysis is outside the present scope, but it should be mentioned that the validity of tree graph series for actions of systems with scalar potentials $v(x, t)$ have been rigorously established [26, 27].

4. A resummation of the expansion

A more general quantum system than the electromagnetic one is considered in this section. For a Hamiltonian which is an arbitrary perturbation of a Laplace–Beltrami operator in $\mathbb{R}^d$, the transport equation for the ratio, F, of the interacting and free propagators is found. While the results of section 2 could then be applied at once, instead, an alternative cluster expansion for F is derived here by summing all the contributions of the free Hamiltonian. This alternative expansion is in agreement with the recent results of Barvinsky and Osborn [13].

Let the physical Hamiltonian be decomposed into the free-plus-perturbative form (1.3). For definiteness, suppose that the perturbing operator has been presented in normal-ordered form,

$$[V(t)\psi](x) = v\left(t, x, \frac{\hbar}{\mathrm{i}}\nabla\right)\psi(x) \tag{4.1}$$

with the corresponding symbol

$$v(t,x,p) = \int_{\mathbb{R}^d} \mathrm{d}^d a\, \tilde{v}(t,x,a)\exp((\mathrm{i}/\hbar)a\cdot p). \tag{4.2}$$

Here a Fourier representation has been employed, instead of a summation of multi-indexed powers of p, for future convenience.

Consider the propagator factorization (1.4) with K_0 again given by (3.5*b*). (Note that, for the problem at hand without gauge fields, a factorization like (3.5*a*) is not appropriate. Similarly the symbol $v(t,x,p)$ should not be confused with the scalar potential $v(x,t)$ of section 3.) The first goal is to derive the transport equation obeyed by configuration function F. In particular the normal-ordered symbol of the ersatz Hamiltonian must be determined. The analogous step in section 3 was much easier. Because of the simple quadratic nature of Hamiltonian (3.2), the normal ordering could be carried out 'by hand'.

If the ansatz (1.4) is substituted into the Schrödinger PDE (3.11), (4.1) and the indicated derivatives are computed, one arrives at the following transport equation for $F(t,s,x,y)$,

$$\partial F(Q) + \frac{x-y}{t-s}\cdot\nabla F = \frac{1}{\mathrm{i}\hbar}\left[\frac{\epsilon}{2}\left\langle\frac{\hbar}{\mathrm{i}}\nabla\right\rangle^2 + K_0(Q)^{-1}v\left(t,x,\frac{\hbar}{\mathrm{i}}\nabla\right)K_0(Q)\right]F. \tag{4.3}$$

Equation (4.3) is not yet in a form to which the results of section 2 are immediately applicable, because the operator on the right-hand side is not in normal-ordered form. Specifically, there is x-dependence in $K_0(Q)$ to the right of gradients in v (which act on K_0 and F).

However, it is possible to 'pull K_0 through' to the left of v using an appropriate operator identity. By employing the explicit formula (3.5*b*) for K_0 one computes the following commutation rule: for $\alpha \in \mathbb{W}^d$ and any smooth F

$$\left(\frac{\hbar}{\mathrm{i}}\nabla\right)^\alpha (K_0 F) = K_0\left(\frac{\mathbf{g}(x-y)}{\epsilon\Delta t} + \frac{\hbar}{\mathrm{i}}\nabla\right)^\alpha F. \tag{4.4}$$

The $|\alpha|$ individual factors comprising $(\cdots)^\alpha$ on the right-hand side may be written in any order—just as they may for ∇^α on the left-hand side. Note that the components of ∇ may act on the xs in any $\mathbf{g}(x-y)$ term to their right, as well as on F. Thus, (4.4) is still not normal-ordered, but it does allow expressing the $K_0^{-1}vK_0$ operator in (4.3) as

$$v\left(t,x,\frac{\mathbf{g}(x-y)}{\epsilon\Delta t} + \frac{\hbar}{\mathrm{i}}\nabla\right) = \int \mathrm{d}^d a\,\tilde{v}(t,x,a)\exp\left\{a\cdot\left(\frac{\mathrm{i}}{\hbar}\frac{\mathbf{g}(x-y)}{\epsilon\Delta t} + \nabla\right)\right\} \tag{4.5}$$

where (4.2) was used. It is now a simple matter to normal-order (4.5) by using the basic Baker–Campbell–Hausdorff formula [28]

$$e^{A+B} = e^{-[A,B]/2} e^A e^B \tag{4.6}$$

in which $A \equiv (\mathrm{i}/\hbar\epsilon\Delta t) a \cdot \mathbf{g}(x-y)$ and $B \equiv a \cdot \nabla$, and the commutator is a multiple of the identity: $[A, B] = (\mathrm{i}\hbar\epsilon\Delta t)^{-1}\langle a\rangle^2$. Thus the normal-ordered form of (4.5) is

$$v\left(t, x, \frac{\mathbf{g}(x-y)}{\epsilon\Delta t} + \frac{\hbar}{\mathrm{i}}\nabla\right) = w\left(t, s, x, y, \frac{\hbar}{\mathrm{i}}\nabla\right) \tag{4.7}$$

where w has the symbol

$$\begin{aligned} w(Q,p) &= \int \mathrm{d}^d a\, \tilde{v}(t,x,a) \exp\left[\frac{\mathrm{i}}{\hbar}\frac{\langle a\rangle^2}{2\epsilon\Delta t}\right] \exp\left\{\frac{\mathrm{i}}{\hbar} a \cdot \left(p + \frac{\mathbf{g}(x-y)}{\epsilon\Delta t}\right)\right\} \\ &= \exp\left[\frac{\hbar}{\mathrm{i}}\frac{1}{2\epsilon\Delta t}\langle\widehat{D}\rangle^2\right] v\left(t, x, p + \frac{\mathbf{g}(x-y)}{\epsilon\Delta t}\right). \end{aligned} \tag{4.8}$$

Once again, $\widehat{D}$ acts on the second vector argument of v. Formula (4.8) shows that the symbol w which expresses $K_0^{-1} v K_0$ in normal-ordered syntax is, in general, a complicated derivative of the original symbol v, has two sources of x- and t-dependence, and depends upon the other parameters $\hbar, \epsilon, y, s$ coming from K_0.

With (4.8) the transport problem for F has been brought to the standard form (2.1), with the ersatz Hamiltonian

$$\tilde{H}(Q,p) = K(p) + w(Q,p) \tag{4.9a}$$

$$K(p) \equiv \tfrac{1}{2}\epsilon\langle p\rangle^2. \tag{4.9b}$$

Note that now $\tilde{H}$ is not simply proportional to ϵ, as it was in the gauge-invariant electromagnetic application of section 3.

If the results of section 2 were applied to this transport problem, an exponentiated cluster solution relative to $\tilde{H}$ would result. Our objective here, however, will be to effect the resummation of all contributions arising from $K(p)$ in (4.9), to obtain the cluster solution relative to perturbation w (or, via (4.8), relative to v). It is very natural, from a computational perspective, to seek such a resummation. For, as was seen in section 3, the effects of the $\frac{1}{2}\epsilon\langle p\rangle^2$ terms are trivial in that for vertices of type-2 they give a contraction of spatial gradients associated with adjacent vertices, cf figure 2. (If the ϵ-expansion for the electromagnetic case is the desired expansion, then a resummation should not be carried out.)

A convenient starting point for the resummation calculation is the following slight modification of (2.15).

$$F(Q) = \sum_{N=0}^{\infty} \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \frac{1}{N!} \int_{I^N} \mathrm{d}^N\xi \left[\prod_{j=1}^{N}\prod_{l=1}^{N} \exp\left(\frac{\hbar}{2\mathrm{i}} S_{j,l}(\xi)\right)\right] \prod_{k=1}^{N} \tilde{H}[\xi_k, 0]. \tag{4.10}$$

Here the double product has been taken over the unrestricted square $\bar{N} \times \bar{N}$ with the aid of (2.14). The $[\cdots]$ operator in (4.10) may be expressed as the exponential of a double sum. If (2.13) is substituted and this sum is indexed so that each $\widehat{D}$ has subscript k, then one finds

$$[\cdots] = \exp\left[\sum_{k=1}^{N}\left\{\frac{\hbar}{\mathrm{i}}\sum_{l=1}^{N}\Theta(\xi_k > \xi_l)\frac{\xi_l}{\xi_k}D_l\right\}\cdot\widehat{D}_k\right]. \tag{4.11}$$

The critical step is now to split the momentum gradient $\widehat{D}$ up into a term $\widehat{D}^{(k)}$ which acts on the 'kinetic' portion $K(p)$ of (4.9), plus a term $\widehat{D}^{(w)}$ which acts on $w(Q,p)$. Thus

$$\widehat{D}_k = \widehat{D}_k^{(k)} + \widehat{D}_k^{(w)} \qquad k \in \bar{N} = \{1, 2, \ldots, N\}. \tag{4.12}$$

Conceptually, decomposition (4.12) is a natural extension of the idea behind the operators D_k and $\widehat{D}_k$: $\widehat{D}^{(k)}$ and $\widehat{D}^{(w)}$ are differential operators acting only on specific arguments of an appropriate multi-variable function.

When (4.9*a*) is substituted into (4.10) the product of symbols $\tilde{H}$ can be grouped into 'powers' of the perturbation w as follows

$$\prod_{k\in\bar{N}}\tilde{H}[\xi_k, 0] = \sum_{J\subset\bar{N}}\left\{\prod_{k\in J}K_k(0)\right\}\prod_{j\in J^c}w[\xi_j, 0]. \tag{4.13}$$

Here $\sum_{J\subset\bar{N}}$ is the sum over all 2^N subsets J of $\bar{N}$, including $\emptyset$ and $\bar{N}$. The complement of J is $J^c = \bar{N}\setminus J$. $K_k(0)$ is the kinetic function (4.9*b*) originating in $\tilde{H}[\xi_k, 0]$. Of course $K_k(0)$ should not be replaced by 0 since K_k is first struck by derivatives $\widehat{D}_k^{(k)}$. Specifically if (4.11)–(4.12) are also now substituted into (4.10) then the $\widehat{D}_k^{(k)}$ part of (4.11) acts as a Taylor-shift taking the argument of K_k from 0 to the $\{\cdots\}$ of (4.11). The result of these substitutions and observations is

$$\begin{aligned}F(Q) = \sum_{N=0}^{\infty}\left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N\frac{1}{N!}\int_{I^N}\mathrm{d}^N\xi\sum_{J\subset\bar{N}}\exp\left[\frac{\hbar}{\mathrm{i}}\sum_{k\in\bar{N}}\sum_{l\in\bar{N}}\Theta(\xi_k > \xi_l)\frac{\xi_l}{\xi_k}D_l\cdot\widehat{D}_k^{(w)}\right]\\ \times\left\{\prod_{k\in J}K_k\left(\frac{\hbar}{\mathrm{i}}\sum_{l\in\bar{N}}\Theta(\xi_k > \xi_l)\frac{\xi_l}{\xi_k}D_l\right)\right\}\prod_{j\in J^c}w[\xi_j, 0].\end{aligned} \tag{4.14}$$

A number of simplifications of (4.14) are now possible. Note that D_l and $\widehat{D}_k^{(w)}$ can only act on $w[\xi_j, 0]$ where $j \in J^c$. Thus the corresponding sums over l and k in $\bar{N}$ may be restricted to J^c. Once that is done, it is seen that the N-dimensional integral in (4.14) can be 'factored' into two integrals, over the components of ξ indexed by J and J^c. The integral over ξ_J must be done inside the ξ_{J^c} integration:

$$\begin{aligned}&\int_{I^{|J|}}\mathrm{d}\xi_J\prod_{k\in J}K\left(\frac{\hbar}{\mathrm{i}}\sum_{l\in J^c}\Theta(\xi_k > \xi_l)\frac{\xi_l}{\xi_k}D_l\right)\\ &\quad = \prod_{k\in J}\int_0^1\mathrm{d}\xi_k\frac{-\epsilon\hbar^2}{2}\sum_{l,l'\in J^c}\Theta(\xi_k > \xi_l)\Theta(\xi_k > \xi_{l'})\frac{\xi_l\xi_{l'}}{\xi_k^{\,2}}\langle D_l, D_{l'}\rangle\\ &\quad = \left(\frac{\epsilon\hbar^2}{2}\sum_{l,l'\in J^c}G(\xi_l, \xi_{l'})\langle D_l, D_{l'}\rangle\right)^{|J|}\end{aligned} \tag{4.15}$$

where $|J|$ is the cardinality of J, and G is the one-dimensional fixed endpoint Green function defined by

$$G(\xi,\xi') \equiv \min\{\xi,\xi'\}(\max\{\xi,\xi'\}-1). \tag{4.16}$$

The result of these manipulations of (4.14) (together with relabelling of the remaining integration variables ξ_{J^c} as $\xi_{\bar{n}}$, $n \equiv N - |J|$) is

$$F(Q) = \sum_{N=0}^{\infty} \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \frac{1}{N!} \sum_{J\subset \bar{N}} \int_{I^n} \mathrm{d}^n\xi \exp\left[\frac{\hbar}{\mathrm{i}} \sum_{k,l\in\bar{n}} \Theta(\xi_k > \xi_l)\frac{\xi_l}{\xi_k} D_l \cdot \widehat{D}_k\right]$$
$$\times \left(\frac{\epsilon\hbar^2}{2} \sum_{l,l'\in J^c} G(\xi_l,\xi_{l'})(D_l, D_{l'})\right)^{N-n} \prod_{j\in\bar{n}} w[\xi_j, 0]. \tag{4.17}$$

Here the superscript $^{(w)}$ on $\widehat{D}_k$ has been dropped; $\widehat{D}_k$ is now the new momentum derivative which acts on $w(Q,\cdot)$.

The next stage of calculation is to complete the exponentiation of the Green function dependent operator which appears under way in (4.17). To this end note that the sum over subsets J can be organized as

$$\sum_{J\subset\bar{N}} = \sum_{n=0}^{N} \sum_{|J|=N-n} .$$

Obviously each term with a given n in (4.17) is identical. Thus the sum over J with $|J| = N - n$ may be replaced by the number of terms in that sum, which is $\binom{N}{n}$. Upon interchanging the remaining sums over N and n in (4.17) and manipulating the summand straightforwardly, the previously mentioned exponentiation is found to occur. The result is

$$F(Q) = \sum_{N=0}^{\infty} \left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \frac{1}{N!} \int_{I^N} \mathrm{d}^N\xi$$
$$\times \exp\left[\sum_{j,l\in\bar{N}} \frac{\hbar}{2\mathrm{i}} \left\{\epsilon\Delta t G(\xi_j,\xi_l)(D_j, D_l) + S_{j,l}(\xi)\right\}\right] \prod_{k\in\bar{N}} w[\xi_k, 0]. \tag{4.18}$$

Here $S_{j,l}(\xi)$ arises as in (4.11), and is defined as in (2.13), but it now acts on the product of w symbols.

Formula (4.18) is expressed in terms of the symbol w that forms part of the ersatz Hamiltonian. Recall that w is related to v by (4.8). In practice, it is preferable to express our results in terms of the symbol v, because v is assumed to be known from the physical Hamiltonian of interest. The computation which implements passing from w to v in (4.18) is, however, somewhat subtle; one cannot just naively substitute (4.8) as it stands. To understand this, notice that (4.18) actually does not require w itself, but rather, arbitrary D and $\widehat{D}$ derivatives of w, which are moreover finally evaluated on the geodesic path $[\xi]$ and at $p = 0$. Thus (4.8) must be used to relate arbitrary derivatives of w and v, evaluated in this way.

From (4.8) it is clear that any $\widehat{D}$ acting on w leads to a $\widehat{D}$ acting on v. On the other hand, a spatial D acting on w may strike either of the two sources of x-dependence in (4.8), thus leading to $D + (\epsilon\Delta t)^{-1}\mathbf{g}\widehat{D}$ acting on v. These necessary replacements of D and $\widehat{D}$ are just consequences of the chain rule, and are valid for arbitrary-order derivatives since $(\epsilon\Delta t)^{-1}\mathbf{g}$ is x, p-independent. Finally such derivatives of w must be evaluated at $(Q, p) = [\xi_k, 0]$. In summary, the relation implied by (4.8) in this way is

$$D^{\alpha}\widehat{D}^{\alpha'}w[\xi_k, 0] = \left(D_k + \frac{1}{\epsilon\xi_k\Delta t}\mathbf{g}\widehat{D}_k\right)^{\alpha}\widehat{D}_k^{\alpha'} \times \exp\left[\frac{\hbar}{2\mathrm{i}}\frac{1}{\epsilon\xi_k\Delta t}\langle\widehat{D}_k\rangle^2\right] v\left({\xi^0}_k, \gamma\xi_k, \frac{\mathbf{g}(x-y)}{\epsilon\Delta t}\right) \tag{4.19}$$

for arbitrary $\alpha, \alpha' \in \mathbb{W}^d$.

Clearly, the effect of using (4.19) in (4.18) will merely be to modify somewhat the quadratic differential operator in the exponent. The resulting formula in terms of v may be written

$$F(Q) = \sum_{N=0}^{\infty}\left(\frac{\Delta t}{\mathrm{i}\hbar}\right)^N \frac{1}{N!}\int_{I^N} \mathrm{d}^N\xi\left[\prod_{1\leqslant j<l\leqslant N}\exp\left(\frac{\hbar}{\mathrm{i}}b_{j,l}(\xi)\right)\right] \times \exp\left(\frac{\hbar}{2\mathrm{i}}c_N(\xi)\right)\prod_{k=1}^{N} v\left[\xi_k, \frac{\mathbf{g}(x-y)}{\epsilon\Delta t}\right] \tag{4.20a}$$

in which the $\epsilon, \Delta t$-dependent differential operators are defined by

$$b_{j,l}(\xi) = \epsilon\Delta t G(\xi_j, \xi_l)\langle D_j, D_l\rangle + (\xi_j - \Theta(\xi_j > \xi_l))D_j \cdot \widehat{D}_l + (\xi_l - \Theta(\xi_l > \xi_j))D_l \cdot \widehat{D}_j + (\epsilon\Delta t)^{-1}\langle\widehat{D}_j, \widehat{D}_l\rangle \tag{4.20b}$$

$$c_N(\xi) = \sum_{k=1}^{N}\left\{\epsilon\Delta t G(\xi_k, \xi_k)\langle D_k\rangle^2 + 2(\xi_k - 1)D_k \cdot \widehat{D}_k + (\epsilon\Delta t)^{-1}\langle\widehat{D}_k\rangle^2\right\}. \tag{4.20c}$$

Formula (4.20) is analogous to (2.15), the main difference being that there are now link operators for $j = l$ (loops), which are gathered in $c_N(\xi)$. Another difference is that the quadratic operator $b_{j,l}(\xi)$ is more elaborate than $S_{j,l}(\xi)$ because it contains couplings of the type $\langle D, D\rangle$ and $\langle\widehat{D}, \widehat{D}\rangle$. The kth term of $c_N(\xi)$ only depends on ξ_k and so it may be grouped with $v[\xi_k, \mathbf{g}(x-y)/\epsilon\Delta t]$ in (4.20a). The standard cluster method is then again applicable to (4.20), and it results in the desired resummed cluster expansion of the configuration function for Hamiltonian (1.3),

$$F(Q) = \exp\left\{\sum_{j=1}^{\infty} L_j(Q)\right\} \tag{4.21a}$$

$$L_j(Q) = \sum_{G_j}\sum_{n=0}^{\infty}\hbar^{r+n-j}\Delta t^j(n!2^n)^{-1}\mathrm{i}^{-r-n-j} \times \int_{Q_j^>}\mathrm{d}^j\xi\left(\prod_{\beta\in E}(l_\beta!)^{-1}b_\beta(\xi)^{l_\beta}\right)c_j(\xi)^n\prod_{k=1}^{j} v\left[\xi_k, \frac{\mathbf{g}(x-y)}{\epsilon\Delta t}\right]. \tag{4.21b}$$

The summation over n originates from a power-series expansion of $\exp\{(\hbar/2\mathrm{i})c_j(\xi)\}$.

Expansion (4.21) is equivalent to the one Barvinsky and Osborn [13] have recently obtained by a derivation somewhat different from the one presented here. The present derivation, while not the shortest route to (4.21), does answer the natural question about the possibility of resumming the transport result (4.10), and it additionally serves to check the correctness and mutual consistency of (4.10) and the result of [13]. The first proof of equivalence between these two expansions was found by Barvinsky [29] using the alternative methods of [13].

Not all of the physical parameter dependence is explicitly visible in (4.21) since b_β and c_j depend on ϵ and Δt. It is possible to modify (4.21) in this regard by rescaling and translating the momentum variable of symbol $v(t,x,p)$. In doing so the kind of arguments leading to (4.19) should be used. Such an improved version of (4.21) will not be displayed or discussed further here; the details may be found in [13].

If the perturbation $v(t,x)$ is momentum-independent, one can set $\widehat{D}=0$ in (4.20). The link and loop operators, $b_{j,l}$ and c_N, then reduce to their pure spatial derivative terms involving the Green function G, and so (4.21) is completely consistent with the previous work of [2].

5. Concluding remarks

While previous connected graph expansion literature [1–3] has been based on the Dyson series [30] representation of the quantum evolution operator, the results presented here have been derived starting from the transport-type PDE obeyed by the quantity of interest. This extends the known range of applicability of cluster methods, since transport PDEs arising outside of quantum mechanical problems can obviously be treated using the same techniques. For example, in section 2 no essential role is played by $\hbar$, and formal self-adjointness of $\tilde{H}$ is not required.

The particular type of transport differential structure considered here, namely the left-hand side of (1.1), is a consequence of (i) considering the quantum propagator in the full configuration (i.e. $\langle x|\cdots|y\rangle$) representation, and (ii) choosing the unperturbed Hamiltonian H_0 to be the free one (i.e. a Laplacian). These assumptions are not essential. It is possible to give parallel treatments for other quantum representations, such as mixed configuration–momentum (e.g. $\langle x|\cdots|p\rangle$) representations, or the phase-space representation of Wigner–Weyl [31–33]. The case of a non-Laplacian unperturbed Hamiltonian has not yet been considered in detail, but it evidently will lead to modified characteristic curves $q(\tau)$ which are unperturbed classical paths, replacing (1.5). Another avenue of extension involves replacing the configuration space $\mathbb{R}^d$ with a different manifold. In [3] connected graph propagator expansions were found (in the coordinate and Wigner–Weyl representations) for systems on tori with scalar potentials.

The cluster expansion method possesses remarkable stability features. First of all, it was seen in section 4 that a cluster expansion survives after the resummation process. Secondly, suppose the electromagnetic problem were treated by the methods of section 4. A cluster expansion of $F=\mathrm{e}^{J/\mathrm{i}\hbar}T$ would result, with an ersatz Hamiltonian given by (4.8)–(4.9) using the perturbation symbol (cf (1.3), (3.2))

$$v(t,x,p)=-\epsilon\langle a(x,t),p\rangle+\tfrac{1}{2}\epsilon(\langle a\rangle^2+\mathrm{i}\hbar\langle\nabla,a\rangle)+v(x,t).$$

Evidently this expansion of F would not be manifestly gauge-covariant, nor would $L_j \propto \epsilon^j$. On the other hand as section 3 shows, after $e^{J/i\hbar}$ is factored out the residual function T still possesses a cluster expansion. Interesting questions can therefore be posed concerning the inter-relation and consistency between these F and T expansions, the possibility of extracting further factors from T, and the widest possible setting admitting this type of stability.

It is of interest to compare the present results with other literature related to propagator expansions involving graphs. Often such literature is concerned with the heat kernel $\langle x|e^{-\beta H}|y\rangle$, where β is the inverse temperature, rather than with the evolution kernel K. The correspondence between the two kernels on a formal level is simply obtained by replacing β with $i\Delta t/\hbar$. (It should be noted, however, that on an analytically rigorous level the heat formalism has the disadvantage that $e^{-\beta H}$ does not exist as a bounded operator when the metric tensor is indefinite.) Some of the available graph expansion literature, e.g. [34, 35], studies the familiar short-time series [11, 12, 36–38]

$$K = K_0 \sum_{j=0}^{\infty} a_j(x,y)(i\Delta t)^j \tag{5.1}$$

and develops systematic procedures for computing the $a_j(x,y)$ coefficient functions. However, closed form solutions for a general a_j are not obtained. One advantage of exponential representations like (1.7) is that the coefficients are generally simpler than the ones in a simple power series like (5.1). The latter are described by disconnected graphs which arise through a cumulant expansion [39] of the exponentiated connected graph series.

A functional integral method of obtaining exponentiated heat kernel expansions has been developed by Roekaerts and collaborators [40–42]. This work considers systems with external electromagnetic fields, and admits the possibility of representing expansion coefficients with diagrams. (An earlier work [43] considered the WKB expansion for arbitrary Hamiltonians, without the introduction of diagrams.) Again, however, a closed symbol calculus determining arbitrary coefficients is not found. Moreover, the diagrams employed have a considerably more intricate structure than just clusters, and the coefficient formulae are not naturally expressed in terms of the Lorentz force. Since the heat problem with its static Hamiltonian is considered, the widest possible $(d+1)$-dimensional gauge transformation is not admitted.

The connected graph representations derived in this paper can reveal the 'multi-scale' behaviour of the propagator by simultaneously displaying its dependence upon a variety of physical parameters, such as ϵ, Δt, $\hbar$ or field coupling constants. These exact results provide a platform for computing *explicit* formulae (e.g. (3.14)–(3.16), (3.18)) for the coefficients of expansions in *any* of these variables. The validity of such expansions can be considered from both a mathematical and a practical perspective. Logically, the mathematical validity is the primary one, because without it there is nothing which can be applied to specific problems. Nevertheless, intuitive understanding about the utility of possible expansions is important. There is a pervasive interplay between these two aspects.

Mathematically, the graphical representation may be exactly valid in some region of the propagator's variables: the infinite graphical series may converge (appropriately) to a fundamental solution of the Schrödinger PDE. For example, for the d-

dimensional harmonic oscillator this series is [1–3] uniformly convergent in x, y if Δt is less than half the oscillator period (i.e. within caustics). Only for relatively trivial Hamiltonians can the series be summed in closed form; generally one looks to retain only a subclass of all the graphs and thereby to obtain an asymptotic expansion. For example, an analysis [14, 15] of the electromagnetic system (3.2) shows that its propagator possesses asymptotic expansions with error proportional to $(\epsilon\Delta t)^N$ if the external fields support smooth bounded derivatives to some order which increases with N.

The expected range of practical validity of a particular formal asymptotic expansion can be approached in two stages. On the simplest level, a dimensional analysis of the Schrödinger equation can be performed with respect to the independent expansion parameter in question. (For such a study of the small ϵ, Δt, $\hbar$ and charge limits for the electromagnetic problem, see section 5c of [9]. See also section 5 of [8].) On a more detailed level, one can examine a particular class of expansion coefficients and determine conditions under which they will be small, and will thus sum to a candidate first neglected term of an asymptotic expansion.

The number of possible expansions extractable from the general results in section 2 is large, and every possible variant cannot be commented upon here. As an illustration, let us summarize the practical limitations and virtues of the $\epsilon \downarrow 0$ propagator expansion found in section 3. It is a generalization [20] of the classic Wigner–Kirkwood [31, 44] ($\beta \downarrow 0$) heat kernel expansion. The applicability of this expansion only for limited time displacements Δt is consistent with its single-term form, $K = K_0 \exp(J/\mathrm{i}\hbar + \sum_j L_j)$, which may be viewed as a small-ϵ re-expansion [9, 20] of the short-time WKB approximation. (For longer times (beyond caustics) the WKB ansatz involves a sum of terms over the multiple interacting classical trajectories from y, s to x, t.) This restriction on Δt prevents the approximation from being used to compute infinite-time properties such as bound state energies. Similarly, quantum mechanical problems in which fixed energies are inherent, e.g. those concerned with tunnelling through turning points into classically inaccessible regions, are not addressable with the evolution kernel for small times. Despite this limitation, the small-time propagator is useful, for example, in the quantum field theoretic renormalization programme [45] of Schwinger–DeWitt. It is used to generate, via integral transforms in t, asymptotic expansions for quantities derived from H, such as the Feynman propagator and the effective Lagrangian.

The $\epsilon \downarrow 0$ expansion is a (gauge invariant) derivative expansion, and as such it is expected to be accurate when the potential fields are slowly varying (even if the potentials are large). This is because all occurrences of undifferentiated fields are completely summed in the exponential gauge-phase $\mathrm{e}^{J/\mathrm{i}\hbar}$, cf (3.5$c$). All higher ϵ-expansion coefficients L_j depend only on derivatives of the potentials; specifically (3.8)–(3.11) show that L_j is constructed from the Lorentz force Ω (and its derivatives), where Ω contains only derivatives of the potential fields a, v. Therefore L_j can be small if the fields are slowly varying. The small-ϵ expansion has a significant practical advantage relative to the short-time WKB expansion. The latter's coefficients, such as the action S, are functionals of the fully interacting classical trajectory satisfying two-point boundary conditions. Such boundary value problems are non-trivial—the trajectory is generally not available in closed form. The $\epsilon \downarrow 0$ expansion, by contrast, is built around the free (geodesic) trajectories $\gamma(\xi; x, y)$ which are (in $\mathbb{R}^d$) extremely simple and always available. Moreover, as indicated at the end of section 3, the graphical representation can be used as a source of formulae for the action. These provide a point of departure for rigorous studies of the classical mechanics [26], or of the WKB asymptotics [27].

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Appendix

Here a general integrand-symmetry theorem will be proved. Special cases of this result were used in section 2. Specifically, the type of integrand symmetrization procedure which allows passing from (2.12) to (2.15) is essential in all derivations leading to an exponential cluster expansion. In addition, the ability to finally express the cluster coefficients L_j in terms of an ordered integration (cf (2.19)) is a practical convenience. After the proof of the theorem, its application in these two situations will be sketched.

Let us begin with some notation, definitions and assumptions which will be used in the theorem. For $n, m, N \geqslant 1$ let

$$V_N : (\mathbb{R}^n \times \mathbb{R}^m)^N \to \mathbb{C}$$

be a smooth function which is symmetric under any permutation of its N arguments. Specifically, if $(z_i, \tau_i) \in \mathbb{R}^n \times \mathbb{R}^m$ for $i \in \bar{N}$, and $\sigma \in S_N$ (the group of permutations of $\bar{N}$), then

$$V_N(z_{\sigma 1}, \tau_{\sigma_1}, \ldots, z_{\sigma_N}, \tau_{\sigma_N}) = V_N(z_1, \tau_1, \ldots, z_N, \tau_N). \tag{A.1}$$

Such function arguments will occur frequently so it is helpful to employ the Cartesian product notation

$$\mathop{\times}_{k=1}^{N} Y_k \equiv (Y_1, Y_2, \ldots, Y_N).$$

The gradient of V_N on its jth $\mathbb{R}^n$-vector argument is denoted by $\mathbb{D}_j$:

$$[\mathbb{D}_j V_N]\left(\mathop{\times}_{k=1}^{N}(z_k, \tau_k)\right) = \nabla_{z_j} V_N\left(\mathop{\times}_{k=1}^{N}(z_k, \tau_k)\right).$$

Assume the existence of paths $\bar{z} : I \to \mathbb{R}^n$ and $\bar{\tau} : I \to \mathbb{R}^m$. For $i, j \in \bar{N}$ and $\xi, \xi' \in I$, assume given a formal differential operator $f(\xi, \xi'; \mathbb{D}_i, \mathbb{D}_j)$ which is symmetric under the interchange of *both* pairs of arguments simultaneously,

$$f(\xi, \xi'; \mathbb{D}_i, \mathbb{D}_j) = f(\xi', \xi; \mathbb{D}_j, \mathbb{D}_i). \tag{A.2}$$

No assumption is made about the effect of $\xi \leftrightarrow \xi'$ or $\mathbb{D}_i \leftrightarrow \mathbb{D}_j$ separately. Note that the $\mathbb{D}$'s commute; this will also be assumed true for the f's.

For the purposes of this appendix, let us adopt the following definitions. A graph is a symmetric map $G : \bar{N}^2 \to \mathbb{W}$. The edge set $E(G)$ of a graph G is the set of unordered pairs $\alpha = \{i, j\} \subset \bar{N}$ such that $G(\alpha) \equiv G(i, j) \geqslant 1$.

This definition of graphs admits loops $[G(j, j) \geqslant 1]$, and multiple edges $[G(i, j) \geqslant 2]$. However, the edge set does *not* contain repetitions of the same edge. Given a graph G and a permutation $\sigma \in \mathcal{S}_N$, define the permuted graph $\sigma^* G \equiv G \circ \sigma^{-1}$. That is, $[\sigma^* G](i, j) = G(\sigma^{-1} i, \sigma^{-1} j)$. Clearly $\sigma^* G$ is a graph too.

Finally, let $\mathcal{F}$ be a family of graphs with the property

$$G \in \mathcal{F} \qquad \sigma \in \mathcal{S}_N \Rightarrow \sigma^* G \in \mathcal{F}. \tag{A.3}$$

Theorem. Under the above assumptions, define for $\xi \in I^N$ the integrand

$$\mathcal{I}(\xi) \equiv \sum_{G \in \mathcal{F}} \mathcal{I}^G(\xi) \tag{A.4a}$$

$$\mathcal{I}^G(\xi) \equiv \left[\prod_{\alpha \in E(G)} f(\xi_{\wedge\alpha}, \xi_{\vee\alpha}; \mathbb{D}_{\wedge\alpha}, \mathbb{D}_{\vee\alpha})^{G(\alpha)} \right] V_N \left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_k), \bar{\tau}(\xi_k)) \right). \tag{A.4b}$$

Then $\mathcal{I}$ is invariant under any permutation of its argument:

$$\mathcal{I}(\xi \circ \sigma) = \mathcal{I}(\xi) \qquad \forall\, \xi \in I^N,\ \sigma \in \mathcal{S}_N.$$

Proof. Begin by computing the effect of the permutation σ on any given term $\mathcal{I}^G(\xi)$ in the sum (A.4*a*). By definition

$$\mathcal{I}^G(\xi \circ \sigma) = \prod_{\alpha \in E(G)} f(\xi_{\sigma(\wedge\alpha)}, \xi_{\sigma(\vee\alpha)}; \mathbb{D}_{\wedge\alpha}, \mathbb{D}_{\vee\alpha})^{G(\alpha)} V_N \left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_{\sigma k}), \bar{\tau}(\xi_{\sigma k})) \right).$$

Due to the symmetry of V_N, its variables can be unpermuted back into standard order provided each $\mathbb{D}_j$ operator acting on it is properly relabelled:

$$\mathbb{D}_j V_N \left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_{\sigma k}), \bar{\tau}(\xi_{\sigma k})) \right) = \mathbb{D}_{\sigma j} V_N \left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_k), \bar{\tau}(\xi_k)) \right).$$

This identity follows since $\mathbb{D}_j$ acts on the jth $\mathbb{R}^n$-argument of V_N, occupied by $\bar{z}(\xi_{\sigma j})$, which after unpermuting the variables of V_N occupies the (σj)th argument. So

$$\mathcal{I}^G(\xi \circ \sigma) = \prod_{\alpha \in E(G)} f(\xi_{\sigma(\wedge\alpha)}, \xi_{\sigma(\vee\alpha)}; \mathbb{D}_{\sigma(\wedge\alpha)}, \mathbb{D}_{\sigma(\vee\alpha)})^{G(\alpha)} V_N \left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_k), \bar{\tau}(\xi_k)) \right). \tag{A.5}$$

Next, it is simple to check that the map $\alpha \mapsto \sigma[\alpha] = \{\sigma i, \sigma j\}$ is a bijection of $E(G)$ onto $E(\sigma^* G)$. Thus the product over edges in (A.5) can be relabelled, yielding

$$\prod_{\beta \in E(\sigma^* G)} f(\xi_{\sigma(\wedge\sigma^{-1}\beta)}, \xi_{\sigma(\vee\sigma^{-1}\beta)}; \mathbb{D}_{\sigma(\wedge\sigma^{-1}\beta)}, \mathbb{D}_{\sigma(\vee\sigma^{-1}\beta)})^{G(\sigma^{-1}\beta)}. \tag{A.6}$$

Now consider the quantities $\sigma(\wedge\sigma^{-1}\beta)$ and $\sigma(\vee\sigma^{-1}\beta)$ which have arisen. If $\beta = \{i, j\}$, fix i to be the vertex whose image under σ^{-1} is the lesser, i.e. $\sigma^{-1}i \leqslant \sigma^{-1}j$ (the equality holds iff β is a loop). Then $\sigma(\wedge\sigma^{-1}\beta) = \sigma(\sigma^{-1}i) = i$ and similarly $\sigma(\vee\sigma^{-1}\beta) = j$. Thus

$$
\begin{aligned}
f(\xi_{\sigma(\wedge\sigma^{-1}\beta)}, \xi_{\sigma(\vee\sigma^{-1}\beta)}; \mathbb{D}_{\sigma(\wedge\sigma^{-1}\beta)}, \mathbb{D}_{\sigma(\vee\sigma^{-1}\beta)}) &= f(\xi_i, \xi_j; \mathbb{D}_i, \mathbb{D}_j) \\
&= f(\xi_{\wedge\beta}, \xi_{\vee\beta}; \mathbb{D}_{\wedge\beta}, \mathbb{D}_{\vee\beta})
\end{aligned}
$$

where the ability to interchange both arguments of f is employed in the event that $i \neq \wedge\beta$. This result, together with the fact that $G(\sigma^{-1}\beta) = \sigma^* G(\beta)$ in the exponent of (A.6), implies

$$
\begin{aligned}
\mathcal{I}^G(\xi \circ \sigma) = & \prod_{\beta \in E(\sigma^* G)} f(\xi_{\wedge\beta}, \xi_{\vee\beta}; \mathbb{D}_{\wedge\beta}, \mathbb{D}_{\vee\beta})^{\sigma^* G(\beta)} \\
& \times V_N\left(\mathop{\times}_{k=1}^{N} (\bar{z}(\xi_k), \bar{\tau}(\xi_k))\right) = \mathcal{I}^{\sigma^* G}(\xi).
\end{aligned}
$$

This is the fundamental behaviour of $\mathcal{I}^G$ under permutation.

Consequently, under a permutation the sum $\mathcal{I}$ takes the form

$$
\mathcal{I}(\xi \circ \sigma) = \sum_{G \in \mathcal{F}} \mathcal{I}^{\sigma^* G}(\xi).
$$

The final step of the proof is to re-order this sum. It is straightforward to check that the map $\sigma^* : G \mapsto \sigma^* G$ is a bijection of $\mathcal{F}$ with itself, and so one has

$$
\mathcal{I}(\xi \circ \sigma) = \sum_{H \in \mathcal{F}} \mathcal{I}^H(\xi) = \mathcal{I}(\xi). \qquad \square
$$

Let us now show how this theorem can be applied in section 2. To begin with, some of the quantities must be identified more specifically. Choose $\mathbb{R}^n$ to be the phase space $\mathbb{R}^{2d} \simeq \mathbb{R}^d_x \times (\mathbb{R}^d_p)^*$ and let $\mathbb{R}^m$ be the time axis $\mathbb{R}^1_\tau$. The symmetric function V_N will be taken to be the product of $\mathbb{C}$-valued symbols $\tilde{H}$,

$$
V_N\left(\mathop{\times}_{k=1}^{N} (x_k, p^k, \tau_k)\right) \equiv \prod_{k=1}^{N} \tilde{H}(\tau_k, s, x_k, y, p^k). \tag{A.7}
$$

Its path arguments should be the geodesics $\bar{z}(\xi) = (\gamma\xi, 0)$ and $\bar{\tau}(\xi) = \xi^0$. Because the N factors in the product (A.7) commute, symmetry property (A.1) is valid.

Before considering the differential operators f, it is first necessary to characterize an appropriate generalization of the link operator $S_\alpha(\xi)$. Corresponding to the phase space splitting $z = (x, p) \in \mathbb{R}^d \times (\mathbb{R}^d)^*$, the $2d$-dimensional gradients decompose into $\mathbb{D}_j = (D_j, \widehat{D}_j)$. The components of $\mathbb{D}_j$ will be indexed by $a \in \overline{2d}$ according to

$$
\mathbb{D}_j^{(a)} = \begin{cases} D_j^{(a)} & a \leqslant d \\ \widehat{D}_j^{(a-d)} & a > d. \end{cases}
$$

A ξ, ξ'-parametrized bilinear function on the abstract algebra of $\mathbb{D}$ operators is defined by

$$B_{\xi,\xi'}(\mathbb{D}_i, \mathbb{D}_j) \equiv \sum_{a,b=1}^{2d} \frac{\min\{\xi, \xi'\}}{\max\{\xi, \xi'\}} (\delta_{a,b-d} + \delta_{a-d,b}) \mathbb{D}_i^{(a)} \mathbb{D}_j^{(b)}.$$

It is easily seen that B possesses the symmetry property

$$B_{\xi,\xi'}(\mathbb{D}_i, \mathbb{D}_j) = B_{\xi',\xi}(\mathbb{D}_j, \mathbb{D}_i). \tag{A.8}$$

A careful check shows that the relation between B and the link operator S defined in (2.13) is

$$S_{i,j}(\xi) = \Theta(i \neq j) B_{\xi_i,\xi_j}(\mathbb{D}_i, \mathbb{D}_j),$$

valid for $i, j \in \bar{N}$ and almost all $\xi \in I^N$.

With this preparation, let us proceed with the first application of the theorem. It must be shown, as stated after (2.14), that the integrand

$$\mathcal{I}(\xi) \equiv \prod_{1 \leqslant j < l \leqslant N} \mathrm{e}^{S_{j,l}(\xi)} \prod_{k=1}^{N} \tilde{H}[\xi_k, 0] \tag{A.9}$$

is a symmetric function of ξ. Comparing (A.9) with (A.4) indicates that if V_N is identified with the product of symbols (A.7), then one should choose

$$f(\xi, \xi'; \mathbb{D}_i, \mathbb{D}_j) \equiv \exp\, B_{\xi,\xi'}(\mathbb{D}_i, \mathbb{D}_j)$$

which (A.8) shows to have the required symmetry (A.2). Since there is no sum over graphs in (A.9), wherein the product over $j < l$ should correspond to products over edges in a graph, choose $\mathcal{F}$ to be the family whose only member G is the complete graph without loops, i.e. $G(j, l) = \Theta(j \neq l)$. Clearly G is invariant under permutations, hence $\mathcal{F}$ obeys property (A.3). With these choices of f and $\mathcal{F}$ the products in (A.4*b*) and (A.9) coincide:

$$\prod_{\alpha \in E(G)} f(\xi_{\wedge\alpha}, \xi_{\vee\alpha}; \mathbb{D}_{\wedge\alpha}, \mathbb{D}_{\vee\alpha})^{G(\alpha)} = \prod_{j<l} \exp\, B_{\xi_j,\xi_l}(\mathbb{D}_j, \mathbb{D}_l) = \prod_{j<l} \mathrm{e}^{S_{j,l}}(\xi).$$

Applying the theorem proves the required symmetry of $\mathcal{I}$.

The second application concerns (2.19), for which the integrand is

$$\mathcal{I}(\xi) = \sum_{G \in C_j} \prod_{\beta \in E(G)} \left[\sum_{l_\beta = 1}^{\infty} (l_\beta!)^{-1} S_\beta(\xi)^{l_\beta} \right] \prod_{k=1}^{j} \tilde{H}[\xi_k, 0]. \tag{A.10}$$

Comparison with (A.4) shows that in this case the family $\mathcal{F}$ of graphs is non-trivial; it is C_j. The clusters G are $\{0, 1\}$-valued, and under permutation produce another cluster so that property (A.3) is valid. Upon choosing

$$f(\xi, \xi'; \mathbb{D}_i, \mathbb{D}_j) \equiv -1 + \exp\, B_{\xi,\xi'}(\mathbb{D}_i, \mathbb{D}_j)$$

and applying the theorem, the symmetry of integrand (A.10) follows immediately.

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