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## HEAT KERNELS AND GREEN FUNCTIONS OF SOME PSEUDO-DIFFERENTIAL OPERATORS IN RELATIVISTIC QUANTUM MECHANICS\*

Qiang Guo, M. W. Wong

A new formula for the Green function of the pseudo-differential operator  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$ , where  $m > 0$ , is derived using its heat kernel, which can be used to obtain  $L^p$ - $L^r$  estimates of the heat semigroup generated by  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$ . The Bessel potential of order 1 is then shown to be equal to the Laplace transform of an upper incomplete gamma function. An explicit formula is given for the kernel of the Schrödinger semigroup generated by the Hamiltonian of a free photon moving in  $\mathbf{R}^n$ . In the case when  $m = 1$ , the trace of the heat semigroup and the zeta function regularized trace of the inverse of the operator  $(-\Delta + 1 + |x|^2)^s$ ,  $s > 0$ , are also given.

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## 1. Introduction

We begin with a relativistic particle of mass  $m$  moving freely in  $\mathbf{R}^n$ . Then the momentum  $\xi$  and the kinetic energy  $E$  are given by

$$\xi = \frac{mv}{\sqrt{1 - \frac{|v|^2}{c^2}}}$$

and

$$E = \frac{mc^2}{\sqrt{1 - \frac{|v|^2}{c^2}}},$$

where  $v$  is the velocity of the particle and  $c$  is the velocity of light. By suitably scaling the units, we let  $c = 1$ . Therefore

$$E^2 = |\xi|^2 + m^2$$

or

$$E = \sqrt{|\xi|^2 + m^2}.$$

By von Neumann's rules of quantization to the effect that  $x$  is kept as is, but  $\xi = (\xi_1, \xi_2, \dots, \xi_n)$  is replaced by  $\left(-i\frac{\partial}{\partial x_1}, -i\frac{\partial}{\partial x_2}, \dots, -i\frac{\partial}{\partial x_n}\right)$ , the energy  $E$  is then the pseudo-differential operator  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$ .

Thus, the simplest example of a pseudo-differential operator studied in [17] plays an important role in relativistic quantum mechanics [1, 3, 5, 6, 8] and in some fairly recently works such as [10, 11]. Its heat kernel is the function  $W_t$  on  $\mathbf{R}^n$  parametrized by time  $t$  given by

$$(1) \quad W_t(x) = \frac{t}{(t^2 + |x|^2)^{(n+1)/2}} \frac{1}{(2\pi)^{(n+1)/2}} \int_0^\infty e^{-\delta/2} e^{-m^2(t^2 + |x|^2)/(2\delta)} \delta^{(n+1)/2} \frac{d\delta}{\delta}$$

for all  $x \in \mathbf{R}^n$ . The beauty of this heat kernel is that it is the product of two fundamentally important functions in analysis and partial differential equations. More precisely,

$$W_t(x) = \gamma_{m,n} P_t(x) G_{2n+1,m,t}(x), \quad x \in \mathbf{R}^n, t > 0.$$

Here,

$$\gamma_{m,n} = 2^{n/2} m^{n+1} \frac{\Gamma((2n+1)/2)}{\Gamma((n+1)/2)},$$

$P_t(x)$  is the Poisson kernel of the Laplacian  $\Delta$  on the upper half space

$$\{(x, t) \in \mathbf{R}^{n+1} : x \in \mathbf{R}^n, t > 0\}$$

given by

$$P_t(x) = \frac{2}{|S^n|} \frac{t}{(t^2 + |x|^2)^{(n+1)/2}},$$

where  $|S^n|$  is the surface area of the unit sphere  $S^n$  in  $\mathbf{R}^{n+1}$  and for all positive numbers  $s$ ,  $m$  and  $t$ ,  $G_{s,m,t}$  is the weighted Bessel potential on  $\mathbf{R}^n$  studied in some detail in [16] and is given by

$$G_{s,m,t}(x) = \frac{m^{n-s}}{2^{s/2}\Gamma(s/2)} \int_0^\infty e^{-r/2} e^{-m^2(t^2+|x|^2)/(2r)} r^{-(n-s)/2} \frac{dr}{r}$$

for all  $x \in \mathbf{R}^n$ . It is called the Bessel–Poisson kernel in [16]. A heat kernel of this form can at least be dated back to [15]. Another formula can be found in [7]. Note that when  $m = 1$  and  $t = 0$ , we get back the Bessel potential  $G_s$  studied in [9, 17]. We should also point out that when  $t = 0$ , it is known in [17] that  $G_{1,m,0}$  is the Green function of the free relativistic Hamiltonian  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$ .

The aim of this paper is to look at some ramifications of the heat kernel and Green function of the pseudo-differential operator  $\sqrt{-\Delta + m^2}$  and its modified operators on  $\mathbf{R}^n$ . In Section 2, we give some  $L^p$ - $L^r$  estimates of the heat semigroup generated by  $\sqrt{-\Delta + m^2}$ . In Section 3, we give another formula for the Green function of the free relativistic Hamiltonian by integrating its heat kernel with respect to time  $t$  from 0 to  $\infty$ . In Section 4, we prove that the new Green function can be used to obtain a new formula for a Bessel potential well studied in [2, 4, 9, 12, 16, 17]. We give in Section 5 an explicit formula for the Schrödinger kernel of the pseudo-differential operator  $\sqrt{-\Delta}$  on  $\mathbf{R}^n$ , which models the Hamiltonian of a free photon moving in  $\mathbf{R}^n$ . Section 6 is devoted to the trace and determinant of the heat kernel and the zeta function regularized trace and determinant of the Green function of the operator  $(-\Delta + 1 + |x|^2)^s$  for  $s > 0$ .

## 2. $L^p$ - $L^r$ Estimates for the Heat Semigroup Generated by $\sqrt{-\Delta + m^2}$ on $\mathbf{R}^n$

We begin with the following estimate.

**Lemma 1.** *The Bessel–Poisson kernel  $W_t$ ,  $t > 0$ , is in  $L^p(\mathbf{R}^n)$  for  $1 \leq p \leq \infty$ . In fact,*

$$\|W_t\|_p \leq C_{n,p}(2|S^n|)^{-1}|S^{n-1}|^{1/p}t^{-n/p'}, \quad t > 0,$$

where  $p'$  is the conjugate index of  $p$  and

$$C_{n,p} = \begin{cases} \left( \int_0^\infty (1+s^2)^{-(n+1)p/2} s^{n-1} ds \right)^{1/p}, & p \neq \infty, \\ 1, & p = \infty. \end{cases}$$

*Proof.* We begin with the observation that

$$W_t(x) \leq \frac{t}{(t^2 + |x|^2)^{(n+1)/2}} \frac{1}{\pi^{(n+1)/2}} \Gamma((n+1)/2), \quad x \in \mathbf{R}^n.$$

So, for  $1 \leq p < \infty$ ,

$$\begin{aligned} & \|W_t\|_p \\ & \leq \pi^{-(n+1)/2} \Gamma((n+1)/2) t \left( \int_{\mathbf{R}^n} \frac{1}{(t^2 + |x|^2)^{(n+1)p/2}} dx \right)^{1/p} \\ & = (2|S^n|)^{-1} t^{-n} \left( |S^{n-1}| \int_0^\infty \left(1 + \frac{r^2}{t^2}\right)^{-(n+1)p/2} r^{n-1} dr \right)^{1/p} \\ & = (2|S^n|)^{-1} |S^{n-1}|^{1/p} t^{-n/p'} \int_0^\infty (1+s^2)^{-(n+1)p/2} s^{n-1} ds \\ & = C_{n,p}(2|S^n|)^{-1} |S^{n-1}|^{1/p} t^{-n/p'} \end{aligned}$$

for all  $t > 0$ . The estimate for  $\|W_t\|_\infty$  is obvious.  $\square$

We denote the heat semigroup of  $\sqrt{-\Delta + m^2}$  by  $e^{-t\sqrt{-\Delta + m^2}}$ ,  $t > 0$ . Using the  $L^\infty$  norm of  $W_t$ ,  $t > 0$ , we get the following estimate.

**Theorem 1.** *Let  $t > 0$ . Then for  $1 \leq p \leq \infty$ , we get*

$$\|e^{-t\sqrt{-\Delta+m^2}}f\|_p \leq (2|S^n|)^{-1}t^{-n}\|f\|_p, \quad f \in L^p(\mathbf{R}^n).$$

The following estimate follows from Young's inequality and the  $L^1$  norm of  $W_t$ ,  $t > 0$ .

**Theorem 2.** *For  $t > 0$ ,*

$$\|e^{-t\sqrt{-\Delta+m^2}}f\|_p \leq C_{n,1}(2|S^n|)^{-1}|S^{n-1}|\|f\|_p, \quad f \in L^p(\mathbf{R}^n),$$

for  $1 \leq p \leq \infty$ .

**Remark.** A comparison of Theorems 1 and 2 is interesting. Both results give an  $L^p$ - $L^p$  estimate for the heat semigroup  $e^{-t\sqrt{-\Delta+m^2}}$  of the pseudo-differential operator  $\sqrt{-\Delta+m^2}$  on  $\mathbf{R}^n$ . Theorem 1 is better than Theorem 2 when  $t \rightarrow \infty$ , whereas, Theorem 2 is better than Theorem 1 when  $t \rightarrow 0+$ .

The following estimate follows from the extended inequality of Young.

**Theorem 3.** *Let  $t > 0$ . Then for  $r > p$ ,*

$$\|e^{-t\sqrt{-\Delta+m^2}}f\|_r \leq C_{n,q}(2|S^{n-1}|)^{-1}|S^{n-1}|^{1/q}t^{-n/q}\|f\|_p, \quad f \in L^p(\mathbf{R}^n),$$

where

$$\frac{1}{p} + \frac{1}{q} = 1 + \frac{1}{r}$$

and  $1 < q \leq \infty$ .

The last estimate follows from Hölder's inequality and the  $L^{p'}$  norm of  $W_t$ ,  $t > 0$ .

**Theorem 4.** *Let  $t > 0$ . Then for  $1 \leq p \leq \infty$ ,*

$$\|e^{-t\sqrt{-\Delta+m^2}}f\|_\infty \leq C_{n,p'}(2|S^n|)^{-1}|S^{n-1}|^{1/p'}t^{-n/p'}\|f\|_p,$$

where

$$\frac{1}{p} + \frac{1}{p'} = 1.$$

### 3. A New Formula for the Green Function

Another formula for the Green function  $G$  of the free Hamiltonian  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$  is given in the following theorem.

**Theorem 5.** *The Green function  $G$  of the free relativistic Hamiltonian  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$  is given by*

$$G(x) = \frac{2m^{n-1}}{(4\pi)^{(n+1)/2}} \int_0^\infty e^{-\delta} \left( \int_{m^2|x|^2/(4\delta)}^\infty e^{-v} v^{(1-n)/2} \frac{dv}{v} \right) d\delta, \quad x \in \mathbf{R}^n.$$

*Proof.* Integrating the heat kernel of  $\sqrt{-\Delta + m^2}$  with respect to time  $t$  from 0 to  $\infty$ , we get for all  $x \in \mathbf{R}^n$ ,

$$(2) \quad \begin{aligned} & (2\pi)^{(n+1)/2} G(x) \\ &= \int_0^\infty \frac{t}{(t^2 + |x|^2)^{(n+1)/2}} \left( \int_0^\infty e^{-\delta/2} e^{-m^2(t^2+|x|^2)/(2\delta)} \delta^{(n+1)/2} \frac{d\delta}{\delta} \right) dt. \end{aligned}$$

By Fubini's theorem,

$$\begin{aligned} & (2\pi)^{(n+1)/2} G(x) \\ &= \int_0^\infty e^{-\delta/2} \delta^{(n+1)/2} \left( \int_0^\infty \frac{t}{(t^2 + |x|^2)^{(n+1)/2}} e^{-m^2(t^2+|x|^2)/(2\delta)} dt \right) \frac{d\delta}{\delta} \end{aligned}$$

for all  $x \in \mathbf{R}^n$ . Let  $u = t^2 + |x|^2$ . Then for all  $x \in \mathbf{R}^n$ ,

$$G(x) = (2\pi)^{-(n+1)/2} \frac{1}{2} \int_0^\infty e^{-\delta/2} \delta^{(n+1)/2} \left( \int_{|x|^2}^\infty u^{-(n+1)/2} e^{-m^2 u/(2\delta)} du \right) \frac{d\delta}{\delta}.$$

Now, we let  $v = m^2 u/(2\delta)$ . Then for all  $x \in \mathbf{R}^n$ ,

$$G(x) = (4\pi)^{-(n+1)/2} \int_0^\infty e^{-\delta/2} \left( \int_{m^2|x|^2/(2\delta)}^\infty m^{n-1} v^{-(n+1)/2} e^{-v} dv \right) d\delta.$$

Finally, let  $r = \delta/2$ . Then

$$G(x) = \frac{2m^{n-1}}{(4\pi)^{(n+1)/2}} \int_0^\infty e^{-r} \left( \int_{m^2|x|^2/(4r)}^\infty e^{-v} v^{(1-n)/2} \frac{dv}{v} \right) dr$$

for all  $x \in \mathbf{R}^n$ .  $\square$

**Remark.** Most importantly, the new formula for the Green function is in fact the Laplace transform evaluated at 1 of the upper incomplete gamma function  $\Gamma(s, \cdot)$  of order  $s \in \mathbf{C}$  defined on  $(0, \infty)$  given by

$$\Gamma(s, \xi) = \int_\xi^\infty e^{-v} v^s \frac{dv}{v}, \quad \xi \in (0, \infty).$$

So,

$$G(x) = \frac{2m^{n-1}}{(4\pi)^{(n+1)/2}} \int_0^\infty e^{-\delta} \Gamma\left(\frac{1-n}{2}, \frac{m^2|x|^2}{4\delta}\right) d\delta, \quad x \in \mathbf{R}^n.$$

#### 4. A New Formula for a Bessel Potential

The following theorem gives another formula for the Bessel potential  $G_{1,m,0}$  of order 1.

**Theorem 6.** *Let  $m > 0$ . Then*

$$G_{1,m,0}(x) = \frac{2m^{n-1}}{(4\pi)^{(n+1)/2}} \int_0^\infty e^{-\delta} \Gamma\left(\frac{1-n}{2}, \frac{m^2|x|^2}{4\delta}\right) d\delta, \quad x \in \mathbf{R}^n.$$

*Proof.* By (2), we get

$$G(x) = (2\pi)^{-(n+1)/2} \int_0^\infty \frac{t}{(t^2 + |x|^2)^{(n+1)/2}} G_{2n+1,m}(t^2 + |x|^2) dt$$

for all  $x \in \mathbf{R}^n$ . Let  $u = t^2 + |x|^2$ . Then

$$G(x) = (2\pi)^{-(n+1)/2} \frac{1}{2} \int_{|x|^2}^\infty u^{-(n+1)/2} G_{2n+1,m}(u) du, \quad x \in \mathbf{R}^n.$$



It is well known [9] that

$$(3) \quad G_{2n+1,m}(x) = O(1)$$

as  $|x| \rightarrow 0$  and for every positive integer  $k$ ,

$$(4) \quad G_{2n+1,m}(x) = O(|x|^{-k})$$

as  $|x| \rightarrow \infty$ . Let  $n > 1$ . Then by (3), we can find positive constants  $\delta$  and  $C$  such that

$$(5) \quad u < \delta \Rightarrow G_{2n+1,m}(u) \leq C.$$

If  $|x|^2 \geq \delta$ , then by (4),

$$(6) \quad G(x) \leq (2\pi)^{-(n+1)/2} \frac{1}{2} \int_{\delta}^{\infty} u^{-(n+1)/2} G_{2n+1,m}(u) du < \infty.$$

If  $|x|^2 < \delta$ , then by (4) and (5),

$$(7) \quad \begin{aligned} G(x) &= (2\pi)^{-(n+1)/2} \frac{1}{2} \int_{|x|^2}^{\infty} u^{-(n+1)/2} G_{2n+1,m}(u) du \\ &= (2\pi)^{-(n+1)/2} \frac{1}{2} \left( \int_{|x|^2}^{\delta} u^{-(n+1)/2} G_{2n+1,m}(u) du + \int_{\delta}^{\infty} u^{-(n+1)/2} G_{2n+1,m}(u) du \right) \\ &= (2\pi)^{-(n+1)/2} \frac{1}{2} \left( \frac{C}{n-1} [\delta^{-(n-1)/2} - |x|^{-(n-1)}] + \int_{\delta}^{\infty} u^{-(n+1)/2} G_{2n+1,m}(u) du \right) \end{aligned}$$

If  $n = 1$ , then the same argument gives

$$(8) \quad G(x) \leq \frac{1}{2} \ln \delta - \ln |x| + \frac{1}{2} \int_{\delta}^{\infty} \frac{1}{u} G_{3,m}(u) du$$

for all  $x \in \mathbf{R}$ . Thus, by (6), (7) and (8),  $G$  is a tempered function on  $\mathbf{R}^n$  and hence a tempered distribution on  $\mathbf{R}^n$ . Therefore

$$(G * \varphi)^{\wedge} = (2\pi)^{n/2} \hat{\varphi} \hat{G}$$

and

$$(G_{1,m,0} * \varphi)^\wedge = (2\pi)^{n/2} \hat{\varphi} \widehat{G_{1,m,0}}$$

for all  $\varphi \in \mathcal{S}$ . Since  $G * \varphi = G_{1,m,0} * \varphi$  for all  $\varphi \in \mathcal{S}$ , it follows that as tempered distributions on  $\mathbf{R}^n$ ,

$$\hat{G} = \widehat{G_{1,m,0}}.$$

Hence  $G = G_{1,m,0}$  in the distribution sense. Since  $G_{1,m,0} \in L^1(\mathbf{R}^n)$ , we can conclude that  $G \in L^1(\mathbf{R}^n)$ .  $\square$

## 5. A Schrödinger Kernel

Let  $m = 0$ . Then the pseudo-differential operator  $\sqrt{-\Delta + m^2}$  becomes  $\sqrt{-\Delta}$  on  $\mathbf{R}^n$ . Thus, we are led to the relativistic Hamiltonian  $\sqrt{-\Delta}$  of a free particle of zero mass, i.e., a photon, moving in  $\mathbf{R}^n$ . We are interested in obtaining an explicit formula for the kernel of the free propagator  $e^{-it\sqrt{-\Delta}}$  for  $-\infty < t < \infty$ .

Putting  $m = 0$  and changing  $t$  to  $-it$  in (1), we obtain the Schrödinger kernel  $S_t$  of  $e^{-it\sqrt{-\Delta}}$  for  $-\infty < t < \infty$  given by

$$S_t(x) = \begin{cases} \frac{2}{|S^n|} \frac{-it}{(|x|^2 - t^2)^{(n+1)/2}}, & x \in \mathbf{R}^n, |x|^2 > t^2, \\ \frac{2}{|S^n|} \frac{-ite^{-(n+1)\pi/2}}{(t^2 - |x|^2)^{(n+1)/2}}, & x \in \mathbf{R}^n, |x|^2 < t^2, \end{cases}$$

where in the case when  $n$  is even and  $t^2 < |x|^2$ , the principal branch of  $(|x|^2 - t^2)^{(n+1)/2}$  is taken.

## 6. Powers of the Hermite Operator

We are interested in the case when the mass  $m$  of a relativistic particle is equal to 1 and we look at the slightly more general operator  $(-\Delta + 1 + |x|^2)^s$ , where  $s > 0$ . It is well known that the eigenvalues are  $2^s |\alpha|^s$ ,  $\alpha \in \mathbf{N}_0$ , where  $\mathbf{N}_0$  is the set of all multi-indices. For each eigenvalue  $2^s |\alpha|^s$ , the corresponding eigenfunctions are  $e_\alpha$ , where

$$e_\alpha(x) = e_{\alpha_1}(x_1) e_{\alpha_2}(x_2) \cdots e_{\alpha_n}(x_n), \quad x \in \mathbf{R}^n.$$

A more in-depth look at the eigenvalues of  $(-\Delta + 1 + |x|^2)^s$  reveals some interesting combinatorial information. The eigenvalues of  $(-\Delta + 1 + |x|^2)^s$  are

$2^s k^s$ ,  $k = 0, 1, \dots$ . For  $k = 0, 1, \dots$ , the eigenvalue  $2^s k^s$  has multiplicity  $m_n(k)$  given by the number of multinomial coefficients

$$\frac{k!}{k_1!k_2!\cdots k_n!},$$

where  $k_1 + k_2 + \cdots + k_n = k$ . So, except for the simple ground state, each eigenvalue has multiplicity given by the number  $m_n(k)$  of multinomial coefficients. Since

$$m_n(k) = \binom{k+n-1}{k},$$

it follows that we have the following theorem.

**Theorem 7.** *For  $t > 0$ , the trace  $\text{tr}(e^{-t(-\Delta+1+|x|^2)^s})$  of the heat semigroup generated by  $(-\Delta + 1 + |x|^2)^s$  is given by*

$$\text{tr}(e^{-t(-\Delta+1+|x|^2)^s}) = \sum_{k=0}^{\infty} e^{-2^s k^s t} m_n(k) = \sum_{k=0}^{\infty} \binom{k+n-1}{k} e^{-2^s k^s t}.$$

Since

$$\binom{k+n-1}{k} = \frac{k^{n-1}}{(n+1)!} \left( 1 + \frac{n(n-1)}{2k} + O(k^{-2}) \right)$$

as  $k \rightarrow \infty$ , it follows that the series in Theorem 7 converges and hence  $e^{-t(-\Delta+1+|x|^2)^s}$  is a trace class operator for  $t > 0$  and its trace is given by Theorem 7.

The inverse of  $(-\Delta + 1 + |x|^2)^s$  for  $s > 0$  is in general not a trace class operator, but we can compute its zeta function regularized trace when  $s \neq n$  and  $s \neq n - 1$ .

**Theorem 8.** *If  $s \neq n$  and  $s \neq n - 1$ , then the zeta function regularized trace  $\text{tr}_R((-\Delta + 1 + |x|^2)^{-s})$  of the inverse  $(-\Delta + 1 + |x|^2)^{-s}$  is given by*

$$\begin{aligned} & \text{tr}_R((-\Delta + 1 + |x|^2)^{-s}) \\ &= \frac{1}{2^s(n+1)!} \left( \zeta(s-n+1) + \frac{n(n-1)}{2} \zeta(s-n+2) + O(\zeta(s+2)) \right), \end{aligned}$$

where  $\zeta$  is the Riemann zeta function [13].

## 7. Conclusions

Notwithstanding the general claim in relativistic quantum mechanics that the square root renders the operator  $\sqrt{-\Delta + m^2}$  on  $\mathbf{R}^n$  difficult to work with and hence a way to deal with it is to square it to the wave operator and hence the Klein–Gordon equation and the Dirac equation. In this paper, we deal with the operator  $\sqrt{-\Delta + m^2}$  directly in the the context of pseudo-differential operators, which have been well studied to date. This paper supplements the available methods to study the Hamiltonians in relativistic quantum mechanics.

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