# 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

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

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  $1 \le f(t) \le 2$  for all  $t \ge 0$ . In particular, one can replace f by 2 for an upper bound.

The functional under consideration is thus

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

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

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

We shall assume that V has finite 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  $|x| \le r$  for some  $r \ge 0$ . 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,

$$e(\beta) \le 8\pi a \left(1 + \frac{a}{\sqrt{3\beta}}\right)^2. \tag{3}$$

For d=2,

$$e(\beta) \le \frac{8\pi}{\ln(1+\beta/a^2)} \left(1 + \frac{1+a^2/\beta}{2\ln(1+\beta/a^2)}\right).$$
 (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

$$\lambda(R) = \inf \left\{ \mathcal{E}_{\infty}(\phi) : \phi(x) = 0 \text{ for } |x| > R \right\}. \tag{5}$$

For d=3, we have, by definition,

$$\lambda(R) = \frac{8\pi a_R}{1 - a_R/R} \tag{6}$$

while for d=2

$$\lambda(R) = \frac{4\pi}{\ln(R/a_R)} \,. \tag{7}$$

It is important to note that  $a_R$  is independent of R in case V has finite range less than R. Note also that  $0 \le a_R \le R$  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

$$\int_{|x|>b} V(x)dx < \infty \qquad (d=3) \tag{8}$$

$$\int_{|x|>b} V(x) \left[ \ln(|x|/b) \right]^2 dx < \infty \qquad (d=2)$$
 (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

$$2\Delta\psi_R(|x|) = V(x)(1 - \psi_R(|x|)) \quad \text{for } |x| \le R$$
 (10)

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

$$1 \ge 1 - \psi_R(|x|) \ge \max\left\{\frac{1 - a_R/|x|}{1 - a_R/R}, 0\right\} \quad \text{for } |x| \le R$$
 (11)

holds. We also have

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

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

$$\int_{R \le |x| \le R_1} V(x) dx \le \frac{1}{1 - \psi_{R_1}(R)} \int_{R \le |x| \le R_1} V(x) (1 - \psi_{R_1}(|x|) dx 
= \frac{1}{1 - \psi_{R_1}(R)} \frac{8\pi a_{R_1}}{1 - a_{R_1}/R_1} - \frac{8\pi a_R}{1 - a_R/R}$$
(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  $|x| \le R$ , and that  $\psi_R(R) = 0$ . Using, in addition, the bound (11) and taking the limit  $R_1 \to \infty$ , we obtain

$$\int_{|x| \ge R} V(x) dx \le \frac{8\pi a}{1 - a/R} - \frac{8\pi a_R}{1 - a_R/R} \tag{14}$$

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

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

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

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

The choice  $R = a + \sqrt{3\beta}$ , together with the bound  $a_R \le a$ , 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

$$1 \ge 1 - \psi_R(|x|) \ge \max\left\{\frac{\ln(|x|/a_R)}{\ln(R/a_R)}, 0\right\} \quad \text{for } |x| \le R.$$
 (17)

Moreover,

$$\int_{|x| \le R} V(x)(1 - \psi_R(|x|))dx = 2\int_{|x| \le R} \Delta \psi_R(|x|)dx = \frac{4\pi}{\ln(R/a_R)}.$$
 (18)

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

$$\int_{R \le |x| \le R_1} V(x) dx \le \frac{1}{1 - \psi_{R_1}(R)} \int_{R \le |x| \le R_1} V(x) (1 - \psi_{R_1}(|x|) dx 
= \frac{1}{1 - \psi_{R_1}(R)} \frac{4\pi}{\ln(R_1/a_{R_1})} - \frac{4\pi}{\ln(R/a_R)}$$
(19)

for  $R_1 > R > 0$ . Inserting (17) and sending  $R_1 \to \infty$  yields

$$\int_{|x| \ge R} V(x) dx \le \frac{4\pi}{\ln(R/a)} - \frac{4\pi}{\ln(R/a_R)}$$
 (20)

for R > a.

Again we use  $\psi_R$  as a trial state for  $\mathcal{E}_{\beta}$ . From (17) it follows that

$$\int_{\mathbb{R}^3} |\psi_R(x)|^2 dx \le \frac{1}{[\ln(R/a_R)]^2} \int_{|x| < R} [\ln(R/x)]^2 dx = \frac{\pi R^2}{2[\ln(R/a_R)]^2}.$$
 (21)

With the aid of (20) and (7) we hence obtain

$$\mathcal{E}_{\beta}(\psi_R) \le \frac{4\pi}{\ln(R/a)} + \frac{\pi R^2}{\beta[\ln(R/a_R)]^2}.$$
 (22)

If we choose  $R = \sqrt{\beta}$  we thus obtain

$$e(\beta) \le \frac{8\pi}{\ln(\beta/a^2)} \left( 1 + \frac{1}{2\ln(\beta/a^2)} \right) \tag{23}$$

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 (4).

## 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  $|x| \le a$  and 0 otherwise. In this case, the minimizer of  $\mathcal{E}_{\beta}$  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  $\mathcal{E}_{\beta}$  for the hard sphere potential is

$$\psi(|x|) = \min \left\{ \frac{K_0(|x|/\sqrt{\beta})}{K_0(a/\sqrt{\beta})}, 1 \right\}, \qquad (26)$$

where  $K_0$  is the modified Bessel function of  $2^{\text{nd}}$  kind. Hence

$$e(\beta) = -\frac{4\pi a}{\sqrt{\beta}} \frac{K_0'(a/\sqrt{\beta})}{K_0(a/\sqrt{\beta})} + \frac{2\pi a^2}{\beta}$$
(27)

in this case. The function  $t \mapsto -tK'_0(t)/K_0(t)$  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 (4)

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  $\int_{|x|>b} V(x) dx < \infty$  for all b > a. On the other hand, if  $\int_{|x| \ge b} V(x) dx < \infty$ , then

$$\frac{8\pi a_R}{1 - a_R/R} \le \frac{8\pi b}{1 - b/R} + \int_{|x| \ge b} V(x) dx \tag{28}$$

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

$$\phi(x) = \begin{cases} 1 & \text{for } |x| \le b \\ \frac{b/|x| - b/R}{1 - b/R} & \text{for } b \le |x| \le R \\ 0 & \text{for } |x| \ge R. \end{cases}$$
 (29)

Hence  $a \le b + (8\pi)^{-1} \int_{|x| \ge b} V(x) dx$ . For d = 2, we can use the trial function

$$\phi(x) = \begin{cases} 1 & \text{for } |x| \le b \\ \frac{\ln(R/|x|)}{\ln(R/b)} & \text{for } b \le |x| \le R \\ 0 & \text{for } |x| \ge R \end{cases}$$
(30)

for R > b. This gives

$$\frac{4\pi}{\ln(R/a_R)} \le \frac{4\pi}{\ln(R/b)} + \frac{1}{[\ln(R/b)]^2} \int_{b \le |x| \le R} V(x) [\ln(|x|/b)]^2 dx. \tag{31}$$

We can rewrite this inequality as

$$4\pi \ln(a_R/b) \le \frac{\ln(R/a_R)}{\ln(R/b)} \int_{b \le |x| \le R} V(x) [\ln(|x|/b)]^2 dx.$$
 (32)

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

$$4\pi \ln(a/b) \le \int_{|x| \ge b} V(x) [\ln(|x|/b)]^2 dx.$$
 (33)

To show that the finiteness of a 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,

$$\frac{4\pi}{\ln(R/a_b)} \le \frac{4\pi}{\ln(R/a_R)} - \int_{b \le |x| \le R} V(x) \left(1 - \psi_R(x)\right)^2 dx. \tag{34}$$

Using (17) this bound implies that

$$4\pi \ln(a_R/a_b) \ge \frac{\ln(R/a_b)}{\ln(R/a_R)} \int_{b < |x| < R} V(x) \left[ \ln(|x|/a_R) \right]^2 dx. \tag{35}$$

Letting  $R \to \infty$  we obtain

$$4\pi \ln(a/a_b) \ge \int_{|x| > b} V(x) [\ln(|x|/a)]^2 dx.$$
 (36)

This completes the proof.

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