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SHORT-TIME ASYMPTOTICS FOR THE TRACE OF ONE- AND MULTI-DIMENSIONAL SCHRÖDINGER SEMIGROUPS

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ABSTRACT. Using Brownian motion we derive the leading asymptotic behaviour, as $t \downarrow 0$, of the (normalized) trace of $e^{tL} - e^{tL^H}$, where L is the operator $\Delta/2 + q(x)$ on $\mathbf{R}^d$ (with zero boundary condition at infinity), H is a hyperplane of $\mathbf{R}^d$ and L^H is the direct sum of $\Delta/2 + q(x)$ acting on H^+, with Dirichlet boundary condition on H (and 0 at infinity), and the same operator acting on $H^-(H^+$ and H^- are the two half-spaces defined by $H)$. The function q is taken bounded and continuous on $\mathbf{R}^d$ and, if $d \geq 2$, we also assume that q is integrable on $\mathbf{R}^d$ (in fact we need a little less than that). We also show how to get higher order terms in our expansion, but in this case q is required to be smoother. In the one-dimensional case our result extends a result of Deift and Trubowitz (see the [D-T, Appendix]), since they proved a similar formula under the additional assumption that $q(x) \to 0$ as $|x| \to \infty$.

The asympotic formula we give implies that q can be recovered from certain spectral properties of L and L^H.

Let $H \subset \mathbf{R}^d$ be a hyperplane (i.e. the graph of $a_1x_1 + \cdots + a_dx_d = b$ in $\mathbf{R}^d$). For convenience (and without loss of generality) we fix H to be

$$H = \{x = (x_1, x_2, \dots, x_d) \in \mathbf{R}^d : x_1 = 0\}. \tag{1}$$

Now, for $f \in L^1(\mathbf{R}^d)$ we consider the following initial-boundary value (parabolic) problems

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) = \frac{1}{2}\Delta u(t,x) + q(x)u(t,x), & (t,x) \in (0,\infty) \times \mathbf{R}^d; \\ u(0,x) = f(x), x \in \mathbf{R}^d; \\ \lim_{|x|\to\infty} u(t,x) = 0, t \in (0,\infty) \end{cases} \tag{2}$$

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(where $|x| = \sqrt{x_1^2 + x_2^2 + \cdots + x_d^2}$) and

$$(3)\qquad \begin{cases} \frac{\partial}{\partial t} v(t,x) = \frac{1}{2} v(t,x) = \frac{1}{2}\Delta v(t,x) + q(x)v(t,x), \\ \qquad\qquad (t,x) \in (0,\infty) \times (\mathbf{R}^d \backslash H); \\ v(0,x) = f(x), x \in (\mathbf{R}^d \backslash H); \\ \lim_{|x|\to\infty} v(t,x) = 0, t \in (0,\infty); \\ v(t,x) = 0, (t,x) \in (0,\infty) \times H. \end{cases}$$

Problem (3) is (a direct sum of) two independent problems, one in H^+ and the other in H^-, where H^+ and H^- are the two half-spaces determined by H, namely

$$H^+ = \{x \in \mathbf{R}^d : x_1 > 0\} \quad \text{and} \quad H^- = \{x \in \mathbf{R}^d : x_1 < 0\}.$$

The function q is bounded and continuous on $\mathbf{R}^d$, symbolically $q \in C_b(\mathbf{R}^d)$. Furthermore, if $d \geq 2$ we also assume $q \in L^1(\mathbf{R}^d)$. Under these assumptions, it will be shown that both problems (2) and (3) have a continuous solution (possibly only in a weak sense) which, in a semigroup notation, can be written respectively as

$$u(t,x) = (S_t f)(x) \quad \text{and} \quad v(t,x) = (S_t^H f)(x).$$

(By a maximum principle, these solutions are also unique—see [P-W]).

Using Brownian motion we can give a very convenient (probabilistic) representation of these semigroups

$$(4)\qquad (S_t f)(x) = E^x\{e_q(t) f(B_t)\}$$

and

$$(5)\qquad (S_t^H f)(x) = E^x\{e_q(t) 1_{[t<T_0]} f(B_t)\},$$

where $B = (B_t, \mathcal{F}_t, P^x)$ is a (standard) Brownian motion process in $\mathbf{R}^d$ starting at x, $e_q(t)$ is the Feynmann-Kac functional of B_t that corresponds to q defined by

$$e_q(t) = \exp\left[\int_0^t q(B_s)\, ds\right]$$

and T_0 is the first hitting time of H, namely

$$T_0(\omega) = \inf\{t > 0 : B_t(\omega) \in H\} = \inf\{t > 0 : B_t^1(\omega) = 0\},$$

where we have set $B_t = (B_t^1, B_t^2, \ldots, B_t^d)$.

The semigroups S_t and S_t^H possess nonnegative continuous kernels

$$k(t,x,y) \text{ and } k^H(t,x,y)$$

respectively, i.e.

$$(S_t f)(x) = \int_{\mathbf{R}^d} k(t,x,y) f(y)\, dy \quad \text{and} \quad (S_t^H f)(x) = \int_{\mathbf{R}^d} k^H(t,x,y) f(y)\, dy.$$

Both kernels are symmetric in x and y and they can be constructed by a standard method which we demonstrate below.

The transition density of B is

$$p(t,x,y) = \frac{1}{(2\pi t)^{d/2}} \exp\left(-\frac{|x-y|^2}{2t}\right), \tag{6}$$

whereas if B is killed at H, its transition density becomes

$$p^H(t,x,y) = \begin{cases} p(t,x,y) - p(t,x,\overline{y}), & \text{if } x_1 y_1 \geq 0; \\ 0, & \text{if } x_1 y_1 < 0, \end{cases} \tag{7}$$

where, for $y = (y_1, y_2, \dots, y_d)$, we denote by $\overline{y}$ its reflection with respect to H, namely $\overline{y} = (-y_1, y_2, \dots, y_d)$. Notice that both $p(t,x,y)$ and $p^H(t,x,y)$ are nonnegative, symmetric in x and y, continuous on $(0,\infty) \times \mathbf{R}^d \times \mathbf{R}^d$ and they decay to 0 if we let $|x| \to \infty$ or $|y| \to \infty$.

To construct $k(t,x,y)$ we first set

$$k_0(t,x,y) = p(t,x,y) \tag{8a}$$

and, for $n = 1, 2, \dots$,

$$k_n(t,x,y) = \int_0^t \int_{\mathbf{R}^d} p(s,x,z) q(z) k_{n-1}(t-s,z,y)\, dz\, ds. \tag{8b}$$

By the Markov property of B and straightforward (rather tedious though) induction on n we get the following key formula

$$\int_{\mathbf{R}^d} k_n(t,x,y) f(y)\, dy = \frac{1}{n!} E^x \left\{ \left[\int_0^t q(B_s)\, ds \right]^n f(B_t) \right\}, \tag{9}$$

which implies that

$$\int_{\mathbf{R}^d} k_n(t,x,y) f(y)\, dy \leq \frac{1}{n!} (t\|q\|)^n E^x\{f(B_t)\} \leq \frac{A}{n!} t^{-d/2} (t\|q\|)^n \|f\|_1, \tag{10}$$

(A is a universal constant and $\|q\| = \|q\|_\infty$) for any $f \in L^1(\mathbf{R}^d)$. Equations (8a) and (8b) imply that each $k_n(t,x,y)$ is continuous on $(0,\infty) \times \mathbf{R}^d \times \mathbf{R}^d$ and symmetric in x and y. Then, since f is arbitrary, formula (10) yields

$$|k_n(t,x,y)| \leq \frac{A}{n!} t^{-d/2} (t\|q\|)^n. \tag{11}$$

Furthermore, by (9) we have

$$k(t,x,y) = \sum_{n=0}^{\infty} k_n(t,x,y)$$

and, because of (11), the series converges (absolutely and) uniformly. Hence $k(t,x,y)$ inherits all the properties of $k_n(t,x,y)$ mentioned above. The nonnegativity follows from (4), since $e_q(t) > 0$.

In exactly the same way (just replace $p(t,x,y)$ and B in the above setup by $p^H(t,x,y)$ and a Brownian motion killed at H) we can construct $k^H(t,x,y)$ and show that it has the same properties. For example, equation (9) becomes

$$(9') \qquad \int_{\mathbf{R}^d} k_n^H(t,x,y)f(y)\,dy = \frac{1}{n!}E^x\left\{\left[\int_0^t q(B_s)\,ds\right]^n 1_{[t<T_0]}f(B_t)\right\}.$$

Notice also that $k(t,x,y) \geq k^H(t,x,y)$, by (4) and (5).

Remark. There is a probabilistic interpretation of these kernels in terms of the Brownian bridge, namely

$$k(t,x,y) = E^x\{e_q(t)|B_t = y\}p(t,x,y),$$
$$k^H(t,x,y) = E^x\{e_q(t)1_{[t<T_0]}|B_t = y\}p(t,x,y).$$

We proceed by defining

$$(12a) \qquad \delta_n^H(t,x,y) = k_n(t,x,y) - k_n^H(t,x,y)$$

and

$$(12b) \qquad \delta^H(t,x,y) = k(t,x,y) - k^H(t,x,y).$$

If H is as in (1), we will write $\delta_n(t,x,y)$ and $\delta(t,x,y)$ instead of $\delta_n^H(t,x,y)$ and $\delta^H(t,x,y)$. (In particular, by (6) and (7)

$$(12c) \qquad \delta_0(t,x,x) = \frac{1}{(2\pi t)^{d/2}}\exp\left(-\frac{2x_1^2}{t}\right),$$

which is in $L^1(\mathbf{R}^d)$ only if $d = 1$ and this is the reason why we need q to be integrable in higher dimensions). The above definitions imply

$$(13) \qquad \int_{\mathbf{R}^d}[\delta(t,x,y) - \delta_0(t,x,y)]f(y)\,dy = \int_{\mathbf{R}^d}\sum_{n=1}^{\infty}\delta_n(t,x,y)f(y)\,dy.$$

We want to estimate $\delta(t,x,y)$ on the "diagonal" $x = y$ (in order to get a trace). From (9), (9′) and the definition of $\delta(t,x,y)$ we have that, for any $f \in L^1(\mathbf{R}^d)$,

$$\int_{\mathbf{R}^d}\delta_n(t,x,y)f(y)\,dy = \frac{1}{n!}E^x\left\{\left[\int_0^t q(B_s)\,ds\right]^n 1_{[t\geq T_0]}f(B_t)\right\}.$$

Now let $n \geq 2$ and choose a constant c such that $c \geq \|q\|^{n-1}/n!$, for all n. Then from the above formula we get

$$\begin{aligned}\left|\int_{\mathbf{R}^d}\delta_n(t,x,y)f(y)\,dy\right| &\leq \frac{1}{n!}(\|q\|t)^{n-1}\left|E^x\left\{\left[\int_0^t q(B_s)\,ds\right]1_{[t\geq T_0]}f(B_t)\right\}\right| \\ &\leq ct^{n-1}\int_{\mathbf{R}^d}|\delta_1(t,x,y)|\,|f(y)|\,dy\end{aligned}$$

and since f is arbitrary,

$$|\delta_n(t,x,y)| \le ct^{n-1}|\delta_1(t,x,y)|, \tag{14}$$

for all (t,x,y) in $(0,\infty) \times \mathbf{R}^d \times \mathbf{R}^d$ (the continuity of $k_n(t,x,y)$ and $k_n^H(t,x,y)$ is crucial here). In particular, if we set $x=y$ we get

$$|\delta_n(t,x,x)| \le ct^{n-1}|\delta_1(t,x,x)|. \tag{14$'$}$$

Therefore, at least for $0 < t \le t_0 < 1$, (13) becomes (because of (14) and the fact that (13) is true for all integrable f)

$$\left|\delta(t,x,y) - \delta_0(t,x,y) - \sum_{j=1}^{n} \delta_j(t,x,y)\right| \le c_0 t^n |\delta_1(t,x,y)|, \tag{15}$$

where we can take $c_0 = c(1-t_0)^{-1}$. Note that (15) remains true if $n = 0$; in this case the sum in the left-hand side is empty, i.e. equals 0.

Next, we want to verify the integrability of $\delta_1(t,\cdot,\cdot)$ on $\mathbf{R}^d$. By (12a), we need to test the integrability of $k_1(t,\cdot,\cdot) - k_1^H(t,\cdot,\cdot)$. Let's start with $k_1(t,\cdot,\cdot)$. From (8a) and (8b) we obtain

$$k_1(t,x,x) = \int_0^t \int_{\mathbf{R}^d} p(s,x,z)q(z)p(t-s,z,x)\,dz\,ds \tag{16}$$

and similarly

$$k_1^H(t,x,x) = \int_0^t \int_{\mathbf{R}^d} p^H(s,x,z)q(z)p^H(t-s,z,x)\,dz\,ds \tag{16$'$}$$

where $p(t,x,y)$ is given by (6) and $p^H(t,x,y)$ by (7).

Case 1. ($q \in C_b(\mathbf{R}^d) \cap L^1(\mathbf{R}^d)$, $d \ge 2$). Without loss of generality we assume that $q(x) \ge 0$ in order to justify the application of Tonelli's Theorem in the analysis done below (the general case follows immediately by expressing q as a difference of two nonnegative terms). Now equation (16) gives

$$\begin{aligned}
\int_{\mathbf{R}^d} k_1(t,x,x)\,dx &= \int_{\mathbf{R}^d}\int_0^t \int_{\mathbf{R}^d} p(s,x,z)q(x)p(t-s,z,x)\,dz\,ds\,dx \\
&= \int_{\mathbf{R}^d} q(z) \int_0^t \int_{\mathbf{R}^d} p(s,x,z)p(t-s,z,x)\,dx\,ds\,dz \\
&= \int_{\mathbf{R}^d} q(z) \int_0^t p(t,z,z)\,ds\,dz \\
&= t\int_{\mathbf{R}^d} q(z)p(t,z,z)\,dz,
\end{aligned} \tag{17}$$

which is finite for any $t > 0$. If we replace $p(t,x,y)$, above, by $p^H(t,x,y)$, we get (in exactly the same way) a similar formula for $k_1^H(t,x,y)$, namely

$$\int_{\mathbf{R}^d} k_1^H(t,x,x)\,dx = t\int_{\mathbf{R}^d} q(z)p^H(t,z,z)\,dz. \tag{17$'$}$$

Remark. In the derivation of (17) and (17′) (and, also, of (21) of Case 2) we have used the fact that since $p(t, x, y)$ and $p^H(t, x, y)$ are kernels of semigroups (that correspond to the standard Brownian motion in $\mathbf{R}^d$ and the Brownian motion killed at H respectively) they, both, satisfy the so-called Chapman–Kolmogorov equation (i.e. the "matrix multiplication" equation), namely

$$r(s+t, x, y) = \int_{\mathbf{R}^d} r(s, x, z) r(t, z, y)\, dz.$$

We stress again that (17) and (17′) are valid for any q (not necessarily nonnegative) that satisfies our initial assumptions, i.e. continuity and integrability. Combining (12a) with (17) and (17′) we obtain

$$\int_{\mathbf{R}^d} \delta_1(t, x, x)\, dx = t \int_{\mathbf{R}^d} q(z) \delta_0(t, z, z)\, dz \tag{18}$$

or, if we want to use (12c),

$$\int_{\mathbf{R}^d} \delta_1(t, x, x)\, dx = \frac{t}{(2\pi t)^{d/2}} \int_{\mathbf{R}^d} q(z) \exp\left(-\frac{2z_1^2}{t}\right) dz.$$

If we set

$$Q(u) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} q(u, z_2, \dots, z_d)\, dz_2 \cdots dz_d, \tag{19}$$

then the previous equation becomes

$$\int_{\mathbf{R}^d} \delta_1(t, x, x)\, dx = \frac{t}{(2\pi t)^{d/2}} \int_{-\infty}^{\infty} Q(u) \exp\left(-\frac{2u^2}{t}\right) du. \tag{20}$$

Notice that we can expand the right-hand side of (20) in powers of t, near $t = 0$, provided that $Q(u)$ is smooth near $u = 0$ (we provide more details later).

Case 2. ($q \in C_b(\mathbf{R}^1)$, $d = 1$). From (16) and (16′) we get

$$\delta_1(t, x, x) = \int_0^t \int_{-\infty}^{\infty} [p(s, x, z) p(t-s, z, x) - p^H(s, x, z) p^H(t-s, z, x)] q(z)\, dz\, ds.$$

Assume (again without loss of generality) that $q(x) \geq 0$. Then, the integrand of the right-hand side of the above equation is nonnegative. Therefore

$$\begin{aligned}\int_{-\infty}^{\infty} \delta_1(t,x,x)\,dx &= \int_{-\infty}^{\infty}\int_0^t\int_{-\infty}^{\infty}[p(s,x,z)p(t-s,z,x) \\ &\qquad - p^H(s,x,z)p^H(t-s,z,x)]q(z)\,dz\,ds\,dx \\ &= \int_{-\infty}^{\infty} q(z)\int_0^t\int_{-\infty}^{\infty}[p(s,x,z)p(t-s,z,x) \\ &\qquad - p^H(s,x,z)p^H(t-s,z,x)]\,dx\,ds\,dz \\ &= \int_{-\infty}^{\infty} q(z)\int_0^t[p(t,z,z)-p^H(t,z,z)]\,ds\,dz \\ &= \int_{-\infty}^{\infty} q(z)\delta_0(t,z,z)\,dz,\end{aligned} \tag{21}$$

or

$$\int_{-\infty}^{\infty}\delta_1(t,x,x)\,dx = \frac{t}{\sqrt{2\pi t}}\int_{-\infty}^{\infty} q(z)\exp\left(-\frac{2z^2}{t}\right)dz, \tag{20$'$}$$

which is finite for all $t > 0$ (remember that $\delta(t,\cdot,\cdot)$ is integrable if $d = 1$). Thus (21) and (20′) say that equations (18) and (20) remain valid for $d = 1$, if we interpret $Q(u)$ of (19) as $q(u)$ which is, of course, perfectly reasonable.

Now we are ready for our main result.

Theorem. *Let $\delta^H(t,x,y)$ and $\delta_n^H(t,x,y)$ be as defined in* (12a) *and* (12b) *and assume that $q \in C_b(\mathbf{R}^1)$, if $d = 1$, or $q \in C_b(\mathbf{R}^d)\cap L^1(\mathbf{R}^d)$, if $d \geq 2$. Then, as $t \downarrow 0$, we have*

$$\int_{\mathbf{R}^d}[\delta^H(t,x,x)-\delta_0^H(t,x,x)]\,dx = \frac{(2\pi)^{(1-d)/2}}{2}\overline{Q}(H)t^{(3-d)/2}+o(t^{(3-d)/2}), \tag{22}$$

where $\overline{Q}(H)$ is the integral of q on the hyperplane H. If H is as in (1), *then, by comparing with* (19),

$$\overline{Q}(H) = Q(0) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} q(0,x_2,\dots,x_d)\,dx_2\cdots dx_d.$$

If $d = 1$ and $H = \{\xi\}$, then $Q(H) = q(\xi)$.

Proof. Without loss of generality H can be taken as in (1). The integrability of

$$F(x) = \delta(t,x,x) - \delta_0(t,x,x)$$

follows by setting $n = 0$ in (15) and by the fact that $\delta_1(t,\cdot,\cdot) \in L^1(\mathbf{R}^d)$, which is a consequence of (20) and (20′).

Now, for $x = y$ and $n = 1$, (15) becomes

$$|[\delta(t,x,x)-\delta_0(t,x,x)]-\delta_1(t,x,x)| \leq c_0 t|\delta_1(t,x,x)|.$$

By integrating we obtain

$$\left|\int_{\mathbf{R}^d}[\delta(t,x,x)-\delta_0(t,x,x)]\,dx-\int_{\mathbf{R}^d}\delta_1(t,x,x)\,dx\right|\le c_0t\int_{\mathbf{R}^d}|\delta_1(t,x,x)|\,dx.$$

Applying (20) and (20′) in the above formula we get that, as $t\downarrow 0$,

(23)

$$\int_{\mathbf{R}^d}[\delta(t,x,x)-\delta_0(t,x,x)]\,dx=\int_{\mathbf{R}^d}\delta_1(t,x,x)\,dx + O(t)\frac{t}{(2\pi t)^{d/2}}\int_{-\infty}^{\infty}|Q(u)|\exp\left(-\frac{2u^2}{t}\right)du,$$

where $Q(u)=q(u)$, if $d=1$. Therefore, to finish the proof, we have to analyze the behaviour of

$$I(t)=\int_{-\infty}^{\infty}Q(u)\exp\left(-\frac{2u^2}{t}\right)du,$$

as $t\downarrow 0$. Substituting $u=v\sqrt{t/2}$, $I(t)$ becomes

$$I(t)=\sqrt{\frac{t}{2}}\int_{-\infty}^{\infty}Q(v\sqrt{t/2})e^{-v^2}dv=\sqrt{\frac{\pi t}{2}}[Q(0)+o(1)],$$

as $t\downarrow 0$ (and to get higher terms we need $Q(u)$ to be smooth near 0). Applying (20), (20′) and the above to (23), we get

$$\int_{\mathbf{R}^d}[\delta(t,x,x)=\delta_0(t,x,x)]\,dx=\frac{t}{(2\pi t)^{d/2}}\sqrt{\frac{\pi t}{2}}Q(0)[1+o(1)] + O(t)\frac{t}{(2\pi t)^{d/2}}\sqrt{\frac{\pi t}{2}}|Q(0)|[1+o(1)],$$

which is (22). ■

Remarks. (a) Formula (22) tells us how to evaluate $\overline{Q}(H)$ by using the leading asymptotic behaviour of the trace of $S_t-S_t^H$. Remember that, if we know $\overline{Q}(H)$ for all hyperplanes $H\subset\mathbf{R}^d$, we can reconstruct q via a Radon transform.

(b) From formulas (15), (20) and the above proof it is clear how we can get higher terms ($t^{(5-d)/2}$, $t^{(7-d)/2}$, etc.) in our asymptotic expansion, if q is sufficiently smooth in an open set containing H.

(c) In the case $d=1$, (12c) implies

$$\int_{-\infty}^{\infty}\delta_0(t,x,x)\,dx=\frac{1}{2}$$

and therefore, if $H=\{0\}$, our asymptotic formula becomes

$$\lim_{t\downarrow 0}\frac{1}{t}\int_{-\infty}^{\infty}\left[\delta(t,x,x)-\frac{1}{2}\right]dx=\frac{q(0)}{2}.$$

The left-hand side in the above formula is the normalized (because of the term 1/2) trace of the difference of the generators of S_t and S_t^H. In the special case where $q(x) \to 0$ as $|x| \to \infty$, this formula was proved (in a different way) by Deift and Trubowitz in the [D-T, Appendix].

(d) In the case $d \geq 2$, let H be an arbitrary hyperplane and n be its unit normal vector (choose arbitrarily one of the two). If we go carefully through the previous analysis, we can see that our theorem remains true under more relaxed assumptions on q, namely we need q in $L^\infty(\mathbf{R}^d)$, continuous near H and such that $\overline{Q}(H + \alpha n)$ (as defined in the statement of the theorem) is continuous in α for α near 0 (notice that, for each α, $H+\alpha n$ is a hyperplane). For example, in the case $d = 2$,

$$q(x) = \frac{1}{1 + x_1^2 + x_2^2}$$

is an acceptable q, although is not in $L^1(\mathbf{R}^2)$.

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