Schrödinger semigroups for vector fields

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Suppose H is the Hamiltonian that generates time evolution in an N-body, spin-dependent, nonrelativistic quantum system. If r is the total number of independent spin components and the particles move in three dimensions, then the Hamiltonian H is an $r \times r$ matrix operator given by the sum of the negative Laplacian $-\Delta_x$ on the $(d = 3N)$-dimensional Euclidean space $\mathbb{R}^d$ plus a Hermitian local matrix potential $W(x)$. Uniform higher-order asymptotic expansions are derived for the time-evolution kernel, the heat kernel, and the resolvent kernel. These expansions are, respectively, for short times, high temperatures, and high energies. Explicit formulas for the matrix-valued coefficient functions entering the asymptotic expansions are determined. All the asymptotic expansions are accompanied by bounds for their respective error terms. These results are obtained for the class of potentials defined as the Fourier image of bounded complex-valued matrix measures. This class is suitable for the N-body problem since interactions of this type do not necessarily decrease as $|x| \to \infty$. Furthermore, this Fourier image class also contains periodic, almost periodic, and continuous random potentials. The method employed is based upon a constructive series representation of the kernels that define the analytic semigroup $\{e^{-zH} | \operatorname{Re} z > 0\}$. The asymptotic expansions obtained are valid for all finite coordinate space dimensions d and all finite vector space dimensions r, and are uniform in $\mathbb{R}^d \times \mathbb{R}^d$. The order of expansion is solely a function of the smoothness properties of the local potential $W(x)$.

I. INTRODUCTION AND SUMMARY

Take H to be the self-adjoint semibounded operator that generates time evolution for the N-body problem in nonrelativistic quantum mechanics and let the complex variable z take values in the open right half-plane D, then the family of bounded operators

$$\{e^{-zH} | z \in D\} \tag{1.1}$$

constitutes the analytic semigroup induced by H. The restriction of z to the positive real axis leads to the one-parameter semigroup associated with the heat transport equation and the partition function of the canonical ensemble. In the heat transport problem the positive value of z is the time variable, whereas in the partition function z is proportional to the inverse temperature of the system. On the other hand, if z belongs to the boundary ∂D and takes on purely imaginary values then the family of operators (1.1) forms the one-parameter unitary group which describes time evolution of the system.

A second, equally basic, family of bounded operators are the resolvent operators

$$\{(H-\lambda)^{-1} | \lambda \in \mathbb{C},\ \operatorname{Im} \lambda \neq 0\} \tag{1.2}$$

that appear in the time-dependent formulation of quantum mechanics. This paper studies the uniform asymptotic expansions of the coordinate-space kernels of both operator families (1.1) and (1.2). For the analytic semigroup $\{e^{-zH} | z \in D\}$ the asymptotic expansion variable is $|z| \to 0$. Physically these expansions are applicable for short times or high temperatures. Asymptotic expansions for the resolvent kernels then result from a Laplace transform of the analytic semigroup kernels. The resolvent kernel expansions are valid for $|\lambda| \to \infty$, or convergent for high energies.

Recently the first of these two problems, (1.1), has been discussed at length for the case of scalar fields by Osborn and Fujiwara in Ref. 1 (hereafter OF). Let x be the generic point in Euclidean space $\mathbb{R}^d$ that specifies the location of all N particles in the system. If each individual particle moves in three dimensions then the Euclidean space dimension is $d = 3N$. The scalar problem for local potentials is realized if the Hamiltonian H is taken to be the self-adjoint extension in $L^2(\mathbb{R}^d)$ of the quadratic elliptic differential form

$$H_{(x)} = -q\Delta_x + v(x). \tag{1.3}$$

Here Δ_x denotes the Laplacian in $\mathbb{R}^d$ and v: $\mathbb{R}^d \to \mathbb{R}$ is the perturbing local potential. In terms of the rationalized value of Planck's constant $\hbar$, and the particle mass m, the quantum scale factor is

$$q = \hbar^2/2m. \tag{1.4}$$

The notationally simplifying device of setting $q = 1$ is avoided because it is illuminating to exhibit explicitly the q dependence of the heat-kernel and resolvent-kernel expansions and thereby see the semiclassical content of these expansions.

However, the general N-body problem is not described by scalar fields unless all the particles are bosons with spin zero. If the ith particle has spin s_i, the resulting N-body wave function is a vector-valued complex function of dimension

$$r = \sum_{i=1}^{N} (2s_i + 1)$$

and an element of the space $L^2(\mathbb{R}^d, \mathbb{C}^r)$. In this circumstance the local perturbation becomes for each x an Hermitian matrix $W(x)$: $\mathbb{C}^r \to \mathbb{C}^r$, and the scalar Laplacian $-\Delta_x$ generalizes to $-\Delta_x I$, where I is the identity on $\mathbb{C}^r$. The matrix-valued analog of (1.3) assumes the form

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$$H_{(x)} = -q\Delta_x I + W(x). \quad (1.5)$$

The appearance of (1.5) seems to assume that all N particles have common mass m. This restriction is apparent rather than real since a scale transformation of the particle coordinates always allows one to write the most general diagonal kinetic energy operator in the form $-q\Delta_x$. The Hamiltonian operator H which defines the physical quantum system is the self-adjoint extension of $H_{(x)}$ in $L^2(\mathbb{R}^d, \mathbb{C}^r)$.

Denote the kernel of the semigroup element e^{-zH} by $U(x,y;z)$: $\mathbb{R}^d \times \mathbb{R}^d \times D \rightarrow \mathbb{C}^{r\times r}$. Similarly if $\rho(H)$ is the resolvent set of H, we define the kernel of the resolvent operator $(H-\lambda)^{-1}$ by $R(x,y;\lambda)$ for all $\lambda \in \rho(H)$. The basic objective of this paper is to derive the precise forms assumed by the natural asymptotic expansions of $U(x,y;z)$ and $R(x,y;\lambda)$. Specifically, we obtain the existence of the kernels, the analytic form (in z) of the asymptotic expansions, explicit closed expressions in terms of $W(x)$ of all the coefficient matrices that enter the asymptotic expansions, and $\mathbb{R}^d \times \mathbb{R}^d$ uniform bounds for the remainder terms. In fact we show that the derivation of these uniform asymptotic expansions requires only continuity and differentiability properties in x of the potential $W(x)$. In particular, there is no necessity to assume that $W(x)$ decays as $|x| \rightarrow \infty$. The restriction we do impose on the allowed form of W is that the potential be the Fourier image of a complex bounded $r\times r$ matrix measure, μ, on $\mathbb{R}^d$.

The analytic semigroup (1.1) is characterized uniquely by its associated family of kernels $\{U(x,y;z) | z \in D\}$. Our approach to determining the existence and the properties of $U(x,y;z)$ is constructive. Let H_0 denote the free kinetic energy operator (the self-adjoint extension of $-q\Delta_x I$). We establish that the kernel analog of the Dyson series[2,3] for e^{-zH} in terms of time-ordered parametric integrals of e^{-zH_0} and W leads to an absolutely and uniformly (in $\mathbb{R}^d \times \mathbb{R}^d$) convergent series representation of $U(x,y;z)$. As an immediate byproduct of this result, it follows that if $W(x)$ has uniformly bounded derivatives of order 2, then $U(x,y;it/\hbar)$, where $t \in \mathbb{R}$ and represents time displacement, constitutes the fundamental solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} U(x,y;it/\hbar) = H_{(x)} U(x,y;it/\hbar) \quad \forall x,y \in \mathbb{R}^d \quad (1.6)$$

obeying the delta-function initial condition

$$U(x,y;it/\hbar) \rightarrow \delta(x-y) I \quad \text{as } t \rightarrow 0. \quad (1.7)$$

Parallel conclusions apply to the heat-conduction problem. The heat-conduction or diffusion problem results if one formally replaces the imaginary time variable with $\beta > 0$. Again $U(x,y;\beta)$ is the fundamental solution of the heat problem. In particle physics terminology, $U(x,y;it/\hbar)$ is the propagator of the N-body system.

The center of interest in this investigation is the small z uniform asymptotic expansion that $U(x,y;z)$ admits. It is well known that these kernels are highly singular in the limit $z \rightarrow 0$. This is evident from the formula for the free heat kernel defined by H_0:

$$U_0(x,y;z) = \left[\frac{1}{(4\pi zq)^{d/2}} \exp\left(\frac{-|x-y|^2}{4zq} \right) \right] I. \quad (1.8)$$

Here $|x-y|$ represents the Euclidean distance in $\mathbb{R}^d$ between x and y. This convolution kernel has an essential singularity at $z=0$. Thus, asymptotic expansions of $U(x,y;z)$ for small z require that this essential singularity structure be explicitly factored out in order to expose a smooth function of z. For this reason it is useful to define a function $F(x,y;z)$: $\mathbb{R}^d \times \mathbb{R}^d \times D \rightarrow \mathbb{C}^{r\times r}$ by

$$U(x,y;z) = U_0(x,y;z) F(x,y;z). \quad (1.9)$$

Both U_0 and F are $r\times r$ matrices. In (1.9) we adopt the hereafter standard convention that $U_0 F$ implies the matrix product. Now if the Dyson series for $U(x,y;z)$ is written in the appropriate form, one finds an explicit series expansion for F. The F-series is uniformly convergent on all compact subsets of $\bar{D}$ (the closure of D). As a consequence it follows that $F(x,y;z)$ is analytic in D, continuous in $\bar{D}$, and $F(x,y;0) = I$ for all $x,y \in \mathbb{R}^d$.

A further restructuring of the F-series leads to the asymptotic expansion

$$F(x,y;z) = \sum_{n=0}^{M} \frac{(-z)^n}{n!} P_n(x,y) + E_M(x,y;z). \quad (1.10)$$

Here, M is an integer proportional to the number of continuous bounded partial derivatives that $W(x)$ supports. The error term is of order $O(|z|^{M+1})$ and has a uniform bound in $\mathbb{R}^d \times \mathbb{R}^d$. In addition, identity (1.10) can be differentiated with respect to x, y, or z as often as desired and the resulting equation is also an asymptotic expansion provided $W(x)$ is sufficiently smooth. This flexible nature of (1.10) permits one to use it as the basis for calculating the small time behavior of correlation functions for an arbitrary pair of observables. The expansion (1.10) has been analyzed extensively in the literature[4-8] for a wide variety of operators H. Generally it is known that the coefficients P_n $[P_0(x,y) = I]$ are functions of $W(x)$ and its partial derivatives up to order $2(n-1)$. A novel feature of the constructive approach is that one can determine for every n explicit expressions of the coefficient matrices $P_n(x,y)$. These expressions are not only applicable when $x=y$, but valid for all $x,y \in \mathbb{R}^d$. Another useful aspect of the constructive approach is that one can prove that expansion (1.10) is uniform in $\arg z$. Thus the short time expansions are on exactly the same analytical footing as the high temperature expansions. In passing we note that the x,y uniform character of expansion (1.10) is a necessary ingredient for the correct description of N-body systems that incorporate the wave function symmetrization required by either fermion or boson statistics.

The study of the resolvent kernel proceeds by using the Laplace transform of $U(x,y;z)$ to determine $R(x,y;z)$, namely,

$$R(x,y;z) = \int_0^\infty e^{\beta z} U(x,y;\beta) d\beta, \quad x \neq y, \quad \operatorname{Re} z < c, \quad (1.11)$$

where c is any negative lower bound for the spectrum of H. The condition $\operatorname{Re} z < c < 0$ ensures that the integral in (1.11) is absolutely convergent. The resolvent kernel is holomorphic in a much larger domain of z, namely $z \in \rho(H)$. Identity (1.11) may be analytically continued to a subset of this larger domain in $\mathbb{C}$ by changing the variable of integration so that the integration contour along the positive real axis is rotated until it becomes a complex ray with origin at $\beta = 0$ and having constant $\arg \beta \in (\pi/2, -\pi/2)$. We find, upon using the analytically extended form of (1.11), that the Laplace image of the heat-kernel asymptotic expansion (1.10) becomes

$$R(x,y;z) = \sum_{n=0}^{M} \frac{(-1)^n}{n!} P_n(x,y) \left(\frac{\partial}{\partial z}\right)^n R_0(x,y;z) + T_M(x,y;z), \quad x \neq y. \tag{1.12}$$

Here, $R_0(x,y;z)$ denotes the kernel defined by $(H_0 - z)^{-1}$. This free resolvent is an analytic function of z in the open cut plane $\mathbb{C}\setminus\mathbb{R}^+$ and for $H_0 = -q\Delta_x I$ it is given by a Bessel function multiplied by I.

Although it is not so apparent from the form of (1.12), the small parameter in the expansion is z^{-1}. Furthermore if $M+2 > d/2$ then the error term in (1.12) has a uniform bound in $\mathbb{R}^d \times \mathbb{R}^d$ and is of the order $(|z|^{-1})^{M+2-d/2}$. The boundedness of the error T_M as $x \to y$ implies that the singularities of $R(x,y;z)$, $R_0(x,y;z)$, and the derivatives of $R_0(x,y;z)$ in the neighborhood of the diagonal $x = y$ are identical on both sides of (1.12). The uniformity in z of (1.12) can be characterized as follows. For any $\delta \in (0,\pi/2)$ let $\widetilde{V}_\delta$ denote the subset of $\mathbb{C}$ given by

$$\{z \mid z \in \mathbb{C}, \quad \arg(z + \|\mu\|(\sin\delta)^{-1}) \in (2\delta, 2\pi - 2\delta)\}.$$

Clearly $\widetilde{V}_\delta$ is the complement of a wedge symmetric about the positive real axis with its apex at $z = -\|\mu\|(\sin\delta)^{-1}$. The expansion (1.12) is uniform for all $z \in \widetilde{V}_\delta$. Although the opening angle of the wedge, 4δ, is arbitrary and can be made as small as desired, there will always be a strip about the positive real axis disjoint from $\widetilde{V}_\delta$. Thus the values of $R(x,y;z)$ as z converges to points on the spectrum, $\sigma(H)$, are not estimated by (1.12). This is to be expected since stating only the smoothness properties of $W(x)$ is insufficient information to determine the detailed nature of the spectrum. In examples where formula (1.12) has been continued to the spectral boundary (such as Buslaev's treatment[9] of $\mathbb{R}^3$), extensive information about the $|x| \to \infty$ decay of $W(x)$ is required in order to extend the z domain of (1.12) to the boundary of the open domain $\mathbb{C}\setminus\sigma(H)$.

A balanced overview of the results outlined above emerges if we consider their connection to the spectral asymptotics of H. Local geometrical spectral asymptotics is the study of the relationships that link three basic structures generated by the differential operator $H_{(x)}$. These structures are (a) the local coefficient functions that define $H_{(x)}$ and the boundary conditions which are obeyed; (b) the Weyl expansion[10,11] predicting the density of eigenvalues λ_i satisfying

$$H\Psi_{\lambda_i} = \lambda_i \Psi_{\lambda_i}, \quad \|\Psi_{\lambda_i}\| = 1, \tag{1.13}$$

as $\lambda_i \to \infty$, or the appropriate generalization of the Weyl expansion when the spectrum has a continuous component; and (c) the asymptotic expansions of the integral kernels for the basic operator functions of H such as the semigroup or resolvent operators.

In general, the coefficient functions that enter $H_{(x)}$ come from the functions that define the Laplace–Beltrami operator for a non-Euclidean manifold (either compact or noncompact), the functions appearing in the first-order terms (such as the magnetic vector potential), and the potential $W(x)$. In our N-body problem the manifold is flat so the Laplace–Beltrami operator reduces to the Laplacian, the first-order derivative terms are absent, and so the only nontrivial coefficient function is $W(x)$. The boundary condition for $\mathbb{R}^d$ reduces to the requirement that $H_{(x)}$ have a unique self-adjoint extension in $L^2(\mathbb{R}^d, \mathbb{C}^r)$. If the manifold supporting the functions on which $H_{(x)}$ acts is noncompact (as in the $\mathbb{R}^d$ case), characteristically one finds that the spectrum has a continuous part. The appropriate extension of the Weyl problem is to replace the study of the density of eigenvalues by the asymptotic expansion of the spectral kernels $e(x,y;\lambda)$ as $\lambda \to \infty$.

In essence the asymptotic expansions (1.10) for the heat kernel and (1.12) for the resolvent kernel display the relationship between (a) and (c). In particular, the explicit expressions we derive later for $P_n(x,y)$ show how the local form of $H_{(x)}$ controls these two expansions. In this sense this paper is a special application of the local geometrical asymptotics program. The approach emphasized in this work is to determine first (via the Dyson expansion) the detailed properties of the semigroup family of kernels and then by various transforms obtain the other asymptotic expansions of interest.

It is worth observing that the connection (a)$\to$(b), although of fundamental importance, is still not well understood in the noncompact domain problems. Following the technique introduced by Carleman,[12] most investigations of the large λ behavior of $e(x,y;\lambda)$ have utilized the Tauberian theorems.[13–16] This approach is capable of predicting only the leading-order behavior of $e(x,y;\lambda)$. An alternate method of investigating the continuum–Weyl problem and obtaining a higher-order asymptotic expansion was developed by Osborn and Wong[17] (hereafter OW). The technique of OW is to obtain the link (a)$\to$(b) by the chain of results (a)$\to$(c) then (c)$\to$(b). In particular, one may prove that the kernel $U(x,y;z)$ has the spectral representation[17,18]

$$U(x,y;z) = \int_{\sigma(H)} e^{-z\lambda}\, de(x,y;\lambda), \quad z \in D. \tag{1.14}$$

In order to implement the stage (c)$\to$(b) the inverse of this transform is required, namely,

$$e(x,y;\lambda) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^{z\lambda}}{z} U(x,y;z)\,dz, \quad c > 0. \tag{1.15}$$

The validity of (1.15) is established in OW. This formula has the feature of transforming semigroup kernels into spectral kernels.

Under the hypothesis that the continuous spectrum contribution to $U(x,y;it/\hbar)$ has nice decay properties as $t \to \pm\infty$ (this assumption just reflects the physically reasonable expectation that particles and stable clusters of particles that belong to the continuum of H will diffuse as $t \to \pm\infty$) then $e(x,y;\lambda)$ admits a higher-order Weyl expansion given by

$$e(x,y;\lambda) = \sum_{n=0}^{M} \frac{(-1)^n}{n!} P_n(x,y) \left(\frac{\partial}{\partial\lambda}\right)^n e_0(x,y;\lambda) + \widetilde{E}_M(x,y;\lambda). \tag{1.16}$$

Here $e_0(x,y;\lambda)$ is the spectral kernel of Hamiltonian H_0 and is a known analytic function of λ. This expansion is uniform within compact regions of $\mathbb{R}^d \times \mathbb{R}^d$. The error term is of order $O(|\lambda|^{-N})$, where N depends in a complicated way on the number of bounded derivatives of $W(x)$ and on the nature of the t-decay of the continuous spectrum contributions to $U(x,y;it/\hbar)$. A more detailed overview of local geometrical spectral asymptotics may be found in the excellent review of Fulling.[4]

The construction of this paper is as follows. In Sec. II the complex matrix-valued measure representation of the potential $W(x)$ is introduced. Section III describes the constructive series representation of the kernel $U(x,y;z)$ and obtains the x,y-uniform asymptotic expansion associated with Eq. (1.10). Furthermore, under appropriate smoothness restrictions on $W(x)$, it is established that $U(x,y;it/\hbar)$ and $U(x,y;\beta)$ are fundamental solutions of their respective partial differential equations. The explicit formulas for the coefficient matrices $P_n(x,y)$ are determined. Finally in Sec. IV we utilize an analytic continuation of the Laplace transform to find the large $|\lambda|$ expansion of the resolvent kernels $R(x,y;\lambda)$. Formulas bounding the total error in the resolvent asymptotic expansion are derived.

II. FOURIER IMAGE POTENTIALS

For a particular class of potentials $W(x)$, the operator $H_{(x)}$ is studied. Let $\mathscr{M}(\mathbb{R}^d,\mathbb{C}^{r\times r})$ be the set of all bounded complex matrix-valued measures defined on the Borel field $\mathscr{B}$ on $\mathbb{R}^d$. Each measure $\mu\in\mathscr{M}$, defines a matrix-valued potential function by the Fourier transform of μ,

$$W(x)=\int_{\mathbb{R}^d} e^{ikx}\,d\mu(k), \tag{2.1}$$

where $k\in\mathbb{R}^d$ and kx denotes the scalar product in $\mathbb{R}^d$. The equality above is understood as that appropriate for the space of complex matrices, $\mathbb{C}^{r\times r}$. If $\nu,\gamma=1,2,\dots,r$ specify the row and column of a matrix, then (2.1) implies

$$W_{\nu\gamma}(x)=\int_{\mathbb{R}^d} e^{ikx}\,d\mu_{\nu\gamma}(k)\quad \text{all } \nu,\gamma. \tag{2.2}$$

Each $\mu_{\nu\gamma}$ is a bounded complex-valued measure on $\mathscr{B}$ and each $\nu\gamma$ component of the matrix W is a complex-valued function of x. Hereafter, in order to simplify our notation the integration domain $\mathbb{R}^d$ will be omitted.

We employ the symbol $|\cdot|$ to represent several different norms. If the argument of $|\cdot|$ is in $\mathbb{C}$, then $|\cdot|$ denotes the absolute value; if the argument is in $\mathbb{C}^r$ or $\mathbb{C}^{r\times r}$ then the norm is the appropriate Euclidean vector length. For example, if E is any set in $\mathscr{B}$,

$$|\mu(E)|=\left\{\sum_{\nu=1}^{r}\sum_{\gamma=1}^{r}|\mu_{\nu\gamma}(E)|^2\right\}^{1/2}. \tag{2.3}$$

A somewhat different meaning of the absolute value sign applies to $|\mu|$. Here, $|\mu|$ is defined to be the total variation of μ, namely the non-negative scalar-valued set function on $\mathscr{B}$ given by

$$|\mu|(E)=\sup\sum_{i=1}^{\infty}|\mu(E_i)|, \tag{2.4}$$

where the supremum is taken over all partitions $\{E_i\}$ of E. The statement that $\mu\in\mathscr{M}$ is bounded means that $|\mu|(\mathbb{R}^d)<\infty$. In fact, the total variation $|\mu|$ may be used to define a norm $\|\cdot\|$ for $\mathscr{M}$ if we set

$$\|\mu\|=|\mu|(\mathbb{R}^d). \tag{2.5}$$

Equipped with this norm $\mathscr{M}$ is a Banach space.[19] It is clear from the definition of (2.1) that the Fourier image of $\mathscr{M}$ consists of $\mathbb{R}^d\to\mathbb{C}^{r\times r}$ functions that are uniformly bounded and uniformly continuous. In particular,

$$|W(x)|\leqslant\|\mu\|,\quad \forall x\in\mathbb{R}^d. \tag{2.6}$$

The transformation (2.1) defines a class of potentials

$$\mathscr{F}=\left\{W(x)=\int e^{ikx}\,d\mu(k)\,|\,\mu\in\mathscr{M}\right\}. \tag{2.7}$$

The elements of the spaces $\mathscr{F}$ and $\mathscr{M}$ are in a one-to-one correspondence. This is a consequence of the uniqueness[20] of the transformation (2.1) that states $W(x)=0$ if and only if $\mu=0$. Again by adjoining norm $\|\mu\|$ to $\mathscr{F}$ one defines a Banach space.

Consider the subset of potentials in $\mathscr{F}$ that are Hermitian matrices for all $x\in\mathbb{R}^d$. For a set $E\in\mathscr{B}$ the reflected set $-E$ is defined to be $-E=\{k\,|\,k\in\mathbb{R}^d,\ -k\in E\}$. We say the measure μ satisfies the reflection property if

$$\mu(-E)=\mu^*(E),\quad \forall E\in\mathscr{B}, \tag{2.8}$$

where * denotes the adjoint on $\mathbb{C}^{r\times r}$. Then the Fourier transform of a μ satisfying the reflection property is a Hermitian matrix for all x. And, conversely an element $W\in\mathscr{F}$ that is Hermitian for all x has an associated measure $\mu\in\mathscr{M}$ that obeys the reflection property. Define the subset of $\mathscr{M}$ that consists of measures μ of the type (2.8) as $\mathscr{M}^*$ and let $\mathscr{F}^*$ be the Fourier image of $\mathscr{M}^*$. The potentials $W\in\mathscr{F}^*$ are the physically significant ones since they comprise all the Hermitian potentials in $\mathscr{F}$.

The asymptotic expansions derived in the next several sections are a manifestation of the smoothness of the potentials $W(x)$. For this reason it is convenient to further classify the potentials in $\mathscr{F}^*$ into subclasses in which derivatives up to order M are bounded. We define $\mathscr{F}^*_M\subseteq\mathscr{F}^*$, $M=0,1,2,\dots$, to be

$$\mathscr{F}^*_M=\left\{W\,|\,W\in\mathscr{F}^*,\int d\,|\mu|(k)|k|^n<\infty,\ n=0,1,\dots,M\right\}. \tag{2.9}$$

In fact, for $W\in\mathscr{F}^*_M$ there exists a smallest finite positive constant $K(W,M)$ such that

$$\int d\,|\mu|(k)|k|^n\leqslant K(W,M)^n\|\mu\|,\quad n=0,1,\dots,M. \tag{2.10}$$

We call $K(W,M)$ the bound constant of potential W in the space $\mathscr{F}^*_M$.

If D^L_x represents an arbitrary partial derivative in $\mathbb{R}^d$, multi-indexed by $L=(l_1,l_2,\dots,l_d)$, $l_i\geqslant 0$, with length $|L|=l_1+l_2+\cdots+l_d$, and given by

$$D^L_x=\left(\frac{\partial}{\partial x_1}\right)^{l_1}\cdots\left(\frac{\partial}{\partial x_d}\right)^{l_d}, \tag{2.11}$$

then $W\in\mathscr{F}^*_M$ implies

$$|(D^L_xW)(x)|\leqslant K(W,M)^{|L|}\|\mu\|,\quad |L|\leqslant M. \tag{2.12}$$

It is useful to decompose the matrix measure μ into the product of the total variation measure $|\mu|$ and a matrix function with unit Euclidean norm.

Lemma 1: Let $\mu\in\mathscr{M}$, then there is a unique $|\mu|$-measurable matrix function $A:\mathbb{R}^d\to\mathbb{C}^{r\times r}$ such that

$$|A(k)|=1,\quad \forall k\in\mathbb{R}^d, \tag{2.13}$$

and

$$\int_E d\mu(k) = \int_E d|\mu|(k)A(k), \quad \forall E \in \mathscr{B}. \tag{2.14}$$

Proof: Since $\mu \ll |\mu|$ the Radon–Nikodym theorem implies the existence of a $|\mu|$-measurable $L^1(|\mu|)$ function $A(k)$. The proof that $A(k)$ has Euclidean norm equal to unity follows from a simple modification of the argument Rudin[21] (Theorem 6.12) gives for the scalar case. □

For scalar problem ($r = 1$) the potential class $\mathscr{F}$ was introduced by Ito[22] to study the Feynman path integral representations of $e^{itH/\hbar}$. Later, Albeverio and Høegh-Krohn[23] used $\mathscr{F}$ for the same purpose and in a fashion similar to our treatment of the kernel form of the Dyson series.

III. ASYMPTOTIC EXPANSIONS FOR e^{-zH}

Throughout the remainder of the paper it is always assumed that $W \in \mathscr{F}^*$. For this class of potentials the Hamiltonian H is defined as the self-adjoint extension of $H_{(x)}$ in $L^2(\mathbb{R}^d, \mathbb{C}^r)$. We also let the symbol W stand for the linear operator on $L^2(\mathbb{R}^d, \mathbb{C}^r)$ given by multiplication in $\mathbb{C}^r$ with the potential function $W(x)$. Inequality (2.6) implies that W has the operator norm bound $\|W\| \leqslant \|\mu\|$; this in turn means that H is semibounded with lower bound $H \geqslant -\|\mu\| I$. Because W is bounded, the unbounded operators H and H_0 have common domains $\mathscr{D}(H) = \mathscr{D}(H_0) \subset L^2(\mathbb{R}^d, \mathbb{C}^r)$. Take $\Lambda = \sigma(H)$ to be the spectrum of H and $\{E_\lambda \,|\, \lambda \in \Lambda\}$ to be the unique family of spectral projectors generated by H. The semiboundedness estimate above tells us that $\Lambda \subseteq [-\|\mu\|, \infty)$. The analytic semigroup operators are then defined by their spectral integrals

$$e^{-zH} = \int_\Lambda e^{-z\lambda}\, dE_\lambda, \quad z \in D. \tag{3.1}$$

Restricting $z = \beta > 0$ gives us the heat operator $e^{-\beta H}$. Replacing H by H_0 in (3.1) determines the free heat operator $e^{-\beta H_0}$.

Before proceeding with the derivations we introduce a number of the notational conventions that will be employed. The Hilbert space on which the semigroup operators act is $\mathscr{H} = L^2(\mathbb{R}^d, \mathbb{C}^r)$. On this space $\langle \cdot,\cdot \rangle$ represents the inner product and $\|f\| = \langle f, f\rangle^{1/2}$ the associated norm. For example, if $f, g \in \mathscr{H}$ then these functions have r components [i.e., $f = (f_1, f_2, \ldots, f_r)$, where $f_i \in L^2(\mathbb{R}^d)$ and similarly for g] and the $\mathscr{H}$-inner product is

$$\langle f, g\rangle = \sum_{i=1}^r (f_i, g_i), \tag{3.2}$$

where $(\cdot,\cdot)$ is the inner product on $L^2(\mathbb{R}^d)$. The general L^p norm for $f \in L^p(\mathbb{R}^d, \mathbb{C}^r)$ will be indicated by $\|f\|_p$. The nth-order iterated parametric integrals which enter the Dyson expansion will be abbreviated by

$$\int_>^1 d^n\xi \equiv \int_0^1 d\xi_1 \int_0^{\xi_1} d\xi_2 \cdots \int_0^{\xi_{n-1}} d\xi_n \tag{3.3}$$

and the iterated μ measure integrals

$$\int d^n\mu \equiv \int d\mu(k_n) \int d\mu(k_{n-1}) \cdots \int d\mu(k_1). \tag{3.4}$$

Note that for differing values of x_1 and x_2, generally

$$W(x_1)W(x_2) \neq W(x_2)W(x_1), \tag{3.5}$$

or equivalently $d\mu(k_1)d\mu(k_2) \neq d\mu(k_2)d\mu(k_1)$. This noncommutivity of the potentials $W(x_1), W(x_2)$ is the most significant structural distinction with the scalar problem. Our choice of the Euclidean norm (2.3) for the matrix measures μ is made on the basis that this norm definition for μ is the one that makes the bound estimates for the vector problem closely parallel to those that enter the scalar case. As a result, we are able to adopt many of the proofs for the scalar problem with only minor alterations.

Several simple mathematical functions occur repeatedly in our analysis so it is convenient to introduce an abbreviated notion for them. For $i = 1, \ldots, n$, let $\xi_i \in [0,1]$, set

$$\Theta(\xi_l, \xi_m) = \min\{\xi_l(1 - \xi_m), \xi_m(1 - \xi_l)\}. \tag{3.6}$$

For $k_i \in \mathbb{R}^d$ define the polynomials in k_i by

$$a_n(\xi_1, \ldots, \xi_n; k_1, \ldots, k_n) = \sum_{l,m=1}^n \Theta(\xi_l, \xi_m) k_l k_m, \tag{3.7}$$

$$b_n(\xi_1, \ldots, \xi_n; k_1, \ldots, k_n) = \sum_{l=1}^n [(1 - \xi_l)x + \xi_l y] k_l, \tag{3.8}$$

where $k_l k_m$ denotes the scalar product in $\mathbb{R}^d$. Furthermore we denote the scalar free diffusion kernel by

$$h(x;z) = (4\pi zq)^{-d/2} \exp\{-|x|^2/4zq\}. \tag{3.9}$$

The Dyson series for $e^{-\beta H}$ is obtained by iterating the identity[24]

$$e^{-\beta H} = e^{-\beta H_0} - \int_0^\beta d\beta_1\, e^{-\beta_1 H} V e^{-(\beta - \beta_1)H_0}. \tag{3.10}$$

The constructive series representation for $U(x,y;z)$ given in Lemma 2 and Theorem 1 results from the analysis of the x,y kernel analog of the Dyson series (3.10) followed by an analytic extension from the positive real axis $\beta \in (0, \infty)$ to $z \in D$. Except for some minor technical details in handling the vector norm on $\mathbb{C}^r$, Lemma 1 permits one to adopt in an obvious way the proofs given in Ref. 1. We have the following results.

Definition 1: Let $W \in \mathscr{F}^*$. For each $z \in \bar{D}$, let $F(\cdot,\cdot;z): \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}^{r \times r}$ be the function defined by the series

$$F(x,y;z) = \sum_{n=0}^\infty B_n(x,y;z), \tag{3.11}$$

where $B_0(x,y;z) = I$ and

$$B_n(x,y;z) = (-z)^n \int_>^1 d^n\xi \int d^n\mu\, e^{-zqa_n + ib_n}. \tag{3.12}$$

Lemma 2: Let $W \in \mathscr{F}^*$. The function $F(x,y;z)$ has the following properties.

(i) Let D_c be any compact subset of $\bar{D}$. The series (3.11) is absolutely and uniformly convergent for all $(x,y;z) \in \mathbb{R}^d \times \mathbb{R}^d \times D_c$. Furthermore, $F_{\nu\gamma}(x,y;z)$ has the bound

$$|F_{\nu\gamma}(x,y;z)| \leqslant e^{|z|\|\mu\|}. \tag{3.13}$$

(ii) $F(x,y;z)$ is a $\mathbb{C}^{r \times r}$ valued holomorphic function in D and continuous in $\bar{D}$. It is jointly continuous in $\mathbb{R}^d \times \mathbb{R}^d$.

In order to proceed further, let us define the free analytic semigroup kernel by

$$U_0(x,y;z) = h(x - y;z)I, \quad z \in \bar{D} \setminus \{0\}, \tag{3.14}$$

where h is (3.9). With this notation we have the following theorem.

Theorem 1: Let $W \in \mathscr{F}^*$. Define the function $U:\mathbf{R}^d \times \mathbf{R}^d \times (\overline{D} \setminus \{0\}) \mapsto \mathbf{C}^{r\times r}$ by

$$U(x,y;z) = U_0(x,y;z)F(x,y;z). \tag{3.15}$$

(i) For all $z \in D$ and all $f \in \mathscr{H}$,

$$(e^{-zH}f)(x) = \int dy\, U(x,y;z)f(y), \quad \text{a.a. } x \in \mathbf{R}^d. \tag{3.16}$$

(ii) Suppose $t \in \mathbf{R}$, $t \neq 0$, and $f \in L^1(\mathbf{R}^d,\mathbf{C}^r) \cap \mathscr{H}$,

$$(e^{-itH}f)(x) = \int dy U(x,y;it)f(y), \quad \text{a.a. } x \in \mathbf{R}^d. \tag{3.17}$$

If $f \in \mathscr{H}$ then

$$(e^{-itH}f)(x) = \text{s-}\lim_{Y\to\infty} \int_{|y|<Y} dy\, U(x,y;it)f(y). \tag{3.18}$$

The form of Theorem 1, in particular part (ii), for time-evolution kernels is the best result that can be expected since if H is replaced by H_0 then (ii) is the standard[25] representation of the free time evolution kernel. Related results on the existence of time evolution kernels have been obtained by Kitada,[26] Kitada and Kumanogo,[27] Fujiwara,[28] and Zelditch.[29]

Turn now to the problem of demonstrating that $U(x,y;it/\hbar)$ and $U(x,y;\beta)$ are fundamental solutions of their respective Schrödinger and heat partial differential equations.

Proposition 1: Let $W \in \mathscr{F}_2^*$, the function $U(x,y;it/\hbar)$ is the fundamental solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} U(x,y;it/\hbar) = H_{(x)} U(x,y;it/\hbar), \quad t \neq 0, \tag{3.19}$$

that satisfies the delta-function initial condition

$$U(x,y;it/\hbar) \to \delta(x-y)I, \quad \text{as } t \to 0. \tag{3.20}$$

Proposition 2: Let $W \in \mathscr{F}_2^*$, the function $U(x,y;\beta)$ is the fundamental solution of the heat equation

$$-\frac{\partial}{\partial \beta} U(x,y;\beta) = H_{(x)} U(x,y;\beta), \quad \beta > 0, \tag{3.21}$$

that satisfies the delta-function initial condition

$$U(x,y;\beta) \to \delta(x-y)I, \quad \text{as } \beta \to 0. \tag{3.22}$$

Proof: Propositions 1 and 2 have similar proofs. We shall write out the proof of Proposition 1. First substitute expression (3.15) into Eq. (3.19). So $U(x,y;it/\hbar)$ is a solution of (3.19) if and only if $F(x,y;it/\hbar)$ is a solution of

$$i\hbar \frac{\partial}{\partial t} F(x,y;it/\hbar) = \left\{ H_{(x)} - \frac{i\hbar}{t}(x-y)\nabla_x I \right\} F(x,y;it/\hbar). \tag{3.23}$$

The function $F(x,y;it/\hbar)$ as defined by series (3.11) converges uniformly in $\mathbf{R}^d \times \mathbf{R}^d$ to I as $t \to 0$. Furthermore it is well known that $U_0(x,y;it/\hbar)$ is a delta function in the limit $t \to 0$. Thus $U(x,y;it/\hbar)$ obeys the initial condition (3.20). So it suffices to prove that $F(x,y;it/\hbar)$ satisfies (3.23) for all t.

To proceed further, consider the terms $B_n(x,y;it/\hbar)$ in the series expansion (3.11) for F. Make the change of variable $\xi_i = (1 - t_i/t)$, $i = 1,\ldots,n$ for the integral expression of B_n. One obtains

$$B_n(x,y;it/\hbar) = \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \times \int d^n\mu \exp\{S_n\}, \tag{3.24}$$

where the exponential argument is

$$S_n(x,y;t_1\ldots t_n;k_1\ldots k_n) = -iq \sum_{l,m=1}^{n} \left(t_l \wedge t_m - \frac{t_l t_m}{t}\right) k_l k_m + i \sum_{l=1}^{n} \left[\frac{t_l}{t} x + \left(1 - \frac{t_l}{t}\right) y\right] k_l. \tag{3.25}$$

Here the notation $t_l \wedge t_m$ is

$$t_l \wedge t_m = \operatorname{sgn}(t) \operatorname{Min}\{|t_l|,|t_m|\}. \tag{3.26}$$

Note that S_n has the algebraic property

$$S_n(x,y;t_1\ldots t_n;k_1\ldots k_n)|_{t_n=t} = S_{n-1}(x,y;t_1\ldots t_{n-1};k_1\ldots k_{n-1}) + ixk_n. \tag{3.27}$$

Now assume $W \in \mathscr{F}_2^*$. Using formula (3.24) together with identity (3.27) gives one the recursion relation for $n \geqslant 1$,

$$i\hbar \frac{\partial}{\partial t} B_n\left(x,y;\frac{it}{\hbar}\right) = [-q\Delta x - (i\hbar/t)(x-y)\nabla_x] B_n(x,y;it/\hbar) + W(x)B_{n-1}(x,y;it/\hbar). \tag{3.28}$$

The assumption $W \in \mathscr{F}_2^*$ is needed in order to justify passing the derivative operators through the multiple integral in (3.24). The last step is to sum (3.28) from $n = 1$ to ∞. If $W \in \mathscr{F}_2^*$, all the infinite sums are absolutely and uniformly convergent in $\mathbf{R}^d \times \mathbf{R}^d$. In addition, the n-summation may be interchanged with all the differential operators appearing in (3.28). Thus (3.23) is satisfied for all x,y,t by $F(x,y;it/\hbar)$ defined through series (3.11). □

The solution of (3.19) and (3.20) is appropriately termed fundamental. All other forms of solution of the time-dependent Schrödinger equation are implied by Proposition 1. For example, one immediately obtains the following statement of the Cauchy-data problem.

Corollary 1: Let $W \in \mathscr{F}_2^*$. Suppose f is any wave packet (element) in $L^1(\mathbf{R}^d,\mathbf{C}^r) \cap \mathscr{H}$. Then

$$\psi(x,t) = \int dy U(x,y;it/\hbar)f(y) \tag{3.29}$$

is a solution of

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = H_{(x)} \psi(x,t), \tag{3.30}$$

with the Cauchy initial data

$$\psi(x,0) = f(x). \tag{3.31}$$

Proof: This follows from an obvious modification of the argument demonstrating Proposition 1. □

The remainder of this section implements a reordering of the series expansion for $F(x,y;z)$ and obtains the higher-order asymptotic expansion (1.10). It is proved that the number of terms M in the expansion is solely a function of the order of the bounded partial derivatives that $W(x)$ supports. Explicit formulas for the diagonal and nondiagonal values of $P_n(x,y)$ for all n are found. The remainder term $E_M(x,y;z)$ is given a bound that is uniform in both $\mathbf{R}^d \times \mathbf{R}^d$ and $\arg z \in [\pi/2, -\pi/2]$. It is observed that the asymptotic expansion (1.10) may be freely differentiated with respect to all the variables of $F(x,y;z)$.

Proposition 3: Let $W \in \mathcal{F}^*_{2(N+1)}$ and let K be the corresponding bound constant of W in the family $\mathcal{F}^*_{2(N+1)}$. For all $z \in \overline{D}$ and $n \geqslant 1$,

$$B_n(x,y;z) = \sum_{m=0}^{N} \frac{(-z)^{n+m}}{(n+m)!} q^m D_{m,n+m}(x,y) + E_{n,N}(x,y;z). \tag{3.32}$$

The coefficient functions $D_{m,n+m}(x,y)$ are jointly and uniformly continuous in $\mathbf{R}^d \times \mathbf{R}^d$ and are represented by the parametric integrals,

$$D_{m,m+n}(x,y) = n! \binom{m+n}{m} \int_{>}^{1} d^n\xi \int d^n\mu(a_n)^m e^{ib_n},$$
$$n > 0, \quad m \geqslant 0, \tag{3.33}$$

where the factor in front of the multiple integral is the binomial coefficient. Furthermore, $D_{0,0}(x,y) = I$, and for $m \geqslant 1$, $D_{m,m}(x,y) = 0$. The coefficient matrices and remainder term have estimates

$$|D_{m,m+n}(x,y)| \leqslant \binom{m+n}{m} \|\mu\|^n \left(\frac{nK}{2}\right)^{2m}, \tag{3.34}$$

$$|E_{n,N}(x,y;z)| \leqslant \frac{(|z|\,\|\mu\|)^n}{n!(N+1)!} \left(\frac{|z|qn^2K^2}{4}\right)^{N+1}, \tag{3.35}$$

for $m \leqslant N$ and $n \geqslant 0$.

Proof: The argument for Proposition 5, Ref. 1, is easily modified to accommodate the matrix nature of (3.32). □

The asymptotic expansion of the analytic semigroup kernel $U(x,y;z)$ follows from Proposition 3 and Lemma 2 for $F(x,y;z)$. Suppose $W \in \mathcal{F}^*_{2(M+1)}$ then F-series (3.11) is decomposed into two parts:

$$F(x,y;z) = \sum_{n=0}^{M} B_n(x,y;z) + \sum_{n=M+1}^{\infty} B_n(x,y;z). \tag{3.36}$$

Inserting (3.32) into (3.36) with $N = M - n$ constructs the M-term power series in z for $F(x,y;z)$ [Eq. (1.10)]. The definition of the error term in (1.10) is then

$$E_M(x,y;z) = \sum_{n=0}^{M} E_{n,M-n}(x,y;z) + \sum_{n=M+1}^{\infty} B_n(x,y;z). \tag{3.37}$$

It is straightforward to see that E_M is of order $O(|z|^{M+1})$. Concise bounds for E_M follow from the bounds (3.35) and the absolutely convergent integrals that define $B_n(x,y;z)$. By this process it is found that the following theorem holds.

Theorem 2: Let $W \in \mathcal{F}^*_{2(M+1)}$ and K be the associated bound constant in the space $\mathcal{F}^*_{2(M+1)}$. Let $U(x,y;z)$ and $U_0(x,y;z)$ be the integral kernels of operators e^{-zH} and e^{-zH_0}, respectively. Then for all $z \in \overline{D} \setminus \{0\}$,

$$U(x,y;z) = U_0(x,y;z) \left\{ \sum_{n=0}^{M} \frac{(-z)^n}{n!} P_n(x,y) + E_M(x,y;z) \right\}, \tag{3.38}$$

where the $\mathbf{C}^{r\times r}$ valued coefficient functions are [$P_0(x,y) = I$]

$$P_n(x,y) = \sum_{m=0}^{n-1} q^m D_{m,n}(x,y), \quad n = 1,\ldots,M. \tag{3.39}$$

The coefficient functions P_n and the remainder E_M have $\mathbf{R}^d \times \mathbf{R}^d$ uniform bounds for $z \in \overline{D}$

$$|P_n(x,y)| \leqslant (\|\mu\| + qn^2K^2/4)^n \tag{3.40}$$

and

$$|E_M(x,y;z)| \leqslant \frac{(|z|\,\|\mu\|)^{M+1}}{(M+1)!} \left\{ \left[1 + \frac{qM^2K^2}{4\|\mu\|}\right]^{M+1} + e^{|z|\|\mu\|} \right\}. \tag{3.41}$$

Several comments are in order. Although we do not formulate it as a theorem, it is apparent that if $W \in \mathcal{F}^*_{2(M+1+j)}$ then one may differentiate the F-asymptotic expansion j times with respect to z (for details see the proof of Theorem 2, Ref. 1). The resultant identity is an asymptotic expansion with uniform (in $x,y,\arg z$) error term of order $O(|z|^{M+1-j})$. Similar conclusions apply to differentiating (1.10) with respect to the variables x and y.

Equation (3.39) contains the general formula for the coefficient matrices that appear in the heat-kernel expansion (3.38). The $x \neq y$ off-diagonal formulas for the coefficients $P_n(x,y)$ have a geometrical character. Denote by $\hat{\xi}_i$ the linear path from x to y parametrized by ξ_i,

$$\hat{\xi}_i = (1-\xi_i)x + \xi_i y. \tag{3.42}$$

In terms of this linear path the formulas for $P_1(x,y)$ and $P_2(x,y)$ become

$$P_1(x,y) = \int_0^1 d\xi_1\, W(\hat{\xi}_1), \tag{3.43}$$

$$P_2(x,y) = 2\int_0^1 d\xi_1 \int_0^{\xi_1} d\xi_2\, W(\hat{\xi}_2)W(\hat{\xi}_1)$$
$$- 2q\int_0^1 d\xi_1\, \xi_1(1-\xi_1)(\Delta W)(\hat{\xi}_1). \tag{3.44}$$

So, $P_1(x,y)$ is just the linear average of W along on the straight line drawn in $\mathbf{R}^d$ between x and y. In $P_2(x,y)$, the q part is an average of ΔW weighted by the polynomial $\xi_1(1-\xi_1)$. Of course, the parametric integrals over ξ_i are inherited from the time-ordered parameters that appear in the Dyson expression (3.11).

The functions simplify markedly on the $x = y$ diagonal. If $x = y$ then $\hat{\xi}_i = x$ and is thus independent of the value of ξ_i. So in the integrals (3.43) and (3.44), and in general, the potentials W can be taken outside the parametric integration $d^n\xi$. The parametric integral $d^n\xi$ multiplies a given polynomial in $\xi_1,\xi_2,\ldots,\xi_n$ and yields a numerical coefficient. In this way one is able to determine all the formulas for diagonal values of P_n. Specific formulas for P_1 through P_4 are

$$P_1(x,x) = W(x), \tag{3.45}$$

$$P_2(x,x) = W^2(x) - \tfrac{1}{3}q(\Delta W)(x), \tag{3.46}$$

$$P_3(x,x) = W^3(x) - q\{\tfrac{1}{2}W(\Delta W) + \tfrac{1}{2}(\Delta W)W + \tfrac{1}{2}(\nabla W)^2\}(x)$$
$$+ \tfrac{1}{10}q^2(\Delta^2 W)(x), \tag{3.47}$$

$$P_4(x,x) = W^4(x) - q\{\tfrac{3}{5}W^2(\Delta W)$$
$$+ \tfrac{4}{5}W(\Delta W)W + \tfrac{3}{5}(\Delta W)W^2$$
$$+ \tfrac{4}{5}W(\nabla W)^2 + \tfrac{2}{5}(\nabla W)W(\nabla W) + \tfrac{4}{5}(\nabla W)^2 W\}(x)$$
$$+ q^2\{\tfrac{1}{5}W(\Delta^2 W) + \tfrac{1}{5}(\Delta^2 W)W + \tfrac{1}{3}(\Delta W)^2$$
$$+ \tfrac{2}{5}(\nabla W)[\nabla(\Delta W)] + \tfrac{2}{5}[\nabla(\Delta W)](\nabla W)$$
$$+ \tfrac{4}{15}(\nabla_2\nabla_1)^2 W_2 W_1\}(x) - \tfrac{1}{35}q^3(\Delta^3 W)(x). \tag{3.48}$$

If these coefficients are compared to the known formulas[8,30] for the $r=1$ case we see the first structural change occurs in the $P_3(x,x)$ coefficient, where the noncommutivity of W and ΔW lead to the symmetric combination $\frac{1}{2}W\Delta W+\frac{1}{2}\Delta WW$ rather than $W\Delta W$. The result available in the literature that comes closest to (3.45)–(3.48) is the determination by Fulling[31] of the coefficient matrices P_n for $r>1$ but with space dimension $d=1$. In this special case, complete agreement is found with Fulling's coefficient expressions, including the $n=5$ coefficient which we have not given above because of its substantial length.

Finally observe the symmetry that the P_n obeys as a consequence of the self-adjoint nature of H. Since H is self-adjoint, so is $e^{-\beta H}$, $\beta>0$. If * denotes the adjoint on $\mathbb{C}^{r\times r}$, then the integral kernel of $e^{-\beta H}$ satisfies

$$U(x,y;\beta)=U(y,x;\beta)^*. \tag{3.49}$$

Inserting (3.15) and series (1.10) in the above identity gives

$$P_n(x,y)=P_n(y,x)^*. \tag{3.50}$$

This follows since $h(x-y;\beta)$ is real and invariant under $x\leftrightarrow y$. If $r=1$, then (3.50) and the symmetry $P_n(x,y)=P_n(y,x)$ requires that the $P_n(x,y)$ be real valued.

The semiclassical facet of the heat-kernel expansion (1.10) resides in the fact that the $P_n(x,y)$ are polynomials in q of order $n-1$. It has been shown[32,33] in the $r=1$ case that if the asymptotic series for (1.10) is exponentiated, then a nonperturbative semiclassical approximation for $U(x,y;z)$ is defined. Furthermore, if $x=y$ the Wigner–Kirkwood semiclassical expansion[34,35] is recovered as a special case.

IV. RESOLVENT KERNEL EXPANSIONS

This section describes the large z asymptotic expansion of the resolvent kernel $R(x,y;z)$. The technique utilized is to investigate the behavior of $R(x,y;z)$ by using the Laplace transform (1.11) that connects the heat kernel to the resolvent kernel. In the first instance, the Laplace transform (1.11) is defined as a convergent integral only on the restricted set $\operatorname{Re} z<-\|\mu\|$. However by exploiting the holomorphic character in z of the kernels $U(x,y;z)$ it is possible to analytically continue the Laplace transform representation of $R(x,y;z)$ to the domain $\widetilde{V}_\delta$. With this approach the Laplace image of asymptotic expansion (3.38) for $U(x,y;z)$ becomes the asymptotic expansions for $R(x,y;z)$. Furthermore the error term bound (3.41) for $E_M(x,y;z)$ suffices to provide an $\mathbb{R}^d\times\mathbb{R}^d$ uniform error term bound for the $R(x,y;z)$ asymptotic expansion.

Let $\{E^0_\lambda|\lambda\geqslant 0\}$ be the family of spectral projectors that is defined by H_0. In terms of E^0_λ, the spectral representation of the free solvent is

$$r_0(z)=(H_0-z)^{-1}=\int_0^\infty\frac{1}{\lambda-z}dE^0_\lambda,\quad z\notin[0,\infty). \tag{4.1}$$

Consider first the kernel representation of the free resolvent.

Lemma 3: Suppose $\operatorname{Re} z<0$, then we have the following.

(i) For each $f\in L^2(\mathbb{R}^d,\mathbb{C}^r)$,

$$(r_0(z)f)(x)=\int_0^\infty e^{\beta z}(e^{-\beta H_0}f)(x)d\beta,\quad \text{a.a. } x. \tag{4.2}$$

(ii) Let $C_0=\{z|z\in\mathbb{C},\operatorname{Re} z<0\}$. Define the function $R_0:\mathbb{R}^d\times\mathbb{R}^d\times C_0\to\mathbb{C}^{r\times r}$ by the integral

$$R_0(x,y;z)=\int_0^\infty e^{\beta z}U_0(x,y;\beta)d\beta. \tag{4.3}$$

$R_0(x,y;z)$ is translation invariant in $\mathbb{R}^d\times\mathbb{R}^d$ (i.e., it depends only on the variable $x-y$). For each pair x,y $(x\neq y)$ $R_0(x,y;z)$ is an analytic function in domain C_0. Finally, $R_0(x,y;z)$ satisfies the integral estimate

$$\int dy\,|R_0(x,y;z)|\leqslant\frac{\sqrt{r}}{-\operatorname{Re} z}. \tag{4.4}$$

(iii) For $z\in C_0$, $r_0(z)$ is an integral operator with an L^1-convolution kernel $R_0(x,y;z)$. For each $f\in L^2(\mathbb{R}^d,\mathbb{C}^r)$,

$$(r_0(z)f)(x)=\int dy\,R_0(x,y;z)f(y),\quad \text{a.a. } x. \tag{4.5}$$

Proof: These results are all elementary but we will write out a detailed proof in a form that allows an easy extension to include the $(H-z)^{-1}$ case. Start with (i). Observe that the right-hand side of (4.2) defines an L^2 function of x:

$$\begin{aligned}\int dx\left|\int_0^\infty e^{\beta z}(e^{-\beta H_0}f)(x)d\beta\right|^2&\leqslant\int_0^\infty d\beta_1\int_0^\infty d\beta_2\,e^{(\beta_1+\beta_2)\operatorname{Re} z}\\&\quad\times\int dx\,|(e^{-\beta_1H_0}f)(x)|\,|(e^{-\beta_2H_0}f)(x)|\\&\leqslant\|f\|^2\left(\int_0^\infty d\beta\,e^{\beta\operatorname{Re} z}\right)^2<\infty.\end{aligned} \tag{4.6}$$

The second inequality follows from $\|e^{-\beta H_0}\|\leqslant 1$. Let g be an arbitrary element of $L^2(\mathbb{R}^d,\mathbb{C}^r)$. Then

$$\begin{aligned}A&\equiv\left\langle g,\int_0^\infty e^{\beta z}(e^{-\beta H_0}f)d\beta\right\rangle\\&=\int dx\,g(x)^*\left\{\int_0^\infty e^{\beta z}(e^{-\beta H_0}f)(x)d\beta\right\}.\end{aligned} \tag{4.7}$$

Using the Schwartz inequality and $\|e^{-\beta H_0}f\|\leqslant\|f\|$ it follows that the $dx\,d\beta$ integral in (4.7) is absolutely convergent. Fubini's theorem allows us to interchange the order of integration giving

$$\begin{aligned}A&=\int_0^\infty e^{\beta z}\langle g,e^{-\beta H_0}f\rangle d\beta\\&=\int_0^\infty e^{\beta z}\left\{\int_0^\infty e^{-\beta\lambda}d\langle g,E^0_\lambda f\rangle\right\}d\beta.\end{aligned} \tag{4.8}$$

The last equality employs the spectral theorem for H_0. The spectral measure has finite total variation bounded by $\|g\|\,\|f\|$. Further, $e^{\beta\operatorname{Re} z}d\beta$ is absolutely integrable, so the order of integration in (4.8) again can be reversed. Using

$$\int_0^\infty e^{\beta(z-\lambda)}d\beta=\frac{1}{\lambda-z}, \tag{4.9}$$

(4.8) takes the form

$$A=\int_0^\infty\frac{1}{\lambda-z}d\langle g,E^0_\lambda f\rangle=\langle g,r_0(z)f\rangle. \tag{4.10}$$

The equality of (4.10) and (4.7) for all $g\in L^2(\mathbb{R}^d,\mathbb{C}^r)$ implies (4.2).

(ii) The expression (3.14) for $U_0(x,y;\beta)$ shows that the integral (4.3) for a fixed pair x,y $(x\neq y)$ is absolutely convergent for $\text{Re}\, z<\epsilon<0$. Since the integrand of (4.3) is analytic in C_0 it follows that the integral defines an analytic function for $\text{Re}\, z<\epsilon$. Since ϵ may be selected to be as small as desired, the allowed domain for z may be extended to C_0. Here, $R_0(x,y;z)$ is translation invariant because $U_0(x,y;\beta)$ is a function of $x-y$. Finally, since $h(x-y;\beta)$ is real and positive,

$$\int dy|R_0(x,y;z)|\leqslant \int_0^\infty e^{\beta\,\text{Re}\, z}\sqrt{r}\left\{\int dy\, h(x-y;\beta)\right\} d\beta. \qquad (4.11)$$

The diffusion function $h(x-y;\beta)$ is normalized so that the dy integral is unity. Equation (4.4) follows by carrying out the $d\beta$ integration.

(iii) Identity (3.16) with $W=0$ states for $f\in L^2(\mathbb{R}^d,\mathbb{C}^r)$

$$(e^{-\beta H_0}f)(x)=\int dy\, U_0(x,y;\beta)f(y), \quad \text{a.a. } x. \qquad (4.12)$$

Combining this with (4.2) gives us

$$(r_0(z)f)(x)=\int_0^\infty e^{\beta z}\left\{\int dy\, U_0(x,y;\beta)f(y)\right\} d\beta. \qquad (4.13)$$

Changing the order of the $d\beta\, dy$ integrals here leads at once to formula (4.5) with $R_0(x,y;\beta)$ defined by (4.3). Now, consider the justification of this interchange of integral order. The iterated integral on the right of (4.13) is majorized by

$$A(x)=\int_0^\infty e^{\beta\,\text{Re}\, z}\left\{\int dy\, h(x-y;\beta)|f(y)|\right\} d\beta. \qquad (4.14)$$

All the functions in (4.14) are non-negative so it may be written

$$A(x)=\int dy\left\{\int_0^\infty e^{\beta\,\text{Re}\, z}h(x-y;\beta)d\beta\right\}|f(y)|$$

$$=\int dy\, r_0(x-y;\text{Re}\, z)|f(y)|, \qquad (4.15)$$

where $r_0(x-y;\text{Re}\, z)$ is just the resolvent kernel $R_0(x,y;\text{Re}\, z)$ in the $r=1$ case. Estimate (4.4) means that (4.15) is an L^1-convolution. Now the Hausdorff–Young inequality for convolutions[36] states that if we have a convolution

$$\psi(x)=\int dy\, K(x-y)\phi(y), \qquad (4.16)$$

where $K\in L^1(\mathbb{R}^d)$ and $\phi\in L^p(\mathbb{R}^d)$, $p\geqslant 1$, then

$$\|\psi\|_p\leqslant\|K\|_1\|\phi\|_p. \qquad (4.17)$$

Applying (4.17) to (4.15) with $p=2$, it follows that $A(x)$ is $L^2(\mathbb{R}^d)$ and thus $A(x)<\infty$ for all but an exceptional set of measure zero in $\mathbb{R}^d$. So, the majorant (4.14) of the iterated integral is absolutely convergent almost everywhere in x. Outside this exception set we apply Fubini's theorem in order to justify the change of integral order in (4.13). □

The next step is to extend our analysis to treat the full resolvent $r(z)$. For the self-adjoint operator H, we let $\{E_\lambda\,|\lambda\geqslant-\|\mu\|\}$ be the family of spectral projectors. The resolvent then has the spectral representation

$$r(z)=(H-z)^{-1}=\int_{-\|\mu\|}^\infty \frac{1}{\lambda-z}dE_\lambda, \quad z\in\rho(H). \qquad (4.18)$$

Lemma 4: Let $W\in\mathscr{F}^*$ and $\text{Re}\, z<-\|\mu\|$, then we have the following.

(i) For each $f\in L^2(\mathbb{R}^d,\mathbb{C}^r)$,

$$(r(z)f)(x)=\int_0^\infty e^{\beta z}(e^{-\beta H}f)(x)d\beta, \quad \text{a.a. } x. \qquad (4.19)$$

(ii) Let $C_\mu=\{z|z\in\mathbb{C},\text{Re}\, z<-\|\mu\|\}$. Define the function $R:\mathbb{R}^d\times\mathbb{R}^d\times C_\mu\to\mathbb{C}^{r\times r}$ by the integral

$$R(x,y;z)=\int_0^\infty e^{\beta z}U(x,y;\beta)d\beta. \qquad (4.20)$$

For each fixed pair x,y $(x\neq y)$, $R(x,y;z)$ is an analytic function of z with domain C_μ. Furthermore, for $z\in C_\mu$, $R(x,y;z)$ satisfies the pointwise bound

$$|R(x,y;z)|\leqslant\sqrt{r}|R_0(x,y;\text{Re}\, z+\|\mu\|)|, \quad \forall x,y\in\mathbb{R}^d. \qquad (4.21)$$

(iii) If $z\in C_\mu$, $r(z)$ is an integral operator with the kernel $R(x,y;z)$. For each $f\in L^2(\mathbb{R}^d,\mathbb{C}^r)$,

$$(r(z)f)(x)=\int dy\, R(x,y;z)f(y), \quad \text{a.a. } x. \qquad (4.22)$$

Proof: The estimate

$$\|e^{-\beta H}f\|\leqslant e^{\text{Re}\,\beta\|\mu\|}\|f\|, \quad f\in\mathscr{H}, \quad \beta\in\overline{D}, \qquad (4.23)$$

and estimate (3.13) for $|F_{\nu\gamma}(x,y;\beta)|$ allow us to follow the same line of argument used to prove Lemma 3 provided that the restriction $\text{Re}\, z<0$ is shifted to $\text{Re}\, z\leqslant-\|\mu\|$. The pointwise bound (4.21) results from

$$\left|\int_0^\infty e^{\beta z}U(x,y;\beta)d\beta\right|\leqslant\int_0^\infty e^{\beta\,\text{Re}\, z}|U(x,y;\beta)|d\beta$$

$$\leqslant\int_0^\infty e^{\beta(\text{Re}\, z+\|\mu\|)}rh(x-y;\beta)d\beta$$

$$\leqslant\sqrt{r}|R_0(x,y;\text{Re}\, z+\|\mu\|)|, \qquad (4.24)$$

where the second inequality is a consequence of (3.15) and (3.13). □

The existence of the Laplace transform (4.2) requires the restriction $\text{Re}\, z<0$. However, the domain of analyticity of $R_0(x,y;z)$ is considerably larger. First fix the polar coordinate representation of z by choosing $\arg z\in[0,2\pi)$ with the positive real axis corresponding to $\arg z=0$. With this notation, the transform (4.3) may be evaluated explicitly[37] yielding a modified Bessel function. For $x\neq y$,

$$R_0(x,y;z)=\frac{2}{(4\pi q)^{d/2}}\left(\frac{i|x-y|}{2q^{1/2}z^{1/2}}\right)^{1-d/2}$$

$$\times K_{(d/2)-1}(-iq^{-1/2}z^{1/2}|x-y|)I, \qquad (4.25)$$

where $z^{1/2}$ is the square root with positive sign. The right side of (4.25) is an analytic function with domain $\mathbb{C}\setminus[0,\infty)$.

In the subsequent anlaysis it is shown that one may exploit the analyticity of $U(x,y;\beta)$ in order to implement an analytic continuation of $R(x,y;z)$ from the domain C_μ to a larger subset of $\mathbb{C}$. The method utilizes contour rotation and depends only on the analytic semigroup properties obtained in Sec. III.

We introduce some convenient terminology. Heretofore, β has denoted a positive number. Now let $\beta\in\overline{D}$ and specify the polar form to be $\beta=|\beta|e^{i\arg\beta}$ with $\arg\beta\in[\pi/2,-\pi/2]$. For any $\delta\in(0,\pi/2]$ define two linear rays in D by

$$L^{\pm}(\delta)=\{\beta\in\overline{D}\,|\,\pm\arg\beta=\pi/2-\delta\}. \qquad (4.26)$$

Here, $L^+(\delta)$ is a ray in the upper right quadrant of the complex β-plane and $L^-(\delta)$ lies in the lower right quadrant. Let us introduce special notations for several different domains in $\mathbb{C}$ for the z-variable appearing in $R(x,y;z)$. For $\delta \in (0,\pi/2]$ define

$$V^+(\delta) = \{z \in \mathbb{C} | 2\delta < \arg z < \pi\}, \tag{4.27}$$

$$V^-(\delta) = \{z \in \mathbb{C} | \pi < \arg z < 2\pi - 2\delta\}. \tag{4.28}$$

Finally indicate by $V^\pm(\delta) + (-z')$ the set in $\mathbb{C}$ defined by translating the set $V^\pm(\delta)$ by $-z' \in \mathbb{C}$, i.e., $z + z' \in V^\pm(\delta)$.

Proposition 4: Let $W \in \mathcal{F}^*$ and parameter $\delta \in (0,\pi/2)$. Define $D_\delta^\pm = V^\pm(\delta) + (-\|\mu\|(\sin\delta)^{-1})$.

(i) If either $z \in D_\delta^+$ or $z \in D_\delta^-$ and $f \in L^2(\mathbb{R}^d, \mathbb{C}^r)$, then

$$(r(z)f)(x) = \int_{L^+(\delta)} e^{\beta z}(e^{-\beta H} f)(x) d\beta, \quad \text{a.a. } x, \tag{4.29}$$

where the integration path $L^+(\delta)$ is applicable for domain D_δ^+ and $L^-(\delta)$ for D_δ^-.

(ii) Define the functions $R^\pm: \mathbb{R}^d \times \mathbb{R}^d \times D_\delta^\pm \to \mathbb{C}^{r\times r}$ by the integral

$$R^\pm(x,y;z) = \int_{L^\pm(\delta)} e^{\beta z} U(x,y;\beta) d\beta. \tag{4.30}$$

For each fixed coordinate pair x,y $(x \neq y)$, $R^+(x,y;z)$ is an analytic function of z in D_δ^+ and $R^-(x,y;z)$ is an analytic function in D_δ^-. The functions $R^\pm$ satisfy for all $z \in D_\delta^\pm$ the pointwise estimate

$$|R^\pm(x,y;z)| \leqslant (\sqrt{r}/(\sin\delta)^{(d/2)-1}) |R_0(x,y; -|z_0|\sin^2\delta)|, \tag{4.31}$$

where $z_0 = z + \|\mu\|(\sin\delta)^{-1}$.

(iii) For z in either D_δ^+ or D_δ^-, then $r(z)$ is an integral operator with a kernel given by $R^+(x,y;z)$ or $R^-(x,y;z)$, respectively. For each $f \in L^2(\mathbb{R}^d, \mathbb{C}^r)$ and z in the appropriate domain D_δ^+ or D_δ^-, then

$$(r(z)f)(x) = \int dy\, R^\pm(x,y;z) f(y), \quad \text{a.a. } x. \tag{4.32}$$

(iv) $R^\pm(x,y;z)$ are analytic continuations of $R(x,y;z)$ from domain C_μ to the domains $D_\delta^\pm$. Specifically, for $x \neq y$,

$$R^+(x,y;z) = R(x,y;z), \quad z \in C_\mu \cap D_\delta^+, \tag{4.33}$$

$$R^-(x,y;z) = R(x,y;z), \quad z \in C_\mu \cap D_\delta^-. \tag{4.34}$$

Proof: (i) Define $u: \mathbb{R}^d \to \mathbb{C}^r$ by the integral

$$u(x) = \int_{L^+(\delta)} e^{\beta z}(e^{-\beta H} f)(x) d\beta. \tag{4.35}$$

By employing the Schwartz inequality it is easily shown that the $L^2(\mathbb{R}^d, \mathbb{C}^r)$ norm of u has the bound

$$\|u\| \leqslant \int_{L^+(\delta)} |e^{\beta z}|\, \|e^{-\beta H} f\|\, |d\beta|. \tag{4.36}$$

In order to establish the finiteness of the $L^+(\delta)$ integral in (4.36) it suffices to find an $|d\beta|$ integrable bound. To this end, introduce the following polar coordinates: $\beta = t\exp[i(\pi/2 - \delta)]$, $t = |\beta|$, $\beta \in L^+(\delta)$; $z_0 = z + \|\mu\|(\sin\delta)^{-1} = |z_0|\exp(i\theta)$. If $z_0 \in V^+(\delta)$, then $\theta \in (2\delta, \pi)$. Thus for all $z \in D_\delta^+$ one has

$$|e^{\beta z}| \leqslant \exp(-t|z_0|\sin(\theta - \delta) - t\|\mu\|). \tag{4.37}$$

Furthermore, inequality (4.23) provides the bound

$$\|e^{-\beta H} f\| \leqslant e^{t\|\mu\|\sin\delta} \|f\|, \quad \beta \in L^+(\delta). \tag{4.38}$$

Taken together, (4.37) and (4.38) give the estimate

$$|e^{\beta z}|\, \|e^{-\beta H} f\| \leqslant \exp(-t|z_0|\sin\delta - t\|\mu\|(1 - \sin\delta))\|f\|, \tag{4.39}$$

where we have used the fact that $\sin(\theta - \delta) \geqslant \sin\delta$ for $z_0 \in V^+(\delta)$. So (4.36) acquires the bound

$$\|u\| \leqslant \|f\|/(\|\mu\|(1 - \sin\delta) + |z_0|\sin\delta) < \infty. \tag{4.40}$$

Let g be an arbitrary $L^2(\mathbb{R}^d, \mathbb{C}^r)$ element. Form the inner product

$$\langle g,u \rangle = \int dx\, g(x)^* \left\{\int_{L^+(\delta)} e^{\beta z}(e^{-\beta H} f)(x) d\beta\right\}. \tag{4.41}$$

Inversion of integral order is permitted here since bound (4.40) together with the Schwartz inequality shows that the $dx|d\beta|$ integral is absolutely convergent. Introducing the spectral representation for $\langle g, e^{-\beta H} f\rangle$ gives

$$\langle g,u \rangle = \int_{L^+(\delta)} e^{\beta z} \left\{\int_{-\|\mu\|}^{\infty} e^{-\beta\lambda} d\langle g, E_\lambda f\rangle\right\} d\beta. \tag{4.42}$$

Upon utilizing

$$\int_{L^+(\delta)} e^{\beta(z-\lambda)} d\beta = \frac{1}{\lambda - z} \tag{4.43}$$

and a final inversion of integral order [valid because the measure $d\langle g, E_\lambda f\rangle$ is of finite total variation and $|e^{\beta z}|$ has estimate (4.37)] one obtains

$$\langle g,u \rangle = \int_{-\|\mu\|}^{\infty} \frac{1}{\lambda - z} d\langle g, E_\lambda f\rangle = \langle g, r(z) f\rangle, \tag{4.44}$$

or since g is arbitrary,

$$u = r(z)f. \tag{4.45}$$

This is (4.29) with contour $L^+(\delta)$ and z-domain D_δ^+. A similar argument applies to contour $L^-(\delta)$ and domain D_δ^-.

(ii) Given relationship (3.15) and estimate (3.13) it follows for $z \in D_\delta^\pm$ that the integral (4.30) is uniformly convergent. Since the integrand is analytic the integral defines a holomorphic function of z. The convolution bound (4.31) results from majorizing the integral with estimate (3.13) and inequality (4.37).

(iii) Combining identity (3.16) of Theorem 1 with Eq. (4.29) leads to

$$(r(z)f)(x) = \int_{L^+(\delta)} e^{\beta z} \left\{\int dy\, U(x,y;\beta) f(y)\right\} d\beta, \quad \text{a.a. } x. \tag{4.46}$$

Inverting the order of integration gives (4.32). In view of estimate (4.37) for $|e^{\beta z}|$ and the bound

$$|F(x,y;\beta) f(y)| \leqslant e^{|\beta|\|\mu\|} |f(y)|, \tag{4.47}$$

the convolution argument given in (4.14) and (4.15) may be used to show that the integral order in (4.46) may be reversed except possibly on a set of x having zero measure.

(iv) Consider the case with $z \in D_\delta^+$. Let s and S be real parameters $0 < s < S < \infty$. Define a closed contour in the analytic semigroup domain D by joining the four segments: $C_1 = \{\beta | s \leqslant \beta \leqslant S\}$, $C_2 = \{\beta | \beta = S e^{i\phi},\ \phi \in [0,(\pi/2) - \delta]\}$, $C_3 = \{\beta | \beta = t e^{i((\pi/2) - \delta)},\ s \leqslant t \leqslant S\}$ and $C_4 = \{\beta | \beta = s e^{i\phi},\ \phi \in [0,(\pi/2) - \delta]\}$. The kernel $U(x,y;\beta)$ is analytic in D.

Cauchy's theorem applied to the contour $C_1 + C_2 + C_3 + C_4$ states

$$\oint e^{\beta z} U(x,y;\beta)d\beta = 0. \tag{4.48}$$

We restrict z so that it lies in a subset of the union of D_δ^+ and C_μ; specifically we take

$$\operatorname{Re} z < -\|\mu\|/\sin\delta, \quad z \in D_\delta^+. \tag{4.49}$$

Now estimate the contribution of the C_2 integral as $S \to \infty$. Let the variable z_0 be that defined after (4.36). Assume $\epsilon > 0$ and note that condition (4.49) is obeyed if

$$z_0 = |z_0| e^{i(\pi/2 + \theta')}, \quad \theta' \in (0,\pi/2), \quad |z_0| > \epsilon. \tag{4.50}$$

Employing estimate (3.13), a computation of the Euclidean norm shows that

$$\left| \int_{C_2} e^{\beta z} U(x,y;\beta)d\beta \right| \leqslant \frac{r(\pi - 2\delta)Se^{-\epsilon a S}}{2(4\pi q S)^{d/2}}, \tag{4.51}$$

where $a > 0$ and is the minimum value of the two numbers $\sin\theta'$ and $\sin(\theta' + \pi/2 - \delta)$. Thus the C_2 contribution to (4.48) vanishes as $S \to \infty$. For $x \neq y$, similar reasoning and conclusions apply to the C_4 contribution as $s \to 0$. Thus after taking the limits $S \to \infty$ and $s \to 0$, (4.48) becomes

$$\int_{L^+(\delta)} e^{\beta z} U(x,y;\beta)d\beta = \int_0^\infty e^{\beta z} U(x,y;\beta)d\beta. \tag{4.52}$$

This is just equality (4.33) for the z allowed by (4.49). For $z \in D_\delta^-$ the argument proceeds by taking the contour in D that is the conjugate image of $C_1 + C_2 + C_3 + C_4$. □

In view of the fact that $R^\pm(x,y;z)$ and $R(x,y;z)$ represent the same analytic function we will drop the $\pm$ superscripts. Furthermore, we denote by $V(\delta)$ the z-plane sector $V^+(\delta) \cup V^-(\delta)$. Observe that inequality (4.31) provides in $V(\delta) + (-\|\mu\|(\sin\delta)^{-1})$ an L^1-convolution bound for the resolvent kernel $R(x,y;z)$. Convolution bounds commonly occur for resolvent kernels of elliptic differential operators. For a recent discussion of this topic see Gurarie.[38]

If the potential $W(x)$ is set equal to zero, the the conclusions of Proposition 4 specialize to the following corollary.

Corollary 2: Let $\delta \in (0,\pi/2)$, then we have the following.

(i) For $z \in V(\delta)$ the resolvent operator $r_0(z)$ has a kernel $R_0: \mathbb{R}^d \times \mathbb{R}^d \times V^\pm \to \mathbb{C}^{r \times r}$ given by the integral representation

$$R_0(x,y;z) = \int_{L^\pm(\delta)} e^{\beta z} U_0(x,y;\beta)d\beta, \tag{4.53}$$

where the path $L^+(\delta)$ is associated with domain $V^+(\delta)$, and $L^-(\delta)$ with $V^-(\delta)$.

(ii) For all x,y with $x \neq y$ and positive integers n,

$$\left(\frac{\partial}{\partial z}\right)^n R_0(x,y;z) = \int_{L^\pm(\delta)} \beta^n e^{z\beta} U_0(x,y;\beta)d\beta, \tag{4.54}$$

for z in the appropriate $V^\pm(\delta)$ domain.

(iii) If $n + 1 > d/2$ and $z \in V(\delta)$,

$$\left| \left(\frac{\partial}{\partial z}\right)^n R_0(x,y;z) \right| \leqslant \frac{\sqrt{r}\Gamma(n + 1 - (d/2))}{(4\pi q)^{d/2}} \left(\frac{1}{|z|\sin\delta}\right)^{n+1-(d/2)} \tag{4.55}$$

uniformly in $\mathbb{R}^d \times \mathbb{R}^d$.

Proof: (i) This is the statement of Proposition 4 that results if $W = 0$.

(ii) The absolute integrability of the integrand of (4.54) justifies passing the partial differentiation $(\partial/\partial z)^n$ through the integral sign in (4.53).

(iii) The right side of (4.55) is the outcome of taking the modulus of the integrand in (4.54) and completing the $|d\beta|$ integration. Symbol Γ denotes the gamma function. □

In the following we set $\tilde{V}_\delta = D_\delta^+ \cup D_\delta^-$. This is the allowed domain for the variation of z. Further it is convenient to denote the nth z-derivative of $R_0(x,y;z)$ by

$$R_0^{(n)}(x,y;z) = \left(\frac{\partial}{\partial z}\right)^n R_0(x,y;z). \tag{4.56}$$

The asymptotic expansion of the resolvent kernel of $r(z)$ for large z is described by the following theorem.

Theorem 3: Let $W \in \mathscr{F}^*_{2(M+1)}$ and let K be the associated bound constant of potential W in space $\mathscr{F}^*_{2(M+1)}$. Suppose $\delta \in (0,\pi/2)$. For $z \in \tilde{V}_\delta$ and all x,y $(x \neq y)$ the resolvent kernel of $(H - z)^{-1}$ admits the expansion

$$R(x,y;z) = \sum_{n=0}^{M} \frac{(-1)^n}{n!} P_n(x,y) R_0^{(n)}(x,y;z) + T_M(x,y;z). \tag{4.57}$$

Define the constant $C = C(\|\mu\|,M)$ by

$$C = \frac{\|\mu\|^{M+1}}{(M+1)!} \left[\left(1 + q\frac{M^2K^2}{4\|\mu\|}\right)^{M+1} + 1 \right]. \tag{4.58}$$

(i) For $z \in \tilde{V}_\delta$ and all integers $M > 0$ the error term has the $x \neq y$ nonuniform bound

$$|T_M(x,y;z)| \leqslant \frac{C(\sin\delta)^{M+2-(d/2)}}{\sqrt{r}} \times |R_0^{(M+1)}(x,y; -|(\sin^2\delta)z + (\sin\delta)\|\mu\||)|. \tag{4.59}$$

(ii) If $M + 2 > d/2$, then for $z \in \tilde{V}_\delta$ the error term has the $\mathbb{R}^d \times \mathbb{R}^d$ uniform bound

$$|T_M(x,y;z)| \leqslant \frac{C\Gamma(M + 2 - (d/2))}{(4\pi q)^{d/2}} \times \frac{1}{|(\sin\delta)z + \|\mu\||^{M+2-(d/2)}}. \tag{4.60}$$

Proof: If $z \in \tilde{V}_\delta$, then either $z \in D_\delta^+$ or $z \in D_\delta^-$. Suppose the first. In this case, the resolvent kernel $R(x,y;z)$ has the integral representation (4.30) with contour $L^+(\delta)$. Since $W \in \mathscr{F}^*_{2(M+1)}$ the semigroup kernel $U(x,y;z)$ obeys the asymptotic expansion (3.38) of Theorem 2. Thus $R(x,y;z)$ may be written

$$R(x,y;z) = \int_{L^+(\delta)} e^{\beta z} U_0(x,y;\beta) \times \left\{ \sum_{n=0}^{M} \frac{(-\beta)^n}{n!} P_n(x,y) + E_M(x,y;\beta) \right\} d\beta. \tag{4.61}$$

The n series is finite and may be passed through the $L^+(\delta)$ integral. Furthermore the individual terms in n are exactly of the form (4.54), so

$$R(x,y;z) = \sum_{n=0}^{M} \frac{(-1)^n}{n!} P_n(x,y) R_0^{(n)}(x,y;z) + T_M(x,y;z), \tag{4.62}$$

where the remainder T_M is defined by

$$T_M(x,y;z) = \int_{L^+(\delta)} e^{\beta z} U_0(x,y;\beta) E_M(x,y;\beta)d\beta. \tag{4.63}$$

If the upper bound (3.41) for E_M is used in (4.63) we have

$$|T_M(x,y;z)| \leqslant C \int_{L^+(\delta)} |e^{\beta z}| \; |h(x-y;\beta)| \times |\beta|^{M+1} e^{|\beta| \|\mu\|} \, |d\beta|, \quad (4.64)$$

where C is (4.58). Formula (4.59) for $|T_M|$ results if $|e^{\beta z}|$ is estimated by (4.37) and $|h|$ is bounded by

$$|h(x-y;\beta)| \leqslant \frac{1}{(4\pi q|\beta|)^{d/2}} \exp\left(-\frac{|x-y|^2}{4q|\beta|} \sin\delta\right). \quad (4.65)$$

Carrying out the $|d\beta|$ integration gives (4.59). Formula (4.60) follows from (4.59) and (4.55). This argument extends to $z \in D_\delta^-$ provided that contour $L^-(\delta)$ is used to represent $R(x,y;z)$. □

A number of comments are in order. An examination of the union of all allowed z domains $\widetilde{V}_\delta$ shows that there is a strip in $\mathbb{C}$ parallel to the positive real axis that is forbidden to z. All z whose least distance to the positive real axis is less than $\|\mu\|$ are in the complement of all $\widetilde{V}_\delta$. Thus Theorem 3 does not allow one to take z arbitrarily close to the real z axis in spite of the fact that $R(x,y;z)$ is analytic for all $z \notin [-\|\mu\|, \infty)$. This domain restriction appears in the analytic continuation technique of this section because of estimate (3.13) for $F(x,y;z)$. An examination of the proof of Lemma 2(see Ref. 1, Proposition 2) shows it has not used the fact that $W(x)$ is Hermitian. Series (3.11) will construct representations of e^{-zH} for non-self-adjoint operators H as well as self-adjoint ones. In the case of non-self-adjoint H the spectrum is not confined to the real axis but may be any point in $\mathbb{C}$ not exceeding a distance $\|\mu\|$ from the positive real axis. Thus the analytic continuation based only on estimate (3.13) cannot penetrate the allowed spectrum of the non-Hermitian operators H.

Consider briefly the behavior of identity (4.57). If $n+1 > d/2$, (4.55) shows that the term $R_0^{(n)}(x,y;z)$ has a $\mathbb{R}^d \times \mathbb{R}^d$ uniform $O(|z|^{-n-1+(d/2)})$ estimate. However, the terms with $n+1 \leqslant d/2$ are singular at $x=y$. Since T_M is bounded at $x=y$, one has the conclusion that the $x=y$ singularities of $R(x,y;z)$ and the singularities of the first $n \leqslant (d/2)-1$ terms of (4.57) must cancel. Finally, it should be recalled that the asymptotic expansion (4.57) has been derived assuming no other information about the potential $W(x)$ except the smoothness properties implied by the condition $W \in \mathscr{F}^*_{2(M+1)}$.

In the physics literature an asymptotic procedure similar to the one used in this section but applicable to quantum field theory in curved space-time may be found in DeWitt[39] and Christensen.[40] In the $r=1$ case, formula (4.57) is given in Ref. 30 and obtained heuristically. The treatment in Ref. 30 gave no estimate of the remainder nor a determination of the allowed z domain. In the $d=3$, $r=1$ case, Buslaev[9] found a formula equivalent to (4.57). Specifically for a C^∞ rapidly decreasing potential Buslaev succeeded in finding a bound of $|T_M|$ for z lying on the spectral boundary ($z = \lambda \pm i0$). This bound decreases as $\lambda \to +\infty$. Agmon and Kannai[41] have obtained a somewhat related expansion for a general class of elliptic differential operators defined on a compact manifold.

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