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Bounds on Green's functions of second-order differential equations

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We estimate the diagonal part of the Green's function for the equation

\[
( - \Delta/2 + V(x) + \partial/\partial t ) \psi(x, t) = 0, \quad t > 0, \quad x \in B,
\]

where \(B\) is a finite region of the Euclidean space \(R^d\) with a regular boundary. In the special case \(V(x) = 0, x \in B\), we also obtain bounds for the non-diagonal part of the Green's function which are uniform in \(t\).

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I. INTRODUCTION

Kac, in unpublished lecture notes summarized in Ref. 1, indicates how Wiener estimates of the Green's function for the one-particle diffusion equation can be used to derive results about the bulk properties of the free boson gas. The mathematical details were supplied in Lewis and Pulè.\(^2\) The same strategy has been used in van den Berg and Lewis\(^3\) to prove results (announced in Ref. 4) about the boson gas in an external potential. For this purpose we require Wiener estimates of the Green's function for the one-particle diffusion equation with an external potential. These estimates may be of use in other fields of application and the purpose of this paper is to provide their proofs.

We estimate the Green's function of the partial differential equation

\[
(L + \partial/\partial t ) \psi(x, t) = 0, \quad x \in B, \quad t > 0,
\]

where \(B\) is a finite region of the Euclidean space \(R^d\) with a regular boundary \(\partial B\). We will restrict ourselves to Dirichlet boundary conditions: \(\psi(x, t) = 0, x \in \partial B\). \(L\) denotes the self-adjoint operator on the space \(L^2(B)\) which is given on smooth functions by the differential operator \(- \Delta/2 + V(x)\) with Dirichlet boundary conditions where \(V(x)\) is a non-negative function (satisfying a Lipschitz condition almost everywhere in \(B\)). This operator has a discrete positive spectrum \(E_1 \leq E_2 \leq \cdots\) and an orthonormal set of eigenfunctions \(\{ \phi_j(x) \}\) forming a basis in \(L^2(B)\) (Davies\(^4\)). Furthermore, the Green's function of (1) has the eigenfunction expansion

\[
K(x, y; t) = \sum_{j=1}^{\infty} \exp(-tE_j) \phi_j(x) \phi_j(y).
\]

Moreover, it has been shown by Rosenblatt\(^6\) and Ray\(^7\) that \(K(x, y; t)\) can be written as

\[
K(x, y; t) = \frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}},
\]

where the quantity

\[
E_j \exp\left[ - \int_0^t V(u(\tau))d\tau \right] : u(0) = x, \quad u(t) = y, \quad u(\tau) \in B
\]

denotes the average value of

\[
\exp\left[ - \int_0^t V(u(\tau))d\tau \right]
\]

for all paths \(u(\cdot)\) of a Wiener process on \(R^d\) subject to \(u(0) = x\) and \(u(t) = y\). Furthermore Ray\(^7\) proved that \(K(x, y; t)\) is continuous (for all \(y\)) at a point \(x_0\) of the boundary \(\partial B\) provided there exists a conical sector with vertex at \(x_0\) entirely outside \(B\). We will assume that this condition holds for all points on the boundary; we call such a boundary regular. Ray\(^7\) has, in addition, results in the case in which \(B\) is an unbounded region of \(R^d\) and \(V(x) \to \infty\) as \(|x| \to \infty\); we will restrict ourselves, however, to the case in which \(B\) is a bounded region.

Our main result is that for \(t\) small

\[
K(x, y; t) \sim e^{-|x-y|^2/(2\pi t)^d/2}
\]

at all points \(x\) which are not too close to the boundary. Expression (4) can easily be understood from formula (3). For small times \(t\) the probability is small that \(|u(\tau)|\) is large, so we may replace \(u(\tau)\) by \(x\) and \(B\) by \(R^d\), provided \(x\) is not too close to \(\partial B\). This has been called the principle of not feeling the boundary.\(^7\) Integrating both sides of (4) with respect to the volume we have, for \(t\) small,

\[
\sum_{j=1}^{\infty} \exp(-tE_j) \sim \frac{1}{(2\pi)^{d/2}} \int_{x \in B} e^{-|x-y|^2} dx.
\]

This is allowed, since most points \(y\) are far from the boundary because the boundary is regular.

In Sec. 2 we will estimate the Green's function of the differential equation (1) for the special case \(V(x) = 0, x \in B\). In Secs. 3 and 4 we will calculate bounds on the correction terms in (4) and (5).

2. A UNIFORM ESTIMATE WHEN \(V\) IS IDENTICALLY ZERO

Theorem 1: Let \(K_0(x, y; t)\) be the Green's function of Eq. (1) with \(V(x) = 0, x \in B\), and with Dirichlet boundary conditions for \(\psi(x, t)\) at \(\partial B\).

Then

\[
K_0(x, y; t) \sim \frac{\exp(-|x-y|^2/2t)}{(2\pi t)^{d/2}}
\]

\[
\leq \frac{2d}{(2\pi)^{d/2}} \exp(4v^2/2 - d^2/2dt), \quad x \in B, \quad y \in B, \quad t > 0,
\]

where \(d\) is the distance of \(x\) from \(\partial B\).

Proof: Let \(\Box_1\) denote a hypercube with center \(x\) which lies entirely inside \(B\) and such that at least one corner vertex lies on \(\partial B\). Then the length \(l_x\) of an edge of the cube is not less than \((2/d)^1\). From (3) we have

\[
\sum_{j=1}^{\infty} \exp(-tE_j) \sim \frac{1}{(2\pi)^{d/2}} \int_{x \in B} e^{-|x-y|^2} dx.
\]
\[0 < K_0(x,y;t) = \exp\left( -\frac{|x-y|^2}{2t} \right) \]
\[\times \mathcal{E}\{u(0) = x, u(t) = y; u(\tau) \in \mathcal{B} \} \]
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\[\exp\left( -\frac{|x-y|^2}{2t} \right)\]
\[\times \mathcal{E}\{u(0) = x, u(t) = y; u(\tau) \in \mathcal{B} \} \]
\[\exp\left( -\frac{|x-y|^2}{2t} \right)\]
Proof: From the theorems of Ray\textsuperscript{7} and Rosenblatt\textsuperscript{6} it follows that
\[\frac{e^{-iV(x)}}{2\pi t^{d/2}} - K(x,x;t) = e^{-iV(x)} \left[ \mathbb{E}\left\{ 1 - \exp\left( - \int_0^t (V(u) - V(x)) \, du \right) : u(0) = u(t) = x; u(t) \in B \right\} \right. \]
\[+ \left. 1 - \mathbb{E}\left\{ u(0) = u(t) = x; u(t) \in B \right\} \right\}\]
\[< \frac{e^{-iV(x)}}{2\pi t^{d/2}} \left[ \mathbb{E}\left\{ \int_0^t (V(u(t)) - V(x)) \, du : u(0) = u(t) = x; u(t) \in B \right\} \right. \]
\[+ 2d \exp\left( - \frac{2d^2}{dt} \right) \left( \mathbb{E}\left\{ \int_0^t e^{-iV(u)} : u(0) = u(t) = x; u(t) \in B \right\} \right)
\[\leq \frac{e^{-iV(x)}}{2\pi t^{d/2}} \left( \mathbb{E}\left\{ \int_0^t \left( \frac{t}{2\pi t(t - \tau)} \right)^{d/2} \exp\left( - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \right\} \right) + 2d \exp\left( - \frac{2d^2}{dt} \right), \quad (13)\]
by the inequality $1 - e^{-x} < x$, Theorem 1, and Fubini's theorem. Moreover
\[K(x,x;t) = \frac{1}{(2\pi t)^{d/2}} \mathbb{E}\left\{ \int_0^t (V(u) - V(x)) \, du : u(0) = u(t) = x; u(t) \in B \right\}
\[< \frac{1}{(2\pi t)^{d/2}} \mathbb{E}\left\{ \int_0^t \frac{dt}{t} \left( \mathbb{E}\left\{ e^{-iV(u(t))} : u(0) = u(t) = x; u(t) \in B \right\} \right) \int_0^t \frac{dt}{t} \int_{u \in B} \exp\left( - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \right\}, \quad (14)\]
by Jensen's inequality and Fubini's theorem. Combining (13) and (14) we have estimate (12).

4. AN ESTIMATE FOR THE PARTITION FUNCTION

In this section we estimate the correction term in (5). This can be done by simply integrating the inequalities (13) and (14) from which an estimate follows. However, due to an inequality of Ray\textsuperscript{7} the result can be improved.

Theorem 3: Let $V(x)$ and $B$ be as in Theorem 2, then
\[\left| \sum_{j=1}^J \exp(-tE_j) - \int_{x \in B} dx \frac{e^{-iV(x)}}{2\pi t^{d/2}} \right| < \frac{1}{(2\pi t)^{d/2}} \int_{u \in B} dx \left( 2d \exp\left( - \frac{2d^2}{dt} \right) \right)
\[+ \left| \int_0^t \frac{dt}{t} \int_{u \in B} du \exp\left( - tV(u) - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \right| \right) \left( \frac{t}{2\pi t(t - \tau)} \right)^{d/2}, \quad (15)\]

Proof: We first prove an upper bound (Ray\textsuperscript{7}).
\[\sum_{j=1}^J \exp(-tE_j)
\[= \int_{x \in B} K(x,x;t) \, dx \leq \frac{1}{(2\pi t)^{d/2}} \int_{u \in B} dx \left( \int_0^t \frac{dt}{t} \mathbb{E}\left\{ e^{-iV(u(t))} : u(0) = u(t) = x; u(t) \in B \right\} \right)
\[= \frac{1}{(2\pi t)^{d/2}} \int_{x \in B} dx \int_0^t \frac{dt}{t} \int_{u \in B} du \exp\left( - tV(u) - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \left( \frac{t}{2\pi t(t - \tau)} \right)^{d/2}
\[= \frac{1}{(2\pi t)^{d/2}} \int_{x \in B} dx \left( \int_0^t \frac{dt}{t} \right) \int_{u \in B} du \exp\left( - tV(u) - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \left( \frac{t}{2\pi t(t - \tau)} \right)^{d/2}
\[= \frac{1}{(2\pi t)^{d/2}} \int_{x \in B} dx \exp\left( - iV(x) \right), \quad (16)\]
by Jensen's inequality. Moreover it follows from (13) that
\[\int_{x \in B} dx \left( K(x,x;t) - \frac{e^{-iV(x)}}{2\pi t^{d/2}} \right) > \int_{x \in B} dx \left( \frac{e^{-iV(x)}}{2\pi t^{d/2}} \right) \left( \int_0^t \frac{dt}{t} \int_{u \in B} du \left( V(u) - V(x) \right) \left( \frac{t}{2\pi t(t - \tau)} \right)^{d/2}
\[\cdot \exp\left( - \frac{t |x - u|^2}{2\pi t(t - \tau)} \right) \right) \right) \right) + 2d \exp\left( - \frac{2d^2}{dt} \right), \quad (17)\]
Combining the bounds (16) and (17) we arrive at (15).
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