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Laplace asymptotic expansions of conditional Wiener integrals and generalised Mehler kernel formulae for Hamiltonians on $L^2(\mathbb{R}^n)$

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Abstract. We extend our previous results to derive Laplace asymptotic expansions for multi-dimensional conditional Wiener integrals. Applications are given to obtaining generalised Mehler kernel formulae, up to arbitrarily high orders in $\hbar$, for the kernels $\exp(-TH(\hbar)/\hbar)(x, y)$ and $\exp(-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar)(x, y)$ for $T>0$, where $H(\hbar)=(-\hbar^2/2)\Delta_3+V(x)$ and $H(\hbar, \boldsymbol{B})=2^{-1}(\mathrm{i}\hbar\nabla+2^{-1}(\boldsymbol{B}\wedge \boldsymbol{x}))^2+V(\boldsymbol{x})$. Here $V\in C^\infty(\mathbb{R}^3)$ is a real-valued potential which is bounded below together with its Hessian matrix and $\boldsymbol{B}$ is a constant vector. We emphasise that these results are valid for non-separable systems.

1. Introduction

In a previous paper (Davies and Truman (I), 1982) we derived generalised Mehler kernel formulae for one-dimensional Hamiltonians $H(\hbar)$ of the form $H(\hbar)=(-\hbar^2/2)\Delta_1+V(x)$ by means of a Laplace asymptotic expansion for one-dimensional conditional Wiener integrals. Following Schilder we required that the functional integrand concerned could be written in a specific form and gave rise to a unique non-degenerate global maximiser. Subsequently (Davies and Truman (II), 1983) we showed how the case of a finite number of non-degenerate global maximisers could be handled in an application to Bender–Wu type formulae. Powerful results, related to those above, for Gaussian integrals with functional integrands having a manifold of extrema have been derived by Ellis and Rosen (1980, 1981, 1984) using abstract results of Donsker and Varadhan (1981). These require one to use L^2-norm estimates as opposed to our use, following Schilder (1965), of the simpler L^∞-norm. We now revert to considering a functional integrand which gives rise to a unique global maximiser but deal with a multi-dimensional conditional Wiener integral.

Our first application extends the results of Davies and Truman (I). We obtain a generalised Mehler kernel formula, up to arbitrarily high order in $\hbar$, for the kernel $\exp[-TH(\hbar)/\hbar](x, y)$ where $H(\hbar)=(-\hbar^2/2)\Delta_3+V(x)$ in terms of corresponding classical mechanical quantities. The potential $V\in C^\infty(\mathbb{R}^3)$ is bounded below with its Hessian bounded below in the sense of quadratic forms. We may easily deal with n-dimensional systems but only work with $n=3$ for the sake of clarity.

The quantum mechanical Hamiltonian $H_F(\hbar, \boldsymbol{B})$ for a charged particle of unit mass moving in a constant magnetic field, $\boldsymbol{B}$, can be written as $H_F(\hbar, \boldsymbol{B})=2^{-1}(\mathrm{i}\hbar\nabla+2^{-1}\boldsymbol{B}\wedge \boldsymbol{x})^2$, $(e=c=1)$. A number of authors (Simon 1979, Avron *et al* 1978, Feynman and Hibbs 1965) have derived in a variety of ways, the following expression for the kernel $\exp[-tH_F(\hbar, \boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$,

$$\begin{aligned}\exp[-tH_F(\hbar, \boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})\\ &= (2\pi\hbar t)^{-1/2}[B4\pi\hbar \sinh(Bt/2)] \exp\{-[(x_3-y_3)^2/2\hbar t]\\ &\quad -[B/4\hbar \sinh(Bt/2)][(x_1-y_1)^2+(x_2-y_2)^2]-\tfrac{1}{2}\mathrm{i}B(x_1y_2-x_2y_1)\},\end{aligned}$$

where the reference frame has been chosen such that $\boldsymbol{B}=(0,0,B)$. One may also derive a similar expression for the kernel $\exp[-tH_F(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$ which, due to the analytic continuation in $\boldsymbol{B}$, does not have a complex exponent. ($\exp[-tH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$ is a convenient shorthand for the Green function of equation (1). We do not wish to imply any analyticity in $\boldsymbol{B}$ by the use of this notation.) This suggests that for some suitable class of potentials, $V(\boldsymbol{x})$, one should be able to derive generalised Mehler kernel formulae for differential operators of the form $[H_F(\hbar, \mathrm{i}\boldsymbol{B})+V(\boldsymbol{x})]$. It is common to require that the potential be axially symmetric about the field, $\boldsymbol{B}$, in problems of this type. We, however, do not require this. We obtain a generalised Mehler kernel formula, up to arbitrarily high orders in $\hbar$, for the kernel $\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$ where $H(\hbar, \mathrm{i}\boldsymbol{B})=2^{-1}[\mathrm{i}\hbar\nabla+2^{-1}(\mathrm{i}\boldsymbol{B}\wedge\boldsymbol{x})]^2+V(\boldsymbol{x})$, the real-valued potential $V\in C^\infty(\mathbb{R}^3)$, together with its Hessian, being bounded below and T being sufficiently small.

For the specific case of $V(\boldsymbol{x})=2^{-1}\boldsymbol{x}^TA^2\boldsymbol{x}$, where A^2 is strictly positive definite, we calculate the kernel and trace exactly, for all $T>0$, giving the spectrum of H in this case.

We point out that the above results are valid for non-separable systems and potentials (in the sense of Stäckel). This may better enable one to study the WKB quantisation condition for three-dimensional (or multi-dimensional) non-separable systems (see Percival (1977) for a short history of the problem).

We state theorems 1, 2, and 3 below together with their attendant conditions but their proofs will be contained in later sections. For ease of notation we will only consider three-dimensional integrals in theorem 1. For an indication of the refinements required in order to obtain the corresponding result, the reader should see Davies (1982). In what follows $C_0[0, T]$ is the Banach space of continuous functions $z:[0,T]\to\mathbb{R}^3$ with $z(0)=z(T)=0$ equipped with the supremum norm, $\|z\|=\sup\{|z(t)|: t\in[0,T]\}$, where $|\ |$ is the usual Euclidean norm on $\mathbb{R}^3$. $C_0[0, T]$ supports the unnormalised conditional Wiener measure $\mathrm{d}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z)$, with covariance

$$\int_{C_0[0,T]} {}^iz(s)\,{}^jz(t)\,\mathrm{d}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z)=\delta_{ij}s(1-t/T)(2\pi T)^{-3/2}, \qquad 0\leq s<t\leq T,$$

where δ_{ij} is the Kronecker delta and $z(\ )$ has the representation $z(\ )=({}^1z(\ ), {}^2z(\ ), {}^3z(\ ))$, with mean zero

$$\int_{C_0[0,T]} z(s)\,\mathrm{d}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z)=\boldsymbol{0}, \qquad 0\leq s\leq T.$$

For the associated probability measure

$$\mu^{-1}_{\boldsymbol{0},0;\boldsymbol{0},T}\{C_0[0,T]\}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z)=(2\pi T)^{3/2}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z),$$

we use the following notation

$$(2\pi T)^{3/2}\int_{C_0[0,\,T]} F(z)\,\mathrm{d}\mu_{\mathbf{0},0;\mathbf{0},T}(z)=\mathbb{E}_z^T\{F(z)\}$$

for suitable functionals F. $C_0^*[0, T]$ is the reproducing kernel Sobolev space associated with $C_0[0, T]$; $z\in C_0^*[0, T]$ if $z\in C_0[0, T]$, ${}^j\dot{z}\in L^2(\mathbb{R})$ and ${}^jz$ is absolutely continuous for $j=1,2,3$.

Theorem 1. Let $F(z)$ be a real-valued, continuous functional defined on $C_0[0, T]$ and suppose that the functional $(F(z)-2^{-1}\int_0^T \dot{z}(s)\cdot\dot{z}(s)\,\mathrm{d}s)$ has a unique maximum at $z_0\in C_0^*[0, T]$ with $(F(z_0)-2^{-1}\int_0^T \dot{z}_0(s)\dot{z}_0(s)\mathrm{d}s)=b$. If F satisfies conditions (1)–(6) below then,

$$\exp(-b\lambda^{-2})\mathbb{E}_z^T[\exp\{\lambda^{-2}F(\lambda z)\}]=\Gamma_0+\lambda\Gamma_1+\lambda^2\Gamma_2+\ldots+\lambda^{n-3}\Gamma_{n-3}+\mathrm{O}(\lambda^{n-2}),$$

as $\lambda\to 0$, where the Γ_i are conditional Wiener integrals dependent only on the functional F and its Frechet derivatives evaluated at z_0.

(i) $F(z)$ is measurable.

(ii) $F(z)\leqslant(b+L_1)+L_2\|z\|^2$, $\mu_{\mathbf{0},0;\mathbf{0},T}$ AE, where L_1 and L_2 are positive real numbers with $L_2<\min\{\gamma/2T, 1/12T\}$, γ being the constant given in lemma 7.

(iii) $F(z)$ is continuous for $\|z\|\leqslant\max\{2(L_1+1)^{1/2}/|L_2-1/2T|^{1/2}, [6T(L_1+1)/\gamma]^{1/2}\}$ and upper semi-continuous elsewhere on $C_0[0, T]$.

(iv) $F(z)$ has $n\geqslant 3$ continuous Frechet derivatives in a ball of radius δ centred at z_0 in $C_0[0, T]$, $\delta>0$. We further assume that the Frechet derivatives D^jF satisfy $D^jF(z_0+\boldsymbol{\eta})(z, z,\ldots, z)=\mathrm{O}(\|z\|^j)$ if $\|\boldsymbol{\eta}\|<\delta$. The bracket $(z, z, \ldots, z)$ contains j arguments.

(v) For some $\varepsilon>0$, for $\|\boldsymbol{\eta}\|<\delta$, $\mathbb{E}_z^T\{\exp[(1+\varepsilon)D^2F(z_0+\boldsymbol{\eta})(z, z)/2]\}$ is uniformly bounded.

(vi) ${}^j\dot{z}_0(\ )$ is of bounded absolute variation on $[0, T]$.

Since we can deduce the above result for $b\neq 0$ from the corresponding theorem with $b=0$ by making the substitution $F(z)\to\{F(z)-b\}$, we will only prove theorem 1 for the case of $b=0$. The net effect of increasing the dimension of the functional integral in theorem 1 is to restrict slightly the choice of possible integrands.

Theorem 2. Let $H(\hbar)$ be the self-adjoint quantum mechanical Hamiltonian $H(\hbar)=(-\hbar^2/2)\Delta_3+V$, where Δ_3 is the three-dimensional Laplacian and $V\in C^\infty(\mathbb{R}^3)$ is, together with its Hessian, bounded below. Let $\boldsymbol{X}_{\min}$ denote the unique minimiser of the functional

$$A(\boldsymbol{X})=\int_0^T [2^{-1}\dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)+V(\boldsymbol{X}(s))]\,\mathrm{d}s$$

over the space of paths $\mathscr{A}=\{\boldsymbol{X}:[0, T]\to\mathbb{R}^3|\boldsymbol{X}(0)=\boldsymbol{x}, \boldsymbol{X}(T)=\boldsymbol{y}, {}^j\boldsymbol{X}(\ )$ is absolutely continuous, $j=1,2,3\}$. Then for sufficiently small time $T>0$,

$$\exp[-TH(\hbar)/\hbar](\boldsymbol{x},\boldsymbol{y})=(2\pi\hbar T)^{-3/2}\exp[-A(\boldsymbol{X}_{\min})/\hbar]\mathbb{E}_z^T\{\exp[\hbar^{-1}F(\hbar^{1/2}z)]\}.$$

where

$$F(z)=-\int_0^T [V(\boldsymbol{X}_{\min}(s)+z(s))-V(\boldsymbol{X}_{\min}(s))-DV(\boldsymbol{X}_{\min}(s))z(s)]\,\mathrm{d}s$$

satisfies the conditions of theorem 1. Hence for each finite integer $n \geq 3$,

$$\exp[-TH(\hbar)/\hbar](x, y)$$

$$= (2\pi\hbar T)^{-3/2} \exp[-A(X_{\min})/\hbar]$$

$$\times\left\{\sum_{j=0}^{n-3} (j!)^{-1}\mathbb{E}_z^T\left[\exp\left(-2^{-1}\int_0^T D^2V(X_{\min}(s))(z(s), z(s))\,\mathrm{d}s\right)\right.\right.$$

$$\times\left(\hbar^{1/2}\int_0^T D^3V(X_{\min}(s))(z(s), z(s), z(s))\,\mathrm{d}s/3! + \cdots + \hbar^{(n-3)/2}\right.$$

$$\left.\left.\times\int_0^T D^{(n-1)}V(X_{\min}(s))(z(s), \ldots, z(s))\,\mathrm{d}s/(n-1)!\right)^j\right] + \mathrm{O}(\hbar^{(n-2)/2})\Bigg\}.$$

Given the constant vector $\boldsymbol{B}$ define the rotation matrix $R(s) \in \mathrm{O}(3)$ to be the rotation about $\boldsymbol{B}$ through $(2^{-1}|\boldsymbol{B}|s)$ radians, so that $R(0) = I$, $R^T(s)R(s) = I$ and $\dot{R}(s)R^T(s)y = 2^{-1}\boldsymbol{B} \wedge y$ for any $y \in \mathbb{R}^3$. Further, define the operator $R_x(\ )$ by $R_x(\ )H(x) = H(R(\ )x)$ for functions $H: \mathbb{R}^3 \to \mathbb{R}$. Also given $V \in C^\infty(\mathbb{R}^3)$ let us define $\tilde{V}(\ ,\ )$ by

$$\tilde{V}(x, t) = V(R(t)x) - (\boldsymbol{B} \wedge x)^2/8.$$

Theorem 3. Let $H(\hbar, \boldsymbol{B})$ be the quantum mechanical Hamiltonian $H(\hbar, \boldsymbol{B}) = 2^{-1}(\mathrm{i}\hbar\nabla + 2^{-1}\boldsymbol{B} \wedge x)^2 + V(x)$, where $V \in C^\infty(\mathbb{R}^3)$ is, together with its Hessian, bounded below and is sufficiently well behaved to ensure that conditions (*) are satisfied. Let $X_{\min}$ be the unique global minimiser of the functional

$$A(X) = \int_0^T [2^{-1}\dot{X}(s)\cdot\dot{X}(s) + \tilde{V}(X(s), T-s)]\,\mathrm{d}s$$

over the space $\mathscr{A}$, as defined previously, given that T is sufficiently small for it to exist. Define $G_0(x, y, T)$ by

$$G_0(x, y, T) = (2\pi\hbar T)^{-3/2} \exp[-A(X_{\min})/\hbar]\mathbb{E}_z^T\{\exp[\hbar^{-1}F(\hbar^{1/2}z)]\},$$

where

$$F(z) = -\int_0^T [\tilde{V}(X_{\min}(s) + z(s), T-s) - \tilde{V}(X_{\min}(s), T-s) - D\tilde{V}(X_{\min}(s), T-s)z(s)]\,\mathrm{d}s$$

satisfies the conditions of theorem 1, and T is sufficiently small to ensure that $G_0(x, y, T)$ exists. Then, for each integer $n \geq 3$,

$$\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](x, y)$$

$$= R_x(T)G_0(x, y, T)$$

$$= R_x(T)\Bigg\{(2\pi\hbar T)^{-3/2}\exp[-A(X_{\min})/\hbar]$$

$$\times\left[\sum_{j=0}^{n-3}(j!)^{-1}\mathbb{E}_z^T\left[\exp\left(2^{-1}\int_0^T D^2F(\mathbf{0})z^2\,\mathrm{d}s\right)\right.\right.$$

$$\times\left(\hbar^{1/2}\int_0^T D^3F(\mathbf{0})z^3\,\mathrm{d}s/3! + \ldots + \hbar^{(n-3)/2}\right.$$

$$\left.\left.\times\int_0^T D^{(n-1)}F(\mathbf{0})z^{n-1}\,\mathrm{d}s/(n-1)!\right)^j\right] + \mathrm{O}(\hbar^{(n-2)/2})\Bigg]\Bigg\},$$

where $\int_0^T D^j F(\mathbf{0}) z^j \, \mathrm{d}s$ is shorthand for

$$\int_0^T D^j \tilde{V}(\boldsymbol{X}_{\min}(s), T-s)(z(s), z(s), \ldots, z(s)) \, \mathrm{d}s.$$

Conditions (*), referred to above, will be stated in detail in § 3.

2. The generalised Mehler kernel formula

In this section we will be concerned with the kernel $\exp[-TH(\hbar)/\hbar](\boldsymbol{x}, \boldsymbol{y})$ where $H(\hbar)$ is the quantum mechanical Hamiltonian $H(\hbar) = (-\hbar^2/2)\Delta_3 + V$ with $V \in C^\infty(\mathbb{R}^3)$ bounded below. We are aiming to express the quantum mechanical Green function in terms of corresponding classical mechanical quantities up to arbitrarily high orders in $\hbar$. If the potential, V, is convex, then the quantum mechanical Green function is shown to satisfy a generalised Mehler kernel formula for arbitrary finite times $T > 0$. If V is not convex, but has its Hessian bounded below, then we must constrain T to be sufficiently small.

We begin with a result from the direct methods of the calculus of variations.

Lemma 1. Fix $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ and $T > 0$. Let the real-valued potential $V \in C^\infty(\mathbb{R}^3)$ be bounded below by $-\beta_0$. Let the functional

$$A(z) = \int_0^T [2^{-1}\dot{z}(s) \cdot \dot{z}(s) + V(z(s))] \, \mathrm{d}s$$

be defined for $z \in \mathscr{A}$, $\mathscr{A}$ being as in the statement of theorem 2. Then A attains its global minimum at at least one path $\boldsymbol{X}_{\min} \in \mathscr{A}$, $\boldsymbol{X}_{\min}$ is smooth and satisfies the Euler–Lagrange equation

$$\ddot{\boldsymbol{X}}_{\min}(s) = \nabla V(\boldsymbol{X}_{\min}(s)), \qquad s \in [0, T].$$

Proof. The method of proof is that used by Akhiezer (1962) when considering the analagous problem in one dimension. The absolute continuity of $\boldsymbol{X}_{\min}$ (by component) follows by the use of the Cauchy–Schwarz inequality and the fact that the minimising subsequence concerned converges uniformly to $\boldsymbol{X}_{\min}$. In the next lemma we will obtain our basic expression for the kernel $\exp[-TH(\hbar)/\hbar](\boldsymbol{x}, \boldsymbol{y})$.

Lemma 2. Let the self-adjoint quantum mechanical Hamiltonian $H(h) = (-h^2/2)\Delta_3 + V$ where the real-valued potential $V \in C^\infty(\mathbb{R}^3)$ is bounded below. Let the wavefunction $\psi \in \mathscr{S}(\mathbb{R}^3)$. Then, for each finite $T > 0$,

$$\exp[-TH(\hbar)/\hbar]\psi(\boldsymbol{x}) = \int \exp[-TH(\hbar)/\hbar](\boldsymbol{x}, \boldsymbol{y})\psi(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}$$

where the kernel is given by

$$\exp[-TH(\hbar)/\hbar](\boldsymbol{x}, \boldsymbol{y}) = \hbar^{-3/2} \exp[-A(\boldsymbol{X}_{\min})/\hbar] \int_{C_0[0, T]} \exp[\hbar^{-1} F(\hbar^{1/2} z)] \, \mathrm{d}\mu_{\mathbf{0},0;\mathbf{0},T}(z),$$

where

$$F(z) = -\int_0^T [V(\boldsymbol{X}_{\min}(s) + z(s)) - V(\boldsymbol{X}_{\min}(s)) - DV(\boldsymbol{X}_{\min}(s)) z(s)] \, \mathrm{d}s,$$

$\boldsymbol{X}_{\min}$ is the global minimiser of A above and $\mu_{\mathbf{0},0;\mathbf{0},T}$ is the unnormalised conditional Wiener measure on $C_0[0, T]$.

Proof. The proof required here is just the three-dimensional analogue of the proof of lemma 2 in Davies and Truman (I). Essentially, one makes use of the Feynman–Kac formula, a Cameron–Martin translation formula and the identity

$$\mathbb{E}_z\{F(z)\} = \int\int \mathrm{d}\mu_{\mathbf{0},0;z(T),T}(z)\,\mathrm{d}z(T)F(z)$$

where $\mathbb{E}_z\{\ \}$ denotes expectation with respect to Wiener measure. Lemma 2 has the following corollary.

Corollary 1. Let $H(\hbar)$ and V be as defined above. Then for $\lambda = \hbar^{1/2}$

$$\exp[-TH(\hbar)/\hbar](\boldsymbol{x}, \boldsymbol{y})$$
$$= (2\pi\hbar T)^{-3/2}\exp[-A(\boldsymbol{X}_{\min})/\hbar]\mathbb{E}_z^T\{\exp[\lambda^{-2}F(\lambda z)]\},$$

where $F(z)$ is as before and

$$F(z) - 2^{-1}\int_0^T \dot{z}(s)\cdot\dot{z}(s)\,\mathrm{d}s = A(\boldsymbol{X}_{\min}) - A(\boldsymbol{X}_{\min} + z),$$

for $z \in C_0^*[0, T]$.

Proof. The first part is obvious and the second part follows after a simple integration by parts.

For us to be able to apply theorem 1 we require the maximum of $[A(\boldsymbol{X}_{\min}) - A(\boldsymbol{X}_{\min} + z)]$ to be unique in $C_0^*[0, T]$. By definition of $\boldsymbol{X}_{\min}$ this maximum will be zero and will be uniquely attained at $z \equiv \mathbf{0}$ iff $\boldsymbol{X}_{\min}$ is the unique global minimiser of A over $\mathcal{A}$. When the Hessian of V is bounded below, in the sense of quadratic forms, the next lemma ensures this uniqueness.

Lemma 3. Let $V \in C^\infty(\mathbb{R}^3)$ be real valued, bounded below and have its Hessian, $\nabla^2 V$, satisfy

$$\boldsymbol{\eta}^{\mathrm{T}}\nabla^2 V\boldsymbol{\eta} \geqslant -|\beta_2|\boldsymbol{\eta}^{\mathrm{T}}\boldsymbol{\eta}, \qquad \text{(T denotes transpose)}$$

for all $\boldsymbol{\eta} \in \mathbb{R}^3$ and some $\beta_2 \in \mathbb{R}$. Then $\boldsymbol{X}_{\min}$, the global minimiser of A over $\mathcal{A}$, is unique for sufficiently small $T > 0$.

Proof. Assume that there are two such global minimisers $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$. Both $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ are absolutely continuous and satisfy the Euler–Lagrange equation

$$\ddot{\boldsymbol{X}}(s) = \nabla V(\boldsymbol{X}(s)) = DV(\boldsymbol{X}(s)), \qquad s \in [0, T].$$

If $\boldsymbol{H}(s) = \boldsymbol{X}_1(s) - \boldsymbol{X}_2(s)$ then $\boldsymbol{H}(0) = \boldsymbol{H}(T) = \mathbf{0}$ and

$$\ddot{\boldsymbol{H}}(s) = DV(\boldsymbol{X}_1(s)) - DV(\boldsymbol{X}_2(s)), \qquad s \in [0, T].$$

Let $G(t)$ be the real valued function

$$G(t) = V(\boldsymbol{X}_2(s) + t\boldsymbol{H}(s)), \qquad t \in [0, 1].$$

Differentiation quickly yields

$$\dot{G}(t) = DV(\boldsymbol{X}_2(s) + t\boldsymbol{H}(s))\boldsymbol{H}(s),$$
$$\ddot{G}(t) = D^2 V(\boldsymbol{X}_2(s) + t\boldsymbol{H}(s))(\boldsymbol{H}(s), \boldsymbol{H}(s)),$$

and from these one obtains

$$\ddot{\boldsymbol{H}}(s)\cdot\boldsymbol{H}(s) = \int_0^1 D^2 V(\boldsymbol{X}_2(s) + t\boldsymbol{H}(s))(\boldsymbol{H}(s), \boldsymbol{H}(s))\,\mathrm{d}t.$$

Integrating with respect to s gives, after an integration by parts,

$$\int_0^T \dot{\boldsymbol{H}}(s)\cdot\dot{\boldsymbol{H}}(s)\,\mathrm{d}s = -\int_0^T\int_0^1 \boldsymbol{H}^T(s)\nabla^2 V(\boldsymbol{X}_2(s) + t\boldsymbol{H}(s))\boldsymbol{H}(s)\,\mathrm{d}t\,\mathrm{d}s.$$

The Rayleigh–Ritz quotient bound for the least eigenvalue, λ, of the equation $\ddot{\boldsymbol{H}}(s) = -\lambda\boldsymbol{H}(s)$, $\boldsymbol{H}(0) = \boldsymbol{H}(T) = \boldsymbol{0}$ gives us

$$\int_0^T \dot{\boldsymbol{H}}(s)\cdot\dot{\boldsymbol{H}}(s)\,\mathrm{d}s \geqslant (\pi/T)^2\int_0^T \boldsymbol{H}(s)\cdot\boldsymbol{H}(s)\,\mathrm{d}s.$$

Using this inequality and $\nabla^2 V \geqslant -|\beta_2| I$ gives

$$(\pi/T)^2\int_0^T \boldsymbol{H}(s)\cdot\boldsymbol{H}(s)\,\mathrm{d}s \leqslant |\beta_2|\int_0^T \boldsymbol{H}(s)\cdot\boldsymbol{H}(s)\,\mathrm{d}s.$$

Thus for $T < \pi|\beta_2|^{-1/2}$ we have $\boldsymbol{X}_1 \equiv \boldsymbol{X}_2$. If V were convex, $\beta_2 = 0$ then $\boldsymbol{X}_1 \equiv \boldsymbol{X}_2$ for all $T > 0$.

Proof of Theorem 2. The majority of the work required to prove theorem 2 has been carried out in proving lemmas 1, 2, and 3 and corollary 1. We need only prove that the functional $F(z)$ satisfies conditions (1)–(6) of theorem 1. Note that we already require $T < \pi|\beta_2|^{-1/2}$. Conditions (1), (3), (4) and (6) are easy to check since F is well behaved. Condition (2) demands that $F(z) \leqslant L_1 + L_2\|z\|^2$ for some positive L_1 and L_2. Recall that

$$F(z) = -\int_0^T [V(\boldsymbol{X}_{\min}(s) + z(s)) - V(\boldsymbol{X}_{\min}(s)) - DV(\boldsymbol{X}(s))z(s)]\,\mathrm{d}s.$$

Using the method employed in the previous lemma with $G(t) = V(\boldsymbol{X}_{\min}(s) + tz(s))$ this time, we get

$$F(z) \leqslant |\beta_2| T\|z\|^2/2 = L_2\|z\|^2, \qquad \text{say.}$$

We must have $L_2 < \min\{\gamma/2T, 1/12T\}$ and so we require $T^2 < \min\{\gamma/|\beta_2|, 1/6|\beta_2|\}$. To satisfy condition (5) we constrain T to be strictly less than $(2\gamma/|\beta_2|)^{1/2}$. Collating all the upper bounds for T we finally have that theorem 2 is valid for $T < (6|\beta_2|)^{-1/2}$, (γ being $\frac{2}{3}$).

The final identity of theorem 2 follows from the final part of the proof of theorem 1.

The following corollary will explicitly show how we connect the result of theorem 2 with a generalised Mehler formula for the kernel $\exp(-TH(\hbar)/\hbar)(\boldsymbol{x}, \boldsymbol{y})$.

Corollary 2. Let $H(\hbar)$ and V be defined as in the statement of theorem 2. Then setting $A(\boldsymbol{X}_{\min}) = A(x, y, T)$ we have, for sufficiently small T,

$$\exp(-TH(\hbar)/\hbar)(x, y) = (2\pi\hbar)^{-3/2}\exp[-A(x, y, T)/\hbar]|-\partial^2 A(x, y, T)/\partial x^j \partial y^k|^{1/2}[1 + \hbar K_1 + O(\hbar^2)],$$

where $|\ |$ represents the determinant and K_1 may be explicitly evaluated in terms of the Frechet derivatives of V of order less than six and $G(\sigma, t)$ (the Feynman–Green function) the Green function of the Sturm–Liouville differential operator $\{[(\mathrm{d}^2/\mathrm{d}\sigma^2) - \nabla_j \nabla_k V(\boldsymbol{X}_{\min}(\sigma))]\}$ with Dirichlet boundary conditions.

Proof. The proof of this result depends on the identity

$$T^{-3/2}\mathbb{E}_z^T\left[\exp\left(\sum_{i=1}^n \alpha_i \cdot z(s_i)\right)\exp\left(-2^{-1}\int_0^T D^2 V(\boldsymbol{X}_{\min}(s))(z(s), z(s))\,\mathrm{d}s\right)\right] = |-\partial^2 A(x, y, T)/\partial x^j \partial y^k|^{1/2}\exp\left(2^{-1}\sum_{i,j=1}^n \boldsymbol{\alpha}_i^{\mathrm{T}} G(s_i, s_j)\boldsymbol{\alpha}_j\right).$$

This identity is proved in exactly the same manner as the analagous one-dimensional result in Davies and Truman (I), and we will not prove it herein. We do not give K_1 explicitly as for general V it involves some unpleasant combinatorics. The necessary combinatorics for the one-dimensional result may be found in Davies (1982). We point out, however, that for a given potential V the calculation of K_1 is straightforward, if tedious.

3. A generalised Mehler kernel formula for Zeeman-effect Hamiltonians

By using similar results to those contained in the previous section we now show how to obtain an asymptotic expansion, in powers of $\hbar$, for the kernel $\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](x, y)$ where $H(\hbar, \mathrm{i}\boldsymbol{B})$ is the quantum mechanical Hamiltonian $H(\hbar, \mathrm{i}\boldsymbol{B}) = 2^{-1}(\mathrm{i}\hbar\nabla + 2^{-1}\mathrm{i}\boldsymbol{B}\wedge \boldsymbol{x})^2 + V$, with $V \in C^\infty(\mathbb{R})$ bounded below. We begin with a short description of the motivation behind our method.

For a charged particle moving in a constant magnetic field $\boldsymbol{B}$ subject to some external potential V, the quantum mechanical Hamiltonian of the system is $H(\hbar, \boldsymbol{B}) = 2^{-1}(\mathrm{i}\hbar\nabla + 2^{-1}\boldsymbol{B}\wedge \boldsymbol{x})^2 + V(\boldsymbol{x})$, where $V \in \mathcal{S}(\mathbb{R}^3)$ say. We may express this Hamiltonian in the form $H(\hbar, \boldsymbol{B}) = (-\hbar^2/2)\Delta_3 + (\boldsymbol{B}\wedge\boldsymbol{x})^2/8 + 2^{-1}\boldsymbol{L}\cdot\boldsymbol{B}$, where $\boldsymbol{L}$ is the angular momentum operator $\boldsymbol{L} = -\mathrm{i}\hbar(\boldsymbol{x}\wedge\nabla)$. If we assume that V is axially symmetric about $\boldsymbol{B}$ and that the spectral projections of $\boldsymbol{L}\cdot\boldsymbol{B}$ commute with the spectral projections of $H_0(\hbar, \boldsymbol{B}) = (-\hbar^2/2)\Delta_3 + (\boldsymbol{B}\wedge\boldsymbol{x})^2/8 + V(\boldsymbol{x})$ then, assuming that the domains are reasonable, we have

$$\exp[-\mathrm{i}tH(\hbar, \boldsymbol{B})/\hbar] \equiv \exp[-\mathrm{i}tH_0(\hbar, \boldsymbol{B})/\hbar]\exp[-\mathrm{i}t(\boldsymbol{L}\cdot\boldsymbol{B})/2\hbar].$$

The effect of $\exp[-\mathrm{i}t(\boldsymbol{L}\cdot\boldsymbol{B})/2\hbar]$ is just a rotation of axes through $|\boldsymbol{B}|t/2$ radians about $\boldsymbol{B}$. Hence for $\psi \in \mathcal{S}(\mathbb{R}^3)$, we may write,

$$\exp[-\mathrm{i}tH(\hbar, \boldsymbol{B})/\hbar]\psi(\boldsymbol{x}) = \exp[-\mathrm{i}tH_0(\hbar, \boldsymbol{B})/\hbar]\psi(R(t)\boldsymbol{x})$$

where R is the matrix that was defined immediately preceeding the statement of theorem 3. This all suggests that a rotation of axes may simplify the evaluation of the kernel $\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](x, y)$.

The diffusion equation corresponding to this kernel is

$$\hbar\, \partial u/\partial t = [(\hbar^2/2)\Delta_3 + (\boldsymbol{B}\wedge \boldsymbol{x})^2/8 - V(\boldsymbol{x}) + 2^{-1}\hbar \boldsymbol{B}\cdot(\boldsymbol{x}\wedge\nabla)]u, \qquad (1)$$

where $u = u(\boldsymbol{x}, t)$. We will not require V to be axially symmetric about $\boldsymbol{B}$ or $V\in \mathscr{S}(\mathbb{R}^3)$. The requirements on V and its derivatives will be given shortly. Let $\boldsymbol{y} = R(t)\boldsymbol{x}$ and set

$$\tilde{u}(\boldsymbol{y}, t) = u(R^{\mathrm{T}}(t)\boldsymbol{y}, t) = u(\boldsymbol{x}, t).$$

Changing independent variables to $\boldsymbol{y}$, we derive the diffusion equation for $\tilde{u}$

$$\hbar\, \partial \tilde{u}/\partial t = [(\hbar^2/2)\Delta_3 + (\boldsymbol{B}\wedge \boldsymbol{y})^2/8 - V(R^{\mathrm{T}}(t)\boldsymbol{y})]\tilde{u}. \qquad (2)$$

If we had chosen V to be axially symmetric about $\boldsymbol{B}$ then the above equation would have been considerably simplified. For convenience we reintroduce $\tilde{V}(\boldsymbol{x}, t) = V(R^{\mathrm{T}}(t)\boldsymbol{x}) - (\boldsymbol{B}\wedge\boldsymbol{x})^2/8$. Following Tingley (1956) the solution of the above diffusion equation is

$$\tilde{u}(\boldsymbol{y}, t) = \mathbb{E}_z\left[\exp\left(-\hbar^{-1}\int_0^t \tilde{V}(x+\hbar^{1/2}z(s), t-s)\,\mathrm{d}s\right)\tilde{u}(\boldsymbol{x}+\hbar^{1/2}\boldsymbol{z}(t), 0)\right], \qquad t < t_{\mathrm{m}},$$

where $\mathbb{E}_z\{\ \}$ denotes expectation with respect to Wiener measure. Note that the second argument of $\tilde{V}$ is $(t-s)$ and not s. We require $\tilde{V}$ and $\tilde{u}$ to satisfy the following

(i) $$-\tilde{V}(\boldsymbol{x}, t) \leq C_1 + \sum_{j=1}^{3} D_{1j}x_j^2$$

(ii) $$|\tilde{V}_t(\boldsymbol{x}, t)|, |\tilde{V}_{x_j}(\boldsymbol{x}, t)|, |\tilde{V}_{x_jx_j}(\boldsymbol{x}, t)| \leq C_2 \exp\left(\sum_{j=1}^{3} D_{2j}x_j^2\right),$$

(iii) $$\tilde{u}(\boldsymbol{x}, 0)\exp\left(-\sum_{j=1}^{3} d_j x_j^2\right) \in L^1(\mathbb{R}^3),$$

where C_1, C_2, D_{1j}, D_{2j} and d_j are non-negative constants for $j = 1, 2, 3$. We denote the above conditions on $\tilde{V}$ as conditions (*). In what follows we choose $\tilde{u}\in C_0^\infty(\mathbb{R}^3)$ and so we may neglect condition (3). Let $t_{\mathrm{m}} = t_{\mathrm{m}}(\tilde{V})$ satisfy the inequalities:

$$D_{1j} + (\hbar\pi^2/t_{\mathrm{m}})D_{2j} < (\hbar\pi/4t_{\mathrm{m}})^2, \qquad j = 1, 2, 3.$$

We now proceed in a similar manner to the previous section. Without loss of generality we may set $\boldsymbol{B} = (0, 0, B)$.

Lemma 4. Fix $\boldsymbol{x}, \boldsymbol{y}\in\mathbb{R}^3$ and $T > 0$. Let the real-valued potential $V\in C^\infty(\mathbb{R}^3)$ be bounded below by $-\beta_1$. Let the functional

$$A(\boldsymbol{X}) = \int_0^T [2^{-1}\dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s) + \tilde{V}(\boldsymbol{X}(s), T-s)]\,\mathrm{d}s,$$

be defined on the space $\mathscr{A}$ where $\mathscr{A} = \{\boldsymbol{X}:[0, T]\to\mathbb{R}^3 | X^j(\ )$ is absolutely continuous, $j = 1, 2, 3$, $\boldsymbol{X}(0) = \boldsymbol{x}$, $\boldsymbol{X}(T) = \boldsymbol{y}\}$. As above $\tilde{V}(\boldsymbol{x}, t) = V(R^{\mathrm{T}}(t)\boldsymbol{x}) - (\boldsymbol{B}\wedge\boldsymbol{x})^2/8$ with $\boldsymbol{B} = (0, 0, B)$. Then, for sufficiently small time $T > 0$, the functional A attains its global minimum at at least one path $\boldsymbol{X}_{\min}\in\mathscr{A}$ with $\boldsymbol{X}_{\min}$ smooth and satisfying the Euler–Lagrange equation

$$\ddot{\boldsymbol{X}}_{\min}(s) = R(T-s)\nabla V(R^{\mathrm{T}}(T-s)\boldsymbol{X}_{\min}(s)) + \boldsymbol{B}\wedge(\boldsymbol{B}\wedge\boldsymbol{X}_{\min}(s))/4, \qquad s\in[0, T],$$

$$\boldsymbol{X}_{\min}(0) = \boldsymbol{x}, \qquad \boldsymbol{X}_{\min}(T) = \boldsymbol{y}.$$

Proof. If we can bound A below in the manner

$$A(\boldsymbol{X}) \geq \alpha \int_0^T \dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)\,\mathrm{d}s + \xi, \qquad \alpha > 0,$$

the problem is solved since we can then mimic the proof of lemma 1. Now,

$$A(\boldsymbol{X}) = 2^{-1}\int_0^T \dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)\,\mathrm{d}s + \int_0^T \{V[R^{\mathrm{T}}(T-s)\boldsymbol{X}(s)] - [\boldsymbol{B}\wedge\boldsymbol{X}(s)]^2/8\}\,\mathrm{d}s$$

$$\geq 2^{-1}\int_0^T \dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)\,\mathrm{d}s - \int_0^T (\boldsymbol{B}\wedge\boldsymbol{X}(s))^2/8\,\mathrm{d}s - \beta_1 T.$$

Using the norm inequality

$$\|\boldsymbol{X}\|^2 \leq T(1+2|\boldsymbol{x}|)\int_0^T \dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)\,\mathrm{d}s + |\boldsymbol{x}|(2+|\boldsymbol{x}|), \qquad \boldsymbol{X}\in\mathscr{A},$$

and

$$\int_0^T (\boldsymbol{B}\wedge\boldsymbol{X}(s))^2\,\mathrm{d}s \leq B^2 T\|\boldsymbol{X}\|^2$$

we get

$$A(\boldsymbol{X}) \geq (2^{-1} - B^2T^2(1+2|\boldsymbol{x}|)/8)\int_0^T \dot{\boldsymbol{X}}(s)\cdot\dot{\boldsymbol{X}}(s)\,\mathrm{d}s + \xi, \qquad \text{say.}$$

For $T < 2/|B|(1+2|\boldsymbol{x}|)^{1/2}$ we have the required inequality. The result now follows as in lemma 1.

Lemma 5. Let $H(\hbar, \boldsymbol{B})$ be the quantum mechanical Hamiltonian $H(\hbar, \boldsymbol{B}) = 2^{-1}(\mathrm{i}\hbar\boldsymbol{\nabla} + 2^{-1}\boldsymbol{B}\wedge\boldsymbol{x})^2 + V(\boldsymbol{x})$ where $V\in C^\infty(\mathbb{R}^3)$ is such that $\tilde{V}$ satisfies conditions (*). Let $\psi\in C_0(\mathbb{R}^3)$. For sufficiently small time $T>0$, the kernel

$$\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y}) = R_x(T)G_0(\boldsymbol{x}, \boldsymbol{y}, T)$$

where $G_0(\boldsymbol{x}, \boldsymbol{y}, T)$ is the Green function for equation (2). Furthermore, $G_0(\boldsymbol{x}, \boldsymbol{y}, T)$ is given by

$$G_0(\boldsymbol{x}, \boldsymbol{y}, T) = \hbar^{-3/2}\exp[-A(\boldsymbol{X}_{\min})/\hbar]\int_{C_0[0,T]} \exp[\hbar^{-1}F(\hbar^{1/2}z)]\}\,\mathrm{d}\mu_{\boldsymbol{0},0;\boldsymbol{0},T}(z),$$

where

$$F(z) = -\int_0^T [\tilde{V}(\boldsymbol{X}_{\min}(s)+z(s), T-s) - \tilde{V}(\boldsymbol{X}_{\min}(s), T-s) - D\tilde{V}(X_{\min}(s), T-s)z(s)]\,\mathrm{d}s,$$

$\boldsymbol{X}_{\min}$ is the global minimiser of A over $\mathscr{A}$ and $\mu_{\boldsymbol{0},0;\boldsymbol{0},T}$ denotes the unnormalised conditional Wiener measure on $C_0[0, T]$.

Proof. We have that

$$\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar]\psi(\boldsymbol{x}) = R_x(T)\int G_0(\boldsymbol{x}, \boldsymbol{y}, T)\psi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y},$$

which leads to

$$\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y}) = R_x(T)G_0(\boldsymbol{x}, \boldsymbol{y}, T),$$

for $T < t_m$. The remainder of the lemma is now a consequence of lemma 2. As in the preceding section the maximiser of $[A(\boldsymbol{X}_{\min}) - A(\boldsymbol{X}_{\min} + \boldsymbol{z})]$ is required to be unique in $C_0^*[0, T]$. By definition of $\boldsymbol{X}_{\min}$ this maximum is zero and will be attained uniquely at $\boldsymbol{z} \equiv \boldsymbol{0}$ if and only if $\boldsymbol{X}_{\min}$ is the unique global minimiser of A over $\mathscr{A}$. If the Hessian of V is bounded below, then we show that $\boldsymbol{X}_{\min}$ is unique for sufficiently small time T.

Lemma 6. Let $V \in C^\infty(\mathbb{R}^3)$ be such that $\tilde{V}$ satisfies conditions (*) and let $\beta_3 \in \mathbb{R}$ be such that $\nabla^2 \tilde{V} \geqslant -|\beta_3| I$, I being the identity. Then, $\boldsymbol{X}_{\min}$, the global minimiser of

$$A(\boldsymbol{X}) = \int_0^T [2^{-1}\dot{\boldsymbol{X}}(s) \cdot \dot{\boldsymbol{X}}(s) + \tilde{V}(\boldsymbol{X}(s), T - s)] \, \mathrm{d}s$$

over $\mathscr{A}$ is unique for $T < \pi(|\beta_3| + B^2/4)^{-1/2}$.

Proof. Defining $\boldsymbol{H}(s) = \boldsymbol{X}_1(s) - \boldsymbol{X}_2(s)$ where $\boldsymbol{X}_1$ and $\boldsymbol{X}_2$ are both global minimisers of A over $\mathscr{A}$ one first shows that

$$\int_0^T \dot{\boldsymbol{H}}(s) \cdot \dot{\boldsymbol{H}}(s) \, \mathrm{d}s \leqslant (|\beta_3| + B^2/4) \int_0^T \boldsymbol{H}(s) \cdot \boldsymbol{H}(s) \, \mathrm{d}s$$

by using the method of lemma 3. It quickly follows that $\boldsymbol{X}_{\min}$ is unique for $T < \pi(|\beta_3| + B^2/4)^{-1/2}$.

Proof of Theorem 3. The proof of theorem 3 is no different in spirit from the proof of theorem 2. The work required to set the result of theorem 3 within the framework of theorem 2 has been carried out in the preceeding three lemmas. The statement of theorem 3 is valid if the time T is bounded above by $\min\{[6/(|\beta_3| + B^2/4)^{1/2}, t_m(\tilde{V})\}$.

We state the following corollary without proof.

Corollary 3. Let H and V be as defined in the hypothesis of theorem 3. Setting $A(\boldsymbol{X}_{\min}) = A(\boldsymbol{x}, \boldsymbol{y}, T)$ we have for T sufficiently small

$$\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y}) = (2\pi\hbar)^{-3/2} R_x(T) \times \{\exp[-A(\boldsymbol{x}, \boldsymbol{y}, T)/\hbar] |J(0)|^{-1/2} [1 + \hbar K_1 + \mathrm{O}(\hbar^2)]\},$$

where $|J(0)|$ denotes the modulus of the determinant of $J(0)$. $J(\ )$ is the matrix which satisfies

$$\ddot{J}(s) = \{R(T-s)\nabla^2 V(R^{\mathrm{T}}(T-s) X_{\min}(s)) R^{\mathrm{T}}(T-s) - B^2 I/4\} J(s), \qquad s \in [0, T],$$

with $J(T) = 0$ and $\dot{J}(T) = I$. K_1 may be determined in terms of the Frechet derivatives of V and the Green function of the above equation which satisfies Dirichlet boundary conditions.

Once again we emphasise that we do not require the system under consideration to be separable.

Example

$$H(\hbar, \boldsymbol{B}) = 2^{-1}(\mathrm{i}\hbar\nabla + 2^{-1}\boldsymbol{B} \wedge \boldsymbol{x})^2 + 2^{-1}\boldsymbol{x}^{\mathrm{T}} A^2 \boldsymbol{x}$$

For the above H, A^2 being a strictly positive definite quadratic form, we will now calculate the kernel $\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$ and use it to determine the spectrum of $H(\hbar, \boldsymbol{B})$. Without loss we may take A^2 to be diagonal, but we now have to accommodate any $B \in \mathbb{R}^3$. This specific form of V allows us to improve upon lemma 6 and prove that the minimiser of the functional $A(\ )$ over $\mathscr{A}$ is unique for all but a discrete series of times in $T>0$.

The kernel $\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar](\boldsymbol{x}, \boldsymbol{y})$ is given by

$$(2\pi\hbar)^{-3/2} R_x(T)\{\exp[-A(\boldsymbol{x}, \boldsymbol{y}, T)/\hbar]|-\partial^2 A(\boldsymbol{x}, \boldsymbol{y}, T)/\partial x^j\, \partial y^k|^{1/2}\}.$$

We must calculate $A(x, y, T) \equiv A(\boldsymbol{X}_{\min})$ and $\boldsymbol{X}_{\min}$. In this particular example it is easier to perform the necessary calculations in the unrotated, original frame of reference. Defining $\boldsymbol{Y}(s) = R^{\mathrm{T}}(T-s)\boldsymbol{X}_{\min}(s)$ we must solve

$$\ddot{\boldsymbol{Y}}(s) = B\dot{\boldsymbol{Y}}(s) + A^2\boldsymbol{Y}(s), \qquad \boldsymbol{Y}(0) = R^{\mathrm{T}}(T)\boldsymbol{x}, \qquad \boldsymbol{Y}(T) = \boldsymbol{y},$$

where $B\dot{\boldsymbol{Y}}(s) = \boldsymbol{B} \wedge \dot{\boldsymbol{Y}}(s)$. If we define the time-dependent matrices E, F, G, and H by

$$\begin{bmatrix} E(s) & F(s) \\ G(s) & H(s) \end{bmatrix} = \exp\left(s\begin{bmatrix} 0 & I \\ A^2 & B \end{bmatrix}\right)$$

then $\boldsymbol{Y}(s) = E(s)\boldsymbol{Y}(0) + F(s)F^{-1}(T)[\boldsymbol{y} - E(T)\boldsymbol{Y}(0)]$, $F(T)$ being invertible for all save a discrete series of times T, and

$$\begin{aligned} A(\boldsymbol{x}, \boldsymbol{y}, T) = 2^{-1}[&\boldsymbol{y}\cdot[G(T)\boldsymbol{Y}(0) + H(T)F^{-1}(T)[\boldsymbol{y} - E(T)\boldsymbol{Y}(0)]] \\ &- \boldsymbol{Y}(0)\cdot[F^{-1}(T)[\boldsymbol{y} - E(T)\boldsymbol{Y}(0)]]]. \end{aligned}$$

The determinant $|\partial^2 A(\boldsymbol{x}, \boldsymbol{y}, T)/\partial x^j \partial y^k|$ is simply

$$|2^{-1}[G(T) - H(T)F^{-1}(T)E(T) - [F^{-1}(T)]^{\mathrm{T}}]|.$$

One may show that $F(-s) = [G(s) - H(s)F^{-1}(s)E(s)]^{-1}$ and that $F(-s) = -F^{\mathrm{T}}(s)$ (see appendix). This leads to

$$|-\partial^2 A(\boldsymbol{x}, \boldsymbol{y}, T)/\partial x^j\, \partial y^k| = |F^{-1}(T)|.$$

Since the above determinant is independent of $\boldsymbol{x}$, the operator $R_x(T)$ acts only on $\exp[-A(\boldsymbol{x}, \boldsymbol{y}, T)/\hbar]$ giving

$$\exp[-A(R_x(T)\boldsymbol{x}, \boldsymbol{x}, T)/\hbar] = \exp\{-\boldsymbol{x}\cdot[G(T) + (H(T) - I)F^{-1}(T)(I - E(T))]\boldsymbol{x}/2\hbar\}.$$

To calculate the trace we must evaluate the integral

$$\int_{\mathbb{R}^3} \exp[-\hbar^{-1}A(R_x(T)\boldsymbol{x}, \boldsymbol{x}, T)]\mathbf{d}\boldsymbol{x}$$

which by the above is simply

$$(2\pi\hbar)^{3/2}|G(T) + (H(T) - I)F^{-1}(T)(I - E(T))|^{-1/2}.$$

It is, however, easy to show that

$$|G(T) + (H(T) - I)F^{-1}(T)(I - E(T))| = -|F^{-1}(T)| \begin{vmatrix} E(T) - I & F(T) \\ G(T) & H(T) - I \end{vmatrix}.$$

This determinant will be positive if A^2 is strictly positive definite. Thus, upon combination of the necessary terms, we have

$$\mathrm{Tr}\{\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar]\} = \left| -\begin{vmatrix} E(T) - I & F(T) \\ G(T) & H(T) - I \end{vmatrix} \right|^{-1/2}.$$

Let α_1^2, α_2^2 and α_3^2 be the positive roots of the equation

$$(a_1^2-\alpha)(a_2^2-\alpha)(a_3^2-\alpha)=\alpha[B_1^2a_1^2+B_2^2a_2^2+B_3^2a_3^2-\alpha|\boldsymbol{B}|^2]$$

where $\boldsymbol{B}=(B_1, B_2, B_3)$ and $A^2=\mathrm{diag}(a_1^2, a_2^2, a_3^2)$. Then

$$\begin{aligned}\mathrm{Tr}\{\exp[-TH(\hbar, \mathrm{i}\boldsymbol{B})/\hbar]\} &= \prod_{j=1} [(\mathrm{e}^{-\alpha_j T}-1)(1-\mathrm{e}^{-\alpha_j T})]^{-1/2}\\ &= \sum_{l,m,n=0}^{\infty} \exp\{-[(l+\tfrac{1}{2})\alpha_1+(m+\tfrac{1}{2})\alpha_2+(n+\tfrac{1}{2})\alpha_3]T\}.\end{aligned}$$

By analytically continuing, we conclude that the eigenvalues of $H(\hbar, \boldsymbol{B})$ are

$$E_{lmn}=\hbar[(l+\tfrac{1}{2})\alpha_1+(m+\tfrac{1}{2})\alpha_2+(n+\tfrac{1}{2})\alpha_3], \qquad l, m, n\in\mathbb{Z}^+.$$

This seems to be a new result.

4. Preliminary lemmas and proof of theorem 1

The lemmas contained in this section are the three-dimensional analogues of those in Davies and Truman (I). We will state all the lemmas required for the proof of theorem 1 but in their proofs, if given, we will only describe any supplementary technical detail necessary to carry the proof through in three dimensions. The following lemma is one of the three critical estimates which we require.

Let χ_A be the characteristic function of the set A. We will sometimes abuse notation by writing $\mathbb{E}_z^T\{\chi_A\}=\mathbb{E}_z^T\{A\}$.

Lemma 7. For some fixed constants c, $\gamma>0$,

$$\mathbb{E}_z^T\{\|z\|>a\}\leqslant c\exp(-\gamma a^2/T).$$

Proof. If $\|z\|>a$ then at least one of the following must be valid also:

$$\|^1z\|>a/\sqrt{3}, \qquad \|^2z\|>a/\sqrt{3}, \qquad \|^3z\|>a/\sqrt{3}.$$

Thus

$$\begin{aligned}\mathbb{E}_z^T\{\|z\|>a\}&\leqslant\mathbb{E}_z^T\{\|^1z\|>a/\sqrt{3} \quad\text{or}\quad \|^2z\|>a/\sqrt{3} \quad\text{or}\quad \|^3z\|>a/\sqrt{3}\}\\ &\leqslant 4\mathbb{E}_z^T\{\|z\|>a/\sqrt{3}\},\end{aligned}$$

where we have used the probabilistic result

$$\begin{aligned}\mathrm{Prob}(A\cup B\cup C)&=\mathrm{Prob}(A)+\mathrm{Prob}(B)+\mathrm{Prob}(C)-\mathrm{Prob}(A\cap B)-\mathrm{Prob}(A\cap C)\\ &\quad-\mathrm{Prob}(B\cap C)+\mathrm{Prob}(A\cap B\cap C).\end{aligned}$$

From Davies and Truman (II) we have $\mathbb{E}_z^T\{\|z\|>a'\}<2\exp(-2a'^2/T)$ and so

$$\mathbb{E}_z^T\{\|z\|>a\}\leqslant 8\exp(-2a^2/3T).$$

Let $z\in C_0[0, T]$, then we define the n-polygonalisation of z, $z^n(\ )$, by

$$z^n(x)=z(jT/n)+(n/T)(s-jT/n)\{z[(j+1)T/n]-z(jT/n)\},$$
$$jT/n\leqslant s\leqslant(j+1)T/n,$$

for $j=0,1,2,\ldots,n-1$. Let $z_j^n=z^n(jT/n)$ for $j=0,1,\ldots,n$. We also define the associated 'vector' ${}^jz^n$ by ${}^jz^n=({}^jz_1^n,{}^jz_2^n,\ldots,{}^jz_n^n)$; note that ${}^jz_n^n=0$ for $j=1,2,3$.

Lemma 8. If

$$\max_{0\leqslant j\leqslant n-1}\left\{\sup_{jT/n\leqslant s\leqslant(j+1)T/n}|z(s)-z(jT/n)|\right\}<\delta/2 \quad \text{then} \quad \|z-z^n(\ )\|<\delta.$$

Proof. Similar to that of lemma 6 in Davies and Truman (I). We now state the second of our three important lemmas.

Lemma 9. Let m be a positive integer, then for $\delta>0$,

$$\mathbb{E}_z^T(\|z-z^m(\ )\|>\delta)<D\exp(-m\delta^2/24T), \qquad D \text{ a positive constant.}$$

Proof. Use the same method as lemma 7 initially and then refer to lemma 8 of Davies and Truman (II).

Lemma 10. For $k,l\in\mathbb{R}$, $\mathbb{E}_z^T[\exp(k\|z\|^2+l\|z\|)]<\infty$ for all l and $k<\gamma/T$, γ as in lemma 4.

Proof. See lemma 9 of Davies and Truman (II).

Lemma 11. Let A_n be the $n\times n$ tridiagonal matrix

$$(n/T)\begin{vmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{vmatrix}.$$

Then for ${}^ks^n$ an n-dimensional vector

$${}^ks^nA_n({}^ks^n)^{\mathrm{T}}=\sum_{j=1}^{n}(n/T)[{}^ks_j^n-{}^ks_{j-1}^n]^2, \qquad {}^ks_0^n=0,$$

$(\ )^{\mathrm{T}}$ is transpose, we postulate that

$$\int_0^T[\mathrm{d}^ks^n(\tau)/\mathrm{d}\tau]^2\,\mathrm{d}\tau={}^ks^nA_n({}^ks^n)^{\mathrm{T}}$$

and

$${}^jz^nA_n({}^jz^n)^{\mathrm{T}}\leqslant\int_0^T[{}^j\dot{z}(\tau)]^2\,\mathrm{d}\tau, \qquad j=1,2,3.$$

${}^ks^n(t)$ is that one-dimensional polygonal path which has ${}^ks^n$ as its associated n-dimensional vector.

Proof. See lemma 4 of Schilder.

Lemma 12. If $z \in C_0^*[0, T]$ then for $s_2 > s_1$

$$\sup_{s_1 \leqslant s \leqslant s_2} |z(s) - z(s_1)|^2 \leqslant (s_2 - s_1) \int_{s_1}^{s_2} \dot{z}(\sigma) \cdot \dot{z}(\sigma) \, d\sigma.$$

Proof. Use the triangle inequality and see lemma 5 of Schilder.

Let us define the function $A(\delta)$ by

$$A(\delta) = \sup_{z \in A_\delta} \left(F(z) - 2^{-1} \int_0^T \dot{z}(s) \cdot \dot{z}(s) \, ds \right)$$

where

$$A_\delta = \{ z \in C_0^*[0, T] \| \| z - z_0 \| \geqslant \delta \}, \qquad \text{for } \delta > 0.$$

Lemma 13. Suppose $F(z)$ satisfies the conditions given in the hypothesis of theorem 1, then $A(\delta) < 0$ for $\delta > 0$.

Proof. See lemma 6 of Schilder.

Lemma 14. If $\| s^n(\ ) - z_0^n(\ ) \| \geqslant \omega$ and $\omega - \delta_n > 0$ then

$$F(s^n(\ )) - 2^{-1} \sum_{j=1}^{3} {}^j s^n A_n ({}^j s^n)^{\mathrm{T}} \leqslant A(\omega - \delta_n), \qquad \delta_n = \| z_0 - z_0^n(\ ) \|,$$

$z_0^n(\ )$ is the n-polygonalisation of z_0.

Proof. Similar to that of lemma 7 of Schilder.

Lemma 15. Let A_n be the $n \times n$ matrix given in lemma 11. Then if ω^n is any n-dimensional vector

$$\omega^n A_n (\omega^n)^{\mathrm{T}} \geqslant T^{-1} \| \omega^n \|_\infty^2, \qquad \| \ \|_\infty \text{ being the sup-norm on } \mathbb{R}^3.$$

Proof. See lemma 13 in Davies and Truman (I).

Let $\chi(\beta, y, z)$, $\beta (\in \mathbb{R}) > 0$ be the characteristic function of the set $\{ z \in C_0[0, T] \| \| y - z \| \leqslant \beta \}$. The next lemma is the last of our crucial estimates.

Lemma 16. Let $F(z)$ be as given in the hypothesis of theorem 1 and let $\delta > 0$. Then for λ sufficiently small,

$$I(\lambda) = \mathbb{E}_z^T \{ [1 - \chi(\delta/\lambda, z_0/\lambda, z)] \exp[\lambda^{-2} F(\lambda z)] \} = O[\exp(\alpha \lambda^{-2})]$$

for some $\alpha < 0$.

Proof. As in the proof of lemma 14 in Davies and Truman (I) we proceed by splitting $I(\lambda)$ into three distinct parts $I_2(\lambda)$, $I_3(\lambda)$ and $I_4(\lambda)$. We deal with $I_2(\lambda)$ and $I_4(\lambda)$ in exactly the same manner as in Davies and Truman (I). $I_3(\lambda)$, however, must be treated with slightly more care as the finite dimensional Lebesgue integral required for the upper bound on $I_3(\lambda)$ is now of dimension $3(n-1)$ and the integration takes place over a more complicated subspace of $\mathbb{R}^{3(n-1)}$. In essence, though, the method of proof is the same.

Lemma 17. If $\dot{z}_0(s)$ is of bounded variation on $[0, T]$ and if

$$\int_0^T f(s)\cdot y(s)\,\mathrm{d}s-\int_0^T \dot{z}_0(s)\cdot \mathrm{d}y(s)=0, \qquad f\in L^2[0,T], \quad \text{for all } y\in C_0^*[0,T],$$

then

$$\int_0^T f(s)\cdot y(s)\,\mathrm{d}s-\int_0^T \dot{z}_0(s)\cdot \mathrm{d}y(s)=0 \quad \text{for AE } y\in C_0[0,T].$$

Proof. Similar to that of lemma 15 in Davies and Truman (I).

Proof of theorem 1. The proof of theorem 1 follows the corresponding proof in Davies and Truman (I). We merely draw on the three-dimensional versions of the lemmas and technical results required. In general, the net effect of extending our original result of Davies and Truman (1) to accommodate functionals of paths in $\mathbb{R}^3$ is to reduce the maximum time, T, for which the result is valid.

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Appendix

The matrices $E(s)$, $F(s)$, $G(s)$ and $H(s)$ were defined by

$$\begin{bmatrix} E(s) & F(s) \\ G(s) & H(s) \end{bmatrix} = \exp\left(s\begin{bmatrix} 0 & I \\ A^2 & B \end{bmatrix}\right).$$

Define the matrices $\bar{E}(s)$, $\bar{F}(s)$, $\bar{G}(s)$, and $\bar{H}(s)$ by

$$\begin{bmatrix} \bar{E}(s) & \bar{F}(s) \\ \bar{G}(s) & \bar{H}(s) \end{bmatrix} = \exp\left(-s\begin{bmatrix} 0 & I \\ A^2 & B \end{bmatrix}\right) = \begin{bmatrix} E(s) & F(s) \\ G(s) & H(s) \end{bmatrix}^{-1}, \qquad \text{if it exists.}$$

By inverting the E, F, G, H matrix we get

$$\bar{F}(s)\equiv (G(s)-H(s)F^{-1}(s)E(s))^{-1}.$$

$\bar{F}(s)$ satisfies the differential equation

$$\ddot{\bar{F}}(s)=A^2\bar{F}(s)-B\dot{\bar{F}}(s), \qquad \bar{F}(0)=0, \qquad \dot{\bar{F}}(0)=-I.$$

However, F satisfies the differential equation

$$\ddot{F}(s)=F(s)A^2+\dot{F}(s)B, \qquad F(0)=0, \qquad \dot{F}(0)=I,$$

and upon taking the transpose of the above we get

$$\ddot{F}^{\mathrm{T}}(s) = A^2 F^{\mathrm{T}}(s) - B\dot{F}^{\mathrm{T}}(s), \qquad F^{\mathrm{T}}(0) = 0, \qquad \dot{F}^{\mathrm{T}}(0) = I.$$

The above yields

$$\bar{F}(s) = -F^{\mathrm{T}}(s),$$

giving us the required result.

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