THE SCATTERING LENGTH AT POSITIVE TEMPERATURE

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Abstract. A positive temperature analogue of the scattering length of a potential $V$ can be defined via integrating the difference of the heat kernels of $-\Delta$ and $-\Delta + \frac{1}{2}V$, with $\Delta$ the Laplacian. An upper bound on this quantity is a crucial input in the derivation of a bound on the critical temperature of a dilute Bose gas [4]. In [4] a bound was given in the case of finite range potentials and sufficiently low temperature. In this paper, we improve the bound and extend it to potentials of infinite range.

1. Introduction and Main Results

Let $\Delta$ denote the usual Laplacian on $\mathbb{R}^d$, and let $V \geq 0$ be a multiplication operator on $L^2(\mathbb{R}^d)$. An important ingredient in the upper bound on the critical temperature for a dilute Bose gas derived in [4] is a bound on the integral of the difference of the heat kernels of $-\Delta$ and $-\Delta + \frac{1}{2}V$. For $\beta > 0$, let

$g(\beta) = \frac{1}{\beta} \int_{\mathbb{R}^{2d}} \left( e^{2\beta\Delta} - e^{\beta(2\Delta - V)} \right) (x, y) \, dx \, dy,$

which is well-defined since the integrand is non-negative, by the Feynman-Kac formula. It was shown in [4, Lemma V.1] that $g(\beta)$ is equal to

$$\inf_{\phi \in H^1(\mathbb{R}^d)} \left\{ \int_{\mathbb{R}^d} \left( 2|\nabla \phi(x)|^2 + V(x)\left(1 - \phi(x)\right)^2 \right) \, dx + \frac{1}{\beta} \langle f(\beta(-2\Delta + V)) \mid \phi \rangle \right\},$$

where $f(t) = t(1 - e^{-t})/(t - 1 + e^{-t})$. This variational principle was used in [4, Lemma V.2] to derive an upper bound on $g(\beta)$ for finite range potentials $V$ and $\beta$ sufficiently large. The function $f$ satisfies $1 \leq f(t) \leq 2$ for all $t \geq 0$. In particular, one can replace $f$ by 2 for an upper bound.

The functional under consideration is thus

$$\mathcal{E}_\beta(\phi) = \int_{\mathbb{R}^d} \left( 2|\nabla \phi(x)|^2 + V(x)|1 - \phi(x)|^2 + \frac{2}{\beta}|\phi(x)|^2 \right) \, dx.$$  \hspace{1cm} (1)

We assume that $V$ is radial and that $V \geq 0$. We are interested in

$$e(\beta) = \inf \left\{ \mathcal{E}_\beta(\phi) : \phi \in H^1(\mathbb{R}^d) \right\}.$$  \hspace{1cm} (2)

We shall assume that $V$ has finite \textit{scattering length} $0 < a < \infty$ (whose definition will be recalled in the next section). No regularity or integrability assumptions have to be imposed, however. In particular, $V$ is allowed to have a hard core, i.e., we allow $V(x)$ to be $\infty$ for $|x| \leq r$ for some $r \geq 0$. The potential $V$ could also be a measure, e.g., a sum of $\delta$-functions.

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Our main result is the following.

**THEOREM 1.** For $d = 3$,  
\[ e(\beta) \leq 8\pi a \left( 1 + \frac{a}{\sqrt{3}\beta} \right)^2. \]  
(3)

For $d = 2$,  
\[ e(\beta) \leq \frac{8\pi}{\ln(1 + \beta/a^2)} \left( 1 + \frac{1 + a^2/\beta}{2\ln(1 + \beta/a^2)} \right). \]  
(4)

Analogous bounds can be derived for $d = 1$ and $d > 3$. Since the bounds have applications in physics [4] only when $d = 2$ or $d = 3$, we shall restrict our attention to these cases for simplicity. The proof of Theorem 1 will be given in Sections 3 and 4 below.

If one is interested in bounds involving only the scattering length of $V$, the bounds of Theorem 1 are optimal in a certain sense. This will be further discussed in Section 5 where we evaluate $e(\beta)$ in the case of a hard core potential.

2. **Scattering Length**

As in [3, 2], the scattering length $a_R$ of the finite range potential $V \chi_{\{|x| \leq R\}}$ is defined via the minimization problem  
\[ \lambda(R) = \inf \{ \mathcal{E}_\infty(\phi) : \phi(x) = 0 \text{ for } |x| > R \}. \]  
(5)

For $d = 3$, we have, by definition,  
\[ \lambda(R) = \frac{8\pi a_R}{1 - a_R/R}. \]  
(6)

while for $d = 2$  
\[ \lambda(R) = \frac{4\pi}{\ln(R/a_R)}. \]  
(7)

It is important to note that $a_R$ is independent of $R$ in case $V$ has finite range less than $R$. Note also that $0 \leq a_R \leq R$ and that $a_R$ is increasing in $R$. The scattering length of $V$ is then defined to be $a = \lim_{R \to \infty} a_R$. The following simple criterion for finiteness holds.

**Lemma 1.** The scattering length $a = \lim_{R \to \infty} a_R$ is finite if and only if  
\[ \int_{|x| > b} V(x) dx < \infty \quad (d = 3) \]  
(8)

\[ \int_{|x| > b} V(x) [\ln(|x|/b)]^2 dx < \infty \quad (d = 2) \]  
(9)

for some $b > 0$.

The proof of this lemma will be given in Section 6.
3. Proof of Theorem 1 in Three Dimensions

It was shown in [3] that there is a unique minimizer $\psi_R$ for (5). The function $\psi_R$ is monotone decreasing, radial, and satisfies

$$2\Delta \psi_R(|x|) = V(x)(1 - \psi_R(|x|)) \quad \text{for } |x| \leq R$$

in the sense of distributions (where the right side is interpreted as 0 if $\psi_R = 1$ and $V = \infty$). Moreover, for $d = 3$ the bound

$$1 \geq 1 - \psi_R(|x|) \geq \max \left\{ \frac{1 - a_R/|x|}{1 - a_R/R}, 0 \right\} \quad \text{for } |x| \leq R$$

holds. We also have

$$\int_{|x| \leq R} V(x)(1 - \psi_R(|x|)) \, dx = 2 \int_{|x| \leq R} \Delta \psi_R(|x|) \, dx = \frac{8\pi a_R}{1 - a_R/R}. \quad (12)$$

From this identity and the monotonicity of $\psi_R$, we have the bound

$$\int_{R \leq |x| \leq R_1} V(x) \, dx \leq \frac{1}{1 - \psi_{R_1}(R)} \int_{R \leq |x| \leq R_1} V(x)(1 - \psi_{R_1}(|x|)) \, dx$$

$$= \frac{1}{1 - \psi_{R_1}(R)} \left[ \frac{8\pi a_{R_1}}{1 - a_{R_1}/R_1} - \frac{8\pi a_R}{1 - a_R/R} \right] \quad (13)$$

for $R_1 > R > 0$. In the last step, we used the fact that $1 - \psi_{R_1}$ and $1 - \psi_R$ are proportional for $|x| \leq R$, and that $\psi_R(R) = 0$. Using, in addition, the bound (11) and taking the limit $R_1 \to \infty$, we obtain

$$\int_{|x| \geq R} V(x) \, dx \leq \frac{8\pi a}{1 - a/R} - \frac{8\pi a_R}{1 - a_R/R} \quad (14)$$

for $R > a$.

As a trial state for $\mathcal{E}_\beta$, we use the function $\psi_R$ for some $R > a$. Using (11), we have

$$\int_{\mathbb{R}^3} |\psi_R(x)|^2 \, dx \leq \frac{4\pi a_R^2}{3} + \frac{a_R^2}{(1 - a_R/R)^2} \int_{a_R \leq |x| \leq R} (1/R - 1/|x|)^2 \, dx = \frac{4\pi a_R^2 R}{3}. \quad (15)$$

With the aid of (14) and (6) we hence obtain

$$\mathcal{E}_\beta(\psi_R) = \frac{8\pi a_R}{1 - a_R/R} + \int_{|x| \geq R} V(x) \, dx + \frac{2}{\beta} \int_{\mathbb{R}^3} |\psi_R(x)|^2 \, dx \leq \frac{8\pi a}{1 - a/R} + \frac{8\pi a_R^2 R}{3\beta}. \quad (16)$$

The choice $R = a + \sqrt{3\beta}$, together with the bound $a_R \leq a$, yields our final result [3].

4. Proof of Theorem 1 in Two Dimensions

The proof for $d = 2$ is similar to the three-dimensional case. Again the minimizer $\psi_R$ for (5) is monotone decreasing and radial, but now it satisfies

$$1 \geq 1 - \psi_R(|x|) \geq \max \left\{ \frac{\ln(|x|/a_R)}{\ln(R/a_R)}, 0 \right\} \quad \text{for } |x| \leq R.$$ 

Moreover,

$$\int_{|x| \leq R} V(x)(1 - \psi_R(|x|)) \, dx = 2 \int_{|x| \leq R} \Delta \psi_R(|x|) \, dx = \frac{4\pi}{\ln(R/a_R)}. \quad (18)$$
From this identity and the monotonicity of $\psi_R$, we thus have the bound
\[
\int_{R \leq |x| \leq R_1} V(x) dx \leq \frac{1}{1 - \psi_R'(R)} \int_{R \leq |x| \leq R_1} V(x)(1 - \psi_R(|x|)) dx \geq \frac{1}{1 - \psi_R'(R)} \ln(R_1/a R_1) - \frac{4\pi}{\ln(R/a R)}
\] (19)
for $R_1 > R > 0$. Inserting (17) and sending $R_1 \to \infty$ yields
\[
\int_{|x| \geq R} V(x) dx \leq \frac{4\pi}{\ln(R/a R)} - \frac{4\pi}{\ln(R/a R)} (20)
\]
for $R > a$.

Again we use $\psi_R$ as a trial state for $E_\beta$. From (17) it follows that
\[
\int_{\mathbb{R}^3} |\psi_R(x)|^2 dx \leq \frac{1}{\ln(R/a R)} \int_{|x| \leq R} |\ln(R/x)|^2 dx = \frac{\pi R^2}{2\ln(R/a R)^2}.
\] (21)
With the aid of (20) and (7) we hence obtain
\[
E_\beta(\psi_R) \leq \frac{4\pi}{\ln(R/a R)} + \frac{\pi R^2}{\beta \ln(R/a R)^2}.
\] (22)
If we choose $R = \sqrt{\beta}$ we thus obtain
\[
e(\beta) \leq \frac{8\pi}{\ln(\beta/a^2)} \left(1 + \frac{1}{2 \ln(\beta/a^2)}\right)
\] (23)
for $\beta > a^2$. To obtain a bound that holds for all $\beta$ we can choose $R = a \sqrt{1 + \beta/a^2}$ instead; this yields (1).

5. The Hard Core Case

As an example, consider the case of a hard sphere potential of range $a > 0$, i.e., $V(x) = \infty$ for $|x| \leq a$ and 0 otherwise. In this case, the minimizer of $E_\beta$ is, for $d = 3$, given by
\[
\psi(|x|) = \min \left\{ \frac{a}{|x|} e^{-(|x| - a)/\sqrt{\beta}}, 1 \right\}
\] (24)
and hence
\[
e(\beta) = -8\pi a^2 \psi'(a) + \frac{8\pi a^3}{3\beta} = 8\pi a \left(1 + \frac{a}{\sqrt{\beta}} + \frac{a^2}{3\beta}\right).
\] (25)
This shows that, except for the value of the constant in the error term, our bound (3) is optimal for large $\beta$. To leading order, $e(\beta)$ equals $8\pi a$, and the relative error is bounded by $O(a/\sqrt{\beta})$.

For $d = 2$, the minimizer of $E_\beta$ for the hard sphere potential is
\[
\psi(|x|) = \min \left\{ \frac{K_0(|x|/\sqrt{\beta})}{K_0(a/\sqrt{\beta})}, 1 \right\},
\] (26)
where $K_0$ is the modified Bessel function of 2nd kind. Hence
\[
e(\beta) = -4\pi a \frac{K_0'(a/\sqrt{\beta})}{\sqrt{\beta} K_0(a/\sqrt{\beta})} + \frac{2\pi a^2}{\beta}
\] (27)
in this case. The function $t \mapsto -t K_0'(t)/K_0(t)$ behaves like $(\ln(2/t) - \gamma + o(1))^{-1}$ as $t \to 0$, where $\gamma$ denotes Euler's constant [1, Eq. 9.6.13]. Again, our bound (1)
reproduces the leading order exactly, and gives the same order of magnitude for the error term as (27).

6. Finiteness of the Scattering Length

In this section we shall prove Lemma 1. Consider first the case $d = 3$. On the one hand, it follows from (13)–(14) that if $a < \infty$ then $\int_{|x| \geq b} V(x) dx < \infty$ for all $b > a$. On the other hand, if $\int_{|x| \geq b} V(x) dx < \infty$, then

$$\frac{8\pi a_R}{1 - a_R/R} \leq \frac{8\pi b}{1 - b/R} + \int_{|x| \geq b} V(x) dx$$

(28)

for all $R > b$, as can be seen by using the trial function

$$\phi(x) = \begin{cases} 
1 & \text{for } |x| \leq b \\
\frac{b|\ln(x/a)|}{\ln(R/a)} & \text{for } b \leq |x| \leq R \\
0 & \text{for } |x| \geq R.
\end{cases}$$

(29)

Hence $a \leq b + (8\pi)^{-1} \int_{|x| \geq b} V(x) dx$.

For $d = 2$, we can use the trial function

$$\phi(x) = \begin{cases} 
1 & \text{for } |x| \leq b \\
\frac{\ln(R/|x|)}{\ln(R/b)} & \text{for } b \leq |x| \leq R \\
0 & \text{for } |x| \geq R
\end{cases}$$

(30)

for $R > b$. This gives

$$\frac{4\pi}{\ln(R/a_R)} \leq \frac{4\pi}{\ln(R/b)} + \frac{1}{\ln(R/b)^2} \int_{b \leq |x| \leq R} V(x) (|x|/b)^2 dx.$$  

(31)

We can rewrite this inequality as

$$4\pi \ln(a_R/b) \leq \frac{\ln(R/|x|)}{\ln(R/a_R)} \int_{b \leq |x| \leq R} V(x) (|x|/b)^2 dx.$$  

(32)

If $\int_{|x| \geq b} V(x) (|x|/b)^2 dx$ is finite, this implies that $a_R$ is bounded independently of $R$. Taking $R \to \infty$ we obtain

$$4\pi \ln(a_R/b) \leq \int_{|x| \geq b} V(x) (|x|/b)^2 dx.$$  

(33)

To show that the finiteness of $a_R$ implies integrability of the right side of (33), we can use $\psi_R$ as a test function for $a_b$, evaluated on a ball of radius $R$, for $R > b > a$. Then,

$$\frac{4\pi}{\ln(R/a_b)} \leq \frac{4\pi}{\ln(R/a_R)} - \int_{b \leq |x| \leq R} V(x) (1 - \psi_R(x))^2 dx.$$  

(34)

Using (17) this bound implies that

$$4\pi \ln(a_R/a_b) \geq \frac{\ln(R/a_b)}{\ln(R/a_R)} \int_{b \leq |x| \leq R} V(x) [\ln(|x|/a_R)]^2 dx.$$  

(35)

Letting $R \to \infty$ we obtain

$$4\pi \ln(a_R/a_b) \geq \int_{|x| \geq b} V(x) [\ln(|x|/a)]^2 dx.$$  

(36)

This completes the proof.
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References

[1] M. Abramowitz, I.A. Stegun, *Handbook of mathematical functions*, Dover (1964).

[2] E.H. Lieb, R. Seiringer, J.P. Solovej, J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, Oberwolfach Seminars, Vol. 34, Birkhäuser (2005); also available at [http://arxiv.org/abs/cond-mat/0610117](http://arxiv.org/abs/cond-mat/0610117).

[3] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Two-dimensional Bose Gas*, J. Stat. Phys. 103, 509 (2001).

[4] R. Seiringer, D. Ueltschi, *Rigorous upper bound on the critical temperature of dilute Bose gases*, Phys. Rev. B 80, 014502 (2009).