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Rigorous Upper Bound on the Critical Temperature of Dilute Bose Gases

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We prove exponential decay of the off-diagonal correlation function in the two-dimensional homogeneous Bose gas when $a^2\rho$ is small and the temperature T satisfies

$$T > \frac{4\pi\rho}{\ln|\ln(a^2\rho)|}.$$

Here, a is the scattering length of the repulsive interaction potential and ρ is the density. To leading order in $a^2\rho$, this bound agrees with the expected critical temperature for superfluidity. In the three-dimensional Bose gas, exponential decay is proved when

$$\frac{T - T_c^{(0)}}{T_c^{(0)}} > 5\sqrt{a\rho^{1/3}},$$

where $T_c^{(0)}$ is the critical temperature of the ideal gas. While this condition is not expected to be sharp, it gives a rigorous upper bound on the critical temperature for Bose-Einstein condensation.

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I. INTRODUCTION

Quantum many-body effects due to particle interactions and quantum statistics make the Bose gas a fascinating system and a challenge to theoretical physics. It is increasingly relevant to experimental physics, especially after the first realization of Bose-Einstein condensation in cold atomic gases.^{1,2} It displays a stunning physical phenomenon: superfluidity. Several mechanisms that are present in the Bose gas also play a rôle in interacting electronic systems and in quantum optics.

Both the two-dimensional and the three-dimensional gas have physical relevance, and they behave rather differently. We consider them separately here. Throughout the paper, we shall assume that units are chosen in such a way that $\hbar = 2m = k_B = 1$, where m is the particle mass.

A. The two-dimensional Bose gas

There is no Bose-Einstein condensation in the two-dimensional Bose gas at positive temperature, as was proved by Hohenberg more than forty years ago.³ In contrast to higher dimensions, the ideal Bose gas offers no intriguing features in two dimensions. But the interacting gas is expected to display a Kosterlitz-Thouless type transition from a normal fluid to a superfluid, where the decay of off-diagonal correlations goes from exponential to power law. The critical temperature T_c depends on the scattering length a of the interaction potential, which we consider to be repulsive. For dilute gases, i.e. when

$a^2\rho \ll 1$, Popov⁴ performed diagrammatic expansions in a functional integral approach, finding that

$$T_c \approx \frac{4\pi\rho}{\ln|\ln(a^2\rho)|}. \quad (1)$$

This formula was confirmed by Fisher and Hohenberg⁵ using Bogoliubov's theory, and by Pilati et al.⁶ using Monte-Carlo simulations. No rigorous proof is available to this date, however.

In this article we prove in a mathematically rigorous fashion that there is exponential decay of the off-diagonal correlation function when the temperature satisfies

$$T \geq \frac{4\pi\rho}{\ln|\ln(a^2\rho)|} \left(1 + O\left(\frac{\ln|\ln|\ln(a^2\rho)||}{\ln|\ln(a^2\rho)|}\right) \right) \quad (2)$$

for small $a^2\rho$. Thus we prove that T_c cannot be bigger than the conjectured value (1), to leading order in $a^2\rho$. The main novel ingredient in our proof is a rigorous bound on the grand-canonical density of the interacting Bose gas. This is explained in the next section.

B. The three-dimensional Bose gas

A three-dimensional Bose gas is interesting even in the absence of particle interactions. Bose-Einstein condensation takes place at the critical temperature $T_c^{(0)} = 4\pi(\rho/\zeta(\frac{3}{2}))^{2/3}$ (where $\zeta(\frac{3}{2}) \approx 2.612$, with ζ the Riemann zeta function). The effects of particle interactions on the critical temperature have been studied by many authors. A consensus has been reached in recent years but it is

tenuous; we give a survey of the main results, both for historical perspective and in order to gain a sense of the solidity of the consensus. Let $\Delta T_c = T_c - T_c^{(0)}$ denote the change of the critical temperature.

1953 Feynman⁷ argued that interactions increase the effective mass of the particles and hence decrease T_c , i.e., $\Delta T_c < 0$.

1958 Lee and Yang⁸ predict that the change of critical temperature is linear in the scattering length, namely

$$\Delta T_c/T_c^{(0)} \approx c a \rho^{1/3}.$$

No information on the constant c is provided, not even its sign.

1960 Glassgold, Kaufman, and Watson⁹ find that the critical temperature increases as $\Delta T_c/T_c^{(0)} \approx C(a\rho^{1/3})^{1/2}$ with $C > 0$.

1964 Huang¹⁰ gives an argument suggesting that $\Delta T_c/T_c^{(0)} \approx C(a\rho^{1/3})^{3/2}$ with $C > 0$.

1971 A Hartree-Fock computation shows that $\Delta T_c < 0$ (Fetter and Walecka¹¹).

1982 A loop expansion of the quantum field representation gives $\Delta T_c/T_c^{(0)} \approx -3.5(a\rho^{1/3})^{1/2}$ (Toyoda¹²).

1992 By studying the evolution of the interacting Bose gas, Stoof¹³ finds that the change of critical temperature is linear in the scattering length with $c = 16\pi/3\zeta(3/2)^{4/3} = 4.66$.

1996 A diagrammatic expansion in the renormalization group yields $\Delta T_c > 0$ (Bijlsma and Stoof¹⁴).

1997 A path integral Monte-Carlo simulation yields $c = 0.34 \pm 0.06$ (Grüter, Ceperley, and Laloë¹⁵).

1999 A virial expansion leads to $c = 0.7$ (Holzmann, Grüter, and Laloë¹⁶). Another virial expansion leads Huang¹⁷ to conclude that $\Delta T_c/T_c^{(0)} \approx 3.5(a\rho^{1/3})^{1/2}$. Interchanging the limit $a \rightarrow 0$ with the thermodynamic limit, and using Monte-Carlo simulations, Holzmann and Krauth¹⁸ find $c = 2.3 \pm 0.25$. The dilute Bose gas can be mapped onto a classical field lattice model (Baym et. al.¹⁹); a self-consistent approach then yields $c = 2.9$.

2000 An experimental realization by Reppy et. al.²⁰ yields $c = 5.1 \pm 0.9$. It was later pointed out that the estimation of the scattering length between particles was not correct, however.²¹

2001 Arnold and Moore,²² and Kashurnikov, Prokof'ev, and Svistunov²¹ performed numerical simulations on the equivalent classical field model;¹⁹ the former get $c = 1.32 \pm 0.02$ and the latter get $c = 1.29 \pm 0.05$.

2003 A variational perturbation theory performed by Kleinert²³ yields $c = 1.14 \pm 0.11$.

2004 By studying the classical field model with variational perturbations, Kastening²⁴ finds $c = 1.27 \pm 0.11$. A path integral Monte-Carlo simulation by Nho and Landau²⁵ yields $c = 1.32 \pm 0.14$.

The last articles essentially agree with one another, and also with more recent articles.⁶ The case for a linear correction with constant $c \approx 1.3$ is made rather convincingly; it is not beyond reasonable doubt, though. Notice that the constant c is *universal* in the sense that it does not depend on such special features as the mass of the particles or the details of the interactions. (The mass enters the scattering length a , however.)

The question of the critical temperature for interacting Bose gases is reviewed in Baym et. al.²⁶ and in Blaizot.²⁷ A comprehensive survey on many aspects of bosonic systems has been written by Bloch, Dalibard, and Zwerger.²⁸ This question is also mentioned in additional articles dealing with certain perturbation methods. The value of c is assumed to be known and its calculation serves to test the method. Some of these references can be found in Blaizot.²⁷

In this article we give a partial rigorous justification of the results in the literature by proving that off-diagonal correlations decay exponentially when

$$\frac{T - T_c^{(0)}}{T_c^{(0)}} \geq 5.09 \sqrt{a\rho^{1/3}} \left(1 + O(\sqrt{a\rho^{1/3}})\right). \quad (3)$$

In particular, there is no Bose-Einstein condensation when (3) is satisfied. This rigorous result is not sharp enough to disprove any of the previous claims that have been just reviewed, although it gets close to Huang's 1999 result. As in the two-dimensional case, the proof is based on bounds of the grand-canonical density for the interacting gas.

C. Outline of this article

In the next section, we shall explain how the exponential decay of correlations can be deduced from appropriate lower bounds on the particle density in the grand-canonical ensemble. These bounds will be proved in the remaining sections. In Section III, we shall state our main result, Theorem III.1, and we shall explain the precise assumptions on the interparticle interactions under which it holds. Our main tool is a path integral representation which is explained in detail in Section IV. Finally, in Section V we investigate certain integrals of the difference between the heat kernel of the Laplacian with and without potential, and obtain bounds that are needed to complete the proof of Theorem III.1.

II. DECAY OF CORRELATIONS

We consider the grand-canonical ensemble at chemical potential μ and we denote the fugacity by $z = e^{\beta\mu}$. Let $\gamma(x, y) = \langle a^\dagger(x)a(y) \rangle$ denote the reduced one-particle density matrix of the interacting system, and $\gamma^{(0)}$ the one of the ideal gas. An important fact is that, when the interactions are repulsive, we have

$$\gamma(x, y) \leq \gamma^{(0)}(x, y) \quad (4)$$

for any $0 < z < 1$. See Bratteli-Robinson,²⁹ Theorem 6.3.17. In d spatial dimensions,

$$\gamma^{(0)}(x, y) = \sum_{n \geq 1} \frac{z^n}{(4\pi\beta n)^{d/2}} e^{-\frac{|x-y|^2}{4\beta n}}$$

which behaves like $\exp(-\sqrt{-\beta^{-1} \ln z} |x-y|)$ for large $|x-y|$. That is, off-diagonal correlations decay exponentially fast when $z < 1$. In particular, the critical fugacity satisfies $z_c \geq 1$.

Next, let $\rho(z)$ denote the grand-canonical density of the interacting system (it depends on β as well, although the notation does not show it explicitly), and let

$$\rho^{(0)}(z) = (4\pi\beta)^{-d/2} g_{d/2}(z) \quad (5)$$

the density of the ideal system. Here, the function $g_{d/2}$ is defined by

$$g_r(z) = \sum_{n \geq 1} \frac{z^n}{n^r}. \quad (6)$$

The density $\rho(z)$ is increasing in z . Then a sufficient condition for the exponential decay of correlations is that, for some $z < 1$,

$$\rho < \rho(z). \quad (7)$$

The obvious problem with this condition is that the density $\rho(z)$ for the interacting system is not given by an explicit function. Our way out is to obtain bounds for $\rho(z)$ (see Theorem III.1 below) and to use them with $z < 1$ suitably chosen.

A. Two dimensions

We now explain the proof of exponential decay of correlations under the condition (2) for $d = 2$. We show below (see Theorem III.1 and the following remarks) that the density satisfies the lower bound

$$\rho(z) \geq \rho^{(0)}(z) - \frac{C}{4\pi\beta} \frac{|\ln(1-z)|}{1-z} \frac{1}{|\ln(a^2/\beta)|}, \quad (8)$$

for some constant $C > 0$ and for $a\beta^{-1/2}$ small enough. Here, a denotes the two-dimensional scattering length, which can be defined similarly to the three-dimensional

case via the solution of the zero-energy scattering equation.^{30,31}

In two dimensions, $\rho^{(0)}(z) = -(4\pi\beta)^{-1} \ln(1-z)$. For the choice $z = z_0$ with

$$z_0 = 1 - \frac{\ln |\ln(a^2/\beta)|}{|\ln(a^2/\beta)|},$$

the criterion (7) is fulfilled when

$$\rho \leq \frac{\ln |\ln(a^2/\beta)|}{4\pi\beta} \left(1 - O\left(\frac{\ln \ln |\ln(a^2/\beta)|}{\ln |\ln(a^2/\beta)|} \right) \right).$$

Since $\beta = 1/T$, one can check that this is equivalent to the condition (2).

The situation is illustrated in Fig. 1 with qualitative graphs of $\rho^{(0)}(z)$ and $\rho(z)$. The critical fugacity z_c is known to be larger than 1. Our density bound holds for $z < 1$, and this yields the lower bound ρ_0 for the critical density. It turns out to be equal to the conjectured critical density (determined by Eq. (1)) to leading order in the small parameter $a\beta^{-1/2}$.

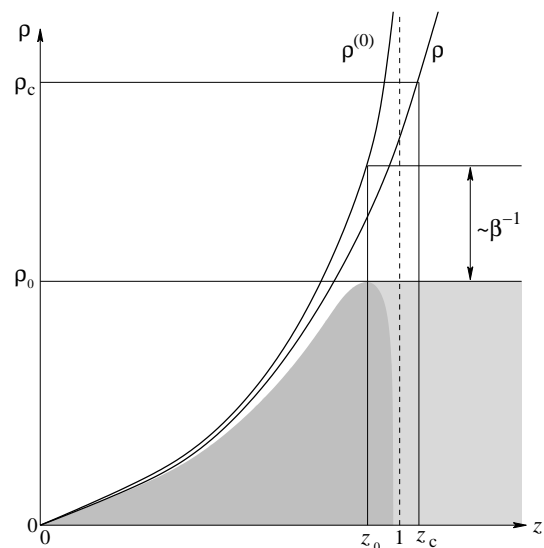


FIG. 1: Qualitative graphs of the grand-canonical density for $d = 2$. The shaded area represents our lower bound for the interacting density — the darker area is the function defined in Eq. (8) and it extends to the lighter area by monotonicity of the grand-canonical density. Our lower bound ρ_0 for the critical density is obtained by choosing $z_0 = 1 - \frac{\ln |\ln(a^2/\beta)|}{|\ln(a^2/\beta)|}$.

B. Three dimensions

We shall prove exponential decay under the condition (3), where the constant 5.09 is really

$$A = \frac{2^{7/2} \pi^{1/2}}{3 \zeta(3/2)^{7/6}} \sqrt{2^{3/2} + \zeta(3/2)} \approx 5.09.$$

It is more convenient to consider the change in the critical density rather than in the temperature. Inequality (3) is equivalent to

$$\frac{\rho - \rho_c^{(0)}}{\rho_c^{(0)}} \leq -A' \sqrt{a\beta^{-1/2}} \left(1 + O(\sqrt{a\beta^{-1/2}})\right), \quad (9)$$

where $\rho_c^{(0)} = \rho^{(0)}(1)$ is the critical density of the ideal Bose gas at temperature T , and where the constants A and A' are related by

$$A' = \frac{3}{2} \frac{\zeta(3/2)^{1/6}}{(4\pi)^{1/4}} A \approx 4.75.$$

We show below that the lower bound

$$\rho(z) \geq \rho^{(0)}(z) - \frac{a}{(2\pi\beta)^2} \left[(2^{3/2} + \zeta(3/2)) \sqrt{\frac{\pi}{-\ln z}} + C \right] \quad (10)$$

holds for some positive constant C and $a\beta^{-1/2}$ small enough (see Theorem III.1 and the following remarks). We use $dg_{3/2}/dz = z^{-1}g_{1/2}(z)$, as well as the bound

$$g_{1/2}(z) \leq \int_0^\infty \frac{z^t}{\sqrt{t}} dt = \sqrt{\frac{\pi}{-\ln z}} \quad (11)$$

to obtain

$$\begin{aligned} \rho^{(0)}(1) - \rho^{(0)}(z) &\leq (4\pi\beta)^{-3/2} \int_z^1 \sqrt{\frac{\pi}{-\ln s}} \frac{ds}{s} \\ &= (4\pi)^{-1} \beta^{-3/2} \sqrt{-\ln z}. \end{aligned}$$

The criterion (7) is thus fulfilled when

$$\begin{aligned} \rho &\leq \rho^{(0)}(1) - (4\pi)^{-1} \beta^{-3/2} \sqrt{-\ln z} \\ &\quad - \frac{a}{(2\pi\beta)^2} \left[(2^{3/2} + \zeta(3/2)) \sqrt{\frac{\pi}{-\ln z}} + C \right] \end{aligned}$$

for some $z < 1$. The right side of this expression depends on z only through $w = \sqrt{-\ln z}$. Since the minimum of $Aw + \frac{B}{w}$ over $w > 0$ is $2\sqrt{AB}$, we get the condition (9). Notice that the optimal choice of z is $z_0 = 1 - \pi^{-1/2}(2^{3/2} + \zeta(3/2))a\beta^{-1/2}$ to leading order in $a\beta^{-1/2}$.

The three-dimensional situation is illustrated in Fig. 2. The critical fugacity z_c is larger than 1 but our density bound holds for $z < 1$. Our lower bound for the critical density, ρ_0 , is close to the conjectured expression for small $a\beta^{-1/2}$.

III. RIGOROUS DENSITY BOUNDS

We are left with proving the lower bounds (8) and (10), respectively. These will be an immediate consequence of Theorem III.1 below. In order to state our results precisely, we shall first give a definition of the model and specify the assumptions on the interaction potential.

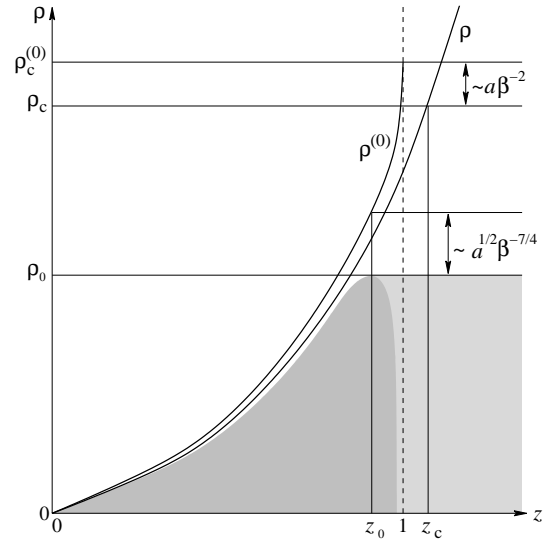


FIG. 2: Qualitative graphs of the grand-canonical density for $d = 3$. The shaded area represents our lower bound for the interacting density — the darker area is the function defined in Eq. (10) and it extends to the lighter area by monotonicity of the grand-canonical density. Our lower bound ρ_0 for the critical density is obtained by choosing $z_0 = 1 - Ca\beta^{-1/2}$. The difference between $\rho_c^{(0)}$ and ρ_c is expected to be of the order $a\beta^{-2}$.

This makes it necessary to adopt a precise mathematical tone from now on. We do so in order to make the results accessible also to readers with a more mathematical background.

Let $\Lambda \subset \mathbb{R}^d$ be an open and bounded domain. The state space for N bosons in Λ is the Hilbert space $L_{\text{sym}}^2(\Lambda^N)$ of square-integrable complex-valued functions that are symmetric with respect to their arguments. The Hamiltonian is

$$H_{\Lambda, N} = - \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} U(x_i - x_j),$$

with Δ_i the Laplacian for the i -th variable, with Dirichlet boundary conditions on the boundary of Λ . The repulsive interaction is given by the multiplication operator $U(x) \geq 0$. We assume that U is radial and has finite range, i.e., $U(x) = 0$ for $|x| > R_0$. No regularity is assumed, however; we only require that the Hamiltonian defines a self-adjoint operator on an appropriate domain, and that the Feynman-Kac formula for the heat kernel applies. In particular, U is allowed to have a hard core. The scattering length of U is denoted by a .

The grand-canonical partition function is

$$Z \equiv Z(\beta, \Lambda, z) = \sum_{N \geq 0} z^N \text{Tr} e^{-\beta H_{\Lambda, N}}.$$

The thermodynamic pressure is defined by

$$p(\beta, z) = \frac{1}{\beta|\Lambda|} \ln Z(\beta, \Lambda, z),$$

and the density is given by

$$\rho(z) = \beta z \frac{\partial}{\partial z} p(\beta, z). \quad (12)$$

We always work in finite volume Λ . The existence of the thermodynamic limit for the pressure, density and reduced density matrix is far from trivial. In particular, the limit for the latter has only been proved when z is small enough.²⁹ This is of no relevance to the present article, however, since our bounds apply to all finite domains uniformly in the volume. The one-particle reduced density matrix can be written in terms of the integral kernels of the operators $e^{-\beta H_{\Lambda, N}}$ as

$$\begin{aligned} \gamma(x, y) &= \frac{1}{Z} \sum_{N \geq 1} N z^N \int_{\Lambda^{N-1}} dx_2 \cdots dx_N \\ &\times e^{-\beta H_{\Lambda, N}}(x, x_2, \dots, x_N; y, x_2, \dots, x_N). \end{aligned}$$

Relatively few rigorous results on interacting homogeneous Bose gases are available to this date. The only proof of occurrence of Bose-Einstein condensation deals with the hard-core lattice model at half-filling.^{32,33} Roepstorff³⁴ used Bogoliubov's inequality to get an upper bound on the condensate density. Several aspects of Bogoliubov's theory^{31,35} have been rigorously justified.^{36,37,38} A rigorous proof of the leading order of the ground state energy per particle in the low density limit was given by Lieb and Yngvason.^{30,39} The next order correction term was recently studied in a certain scaling limit.⁴⁰ Bounds of the free energy at positive temperature were given in⁴¹. Cluster expansions give informations on the phase without Bose-Einstein condensation, for repulsive or stable potentials.^{42,43} Recently there has been interest in Feynman cycles which should be related to Bose-Einstein condensation.⁴⁴ The conditions (2) and (3) guarantee the absence of infinite cycles. This follows from the considerations here, and from the proof that all cycles are finite when the chemical potential is negative.⁴⁵

The following theorem gives bounds on the density $\rho(z)$. Recall the function g_r defined in (6). Let us define the following small parameter $\tilde{a}(\beta)$, which is associated with the scattering length a : for $d = 2$,

$$\tilde{a}(\beta) = \left(|\ln(a^2/\beta)| - 2 \ln |\ln(a/\sqrt{\beta})| \right)^{-1} + |\ln(a^2/\beta)|^{-2};$$

and for $d = 3$,

$$\tilde{a}(\beta) = a \left([1 - (a/\sqrt{\beta})^{1/2}]^{-1} + \frac{1}{3} (a/\sqrt{\beta})^{1/2} \right).$$

Theorem III.1. *Let us assume that $\sqrt{\beta} |\ln(a/\sqrt{\beta})|^{-1} > R_0$ when $d = 2$, or that $a\sqrt{\beta} > R_0^2$ when $d = 3$. Then we have, for $0 < z < 1$,*

$$\rho(z) \geq \rho^{(0)}(z) - \frac{4z^2}{(4\pi\beta)^{d-1}} \left(h_d(z) \tilde{a}(\beta) + 2^{d/2} \tilde{a}(\beta/2) \right), \quad (13)$$

where

$$h_d(z) = \left(2^{\frac{d}{2}} + g_{\frac{d}{2}}(z) \right) g_{\frac{d}{2}-1}(z) + 2^{\frac{d}{2}+1} g_{\frac{d}{2}}(z) + g_{\frac{d}{2}}(z)^2. \quad (14)$$

Notice that $\rho(z) \leq \rho^{(0)}(z)$; this is an immediate consequence of (4). For $d = 2$ we believe that for z close to 1 the lower bound is optimal up to terms of higher order in $\tilde{a}(\beta)$, while for $d = 3$ the prefactor is not optimal. This is based on the (yet unproved) assumption that the leading order correction to the pressure is equal to $-8\pi\tilde{a}(\beta)\rho^{(0)}(z)^2$ for $z < 1$.^{30,41,46} Using (5) and (12), this suggests that $\rho(z) \approx \rho^{(0)}(z) - 4\tilde{a}(\beta)(4\pi\beta)^{1-d} g_{d/2}(z) g_{d/2-1}(z)$. If this indeed holds as a lower bound, one can replace the constant 5.09 in (3) by 3.52, yielding a bound in agreement with Huang's prediction.¹⁷

From Theorem III.1, we can easily deduce the bounds (8) and (10), which we have used in the previous section. Since $g_0(z) = z/(1-z)$ and $g_1(z) = -\ln(1-z)$, we see that the function h_2 is bounded by

$$h_2(z) \leq C(1-z)^{-1} |\ln(1-z)|$$

for some constant $C < \infty$, which implies (8). To obtain (10), note that the function $g_{3/2}(z)$ converges to $\zeta(3/2)$ as $z \rightarrow 1$. Using the bound (11) we see that h_3 is less than

$$h_3(z) \leq \left(2^{3/2} + \zeta\left(\frac{3}{2}\right) \right) \sqrt{\frac{\pi}{-\ln z}} + 2^{5/2} \zeta\left(\frac{3}{2}\right) + \zeta\left(\frac{3}{2}\right)^2.$$

We are left with the proof of Theorem III.1. In Section IV we use the Feynman-Kac representation of the Bose gas to obtain bounds on the density. These bounds are expressed in terms of integrals of the difference between the heat kernel of the Laplacian with and without potential. Section V deals with bounds of these integrals. It contains a novel variational principle for integrals over heat kernel differences (Lemma V.1), which allows to bound these in terms of the scattering length of the interaction potential. Theorem III.1 then follows directly from Proposition IV.2 and from Lemmas V.2 and V.3.

IV. FEYNMAN-KAC REPRESENTATION OF THE INTERACTING BOSE GAS

From now on we shall work in arbitrary dimension $d \geq 1$. Let $W_{x,y}^t$ denote the Wiener measure for the Brownian bridge from x to y in time t ; the normalization is chosen so that

$$\int dW_{x,y}^t(\omega) = (2\pi t)^{-d/2} e^{-|x-y|^2/2t} \equiv \pi_t(x-y).$$

The integral kernel of $e^{2\beta\Delta} - e^{\beta(2\Delta-U)}$ will be denoted by $K(x, y)$. By the Feynman-Kac formula, it can be expressed as

$$K(x, y) = \int (1 - e^{-\frac{1}{4} \int_0^{4\beta} U(\omega(s)) ds}) dW_{x,y}^{4\beta}(\omega). \quad (15)$$

Let us introduce the interaction $\bar{U}(\omega, \omega')$ between two paths ω and ω' : $[0, 2\beta] \rightarrow \mathbb{R}^d$. Namely,

$$\bar{U}(\omega, \omega') = \frac{1}{2} \int_0^{2\beta} U(\omega(s) - \omega'(s)) ds.$$

The following identity, which will prove useful in the sequel, is obtained by changing to center-of-mass and relative coordinates.

Lemma IV.1. *For any $x, y, x', y' \in \mathbb{R}^d$,*

$$\begin{aligned} & \int dW_{x,y}^{2\beta}(\omega) \int dW_{x',y'}^{2\beta}(\omega') (1 - e^{-\bar{U}(\omega, \omega')}) \\ &= 2^d \pi_{4\beta}(x - y + x' - y') K(x - x', y - y'). \end{aligned}$$

Proof. The difference $\omega - \omega'$ of two Brownian bridges is a Brownian bridge with double variance. Precisely, we have

$$\begin{aligned} & \int \frac{dW_{x,y}^{2\beta}(\omega)}{\pi_{2\beta}(x - y)} \int \frac{dW_{x',y'}^{2\beta}(\omega')}{\pi_{2\beta}(x' - y')} (1 - e^{-\bar{U}(\omega, \omega')}) \\ &= \int \frac{dW_{x-x', y-y'}^{4\beta}(\omega)}{\pi_{4\beta}(x - x' - y + y')} \left(1 - e^{-\frac{1}{2} \int_0^{2\beta} U(\omega(2s)) ds}\right). \end{aligned}$$

By the parallelogram identity,

$$\frac{\pi_{2\beta}(x - y) \pi_{2\beta}(x' - y')}{\pi_{4\beta}(x - x' - y + y')} = 2^d \pi_{4\beta}(x - y + x' - y').$$

The result then follows from (15). \square

We also use the Feynman-Kac formula for the canonical partition function. Namely,

$$\begin{aligned} \text{Tr } e^{-\beta H_{\Lambda, N}} &= \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} \int_{\Lambda^N} dx_1 \cdots dx_N \\ &\times \int dW_{x_1, x_{\pi(1)}}^{2\beta}(\omega_1) \cdots \int dW_{x_N, x_{\pi(N)}}^{2\beta}(\omega_N) \\ &\times \left(\prod_{i=1}^N \chi_{\Lambda}(\omega_i) \right) \exp \left\{ - \sum_{1 \leq i < j \leq N} \bar{U}(\omega_i, \omega_j) \right\}. \end{aligned} \quad (16)$$

Here, \mathcal{S}_N is the set of permutations of N elements; $\chi_{\Lambda}(\omega)$ is equal to one if $\omega(s) \in \Lambda$ for all $0 \leq s \leq 2\beta$, and it is zero otherwise. Eq. (16) makes sense for general measurable functions $U : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{\infty\}$. In particular, we can consider the case of the hard-core potential of radius a . An introduction to the Feynman-Kac formula in the context of bosonic quantum systems can be found in Ginibre's survey.⁴²

We now rewrite the grand-canonical partition function in terms of winding loops. Let Ω_k be the set of continuous paths $[0, 2\beta k] \rightarrow \mathbb{R}^d$ that are closed. Its elements are denoted by $\omega = (x, k, \omega)$, with $x \in \mathbb{R}^d$ the starting point and k the winding number; we have $\omega(0) = \omega(2\beta k) = x$.

For $0 \leq \ell \leq k - 1$, we also let ω_{ℓ} denote the ℓ -th leg of ω ,

$$\omega_{\ell}(s) = \omega(2\beta\ell + s),$$

with $0 \leq s \leq 2\beta$. We consider the measure μ given by

$$d\mu(\omega) = \frac{z^k}{k} dx \chi_{\Lambda}(\omega) dW_{x,x}^{2\beta k}(\omega) e^{-V(\omega)}.$$

Here, $V(\omega)$ is a self-interaction term that is defined below in Eq. (17). Let $\Omega = \cup_{k \geq 1} \Omega_k$; the measure μ above naturally extends to a measure on Ω . The grand-canonical partition function can then be written as⁴²

$$\begin{aligned} Z &= \sum_{n \geq 0} \frac{1}{n!} \int_{\Omega^n} d\mu(\omega_1) \cdots d\mu(\omega_n) \\ &\times \exp \left\{ - \sum_{1 \leq i < j \leq n} V(\omega_i, \omega_j) \right\}. \end{aligned}$$

The self-interaction $V(\omega)$ and the 2-path interaction $V(\omega, \omega')$ are given by

$$\begin{aligned} V(\omega) &= \sum_{0 \leq \ell < m \leq k-1} \bar{U}(\omega_{\ell}, \omega_m), \\ V(\omega, \omega') &= \sum_{\ell=0}^{k-1} \sum_{\ell'=0}^{k'-1} \bar{U}(\omega_{\ell}, \omega'_{\ell'}). \end{aligned} \quad (17)$$

We shall denote $V_{ij} \equiv V(\omega_i, \omega_j)$ for short. Using (12) one obtains an expression for the grand-canonical density, namely

$$\begin{aligned} \rho(z) &= \frac{1}{|\Lambda|Z} \sum_{n \geq 1} \frac{1}{(n-1)!} \int d\mu(\omega_1) k_1 \\ &\times \int d\mu(\omega_2) \cdots \int d\mu(\omega_n) e^{-\sum_{i < j} V_{ij}}. \end{aligned} \quad (18)$$

From the representation (18) it is easy to see that $\rho(z) \leq \rho^{(0)}(z)$. One uses the positivity of V_{ij} to bound $\sum_{1 \leq i < j \leq N} V_{ij} \geq \sum_{2 \leq i < j \leq N} V_{ij}$. For fixed ω_1 , the integration over ω_j with $j \geq 2$ then yields Z , and hence

$$\rho(z) \leq \frac{1}{|\Lambda|} \int d\mu(\omega_1) k_1 \leq \rho^{(0)}(z).$$

The last inequality follows since the self-interaction $V(\omega)$ is also positive.

In the following proposition we shall derive a *lower* bound on $\rho(z)$. We use the function h_d defined in (14), as well as the integral kernel $K(x, y)$ in (15).

Proposition IV.2. *For $d \geq 1$, $\beta > 0$ and $0 < z < 1$, we have the lower bound*

$$\begin{aligned} \rho(z) &\geq \rho^{(0)}(z) - \frac{2z^2}{(4\pi\beta)^d} \left(h_d(z) \int K(x, y) dx dy \right. \\ &\quad \left. + \frac{1}{2} (8\pi\beta)^{d/2} \int [K(x, x) + K(x, -x)] dx \right) \end{aligned}$$

for any bounded (and measurable) $\Lambda \subset \mathbb{R}^d$.

Proof. Isolating the interactions between the first path and the others, we can bound $\exp\{-\sum_{1 \leq i < j \leq n} V_{ij}\}$ from below as

$$\begin{aligned} & \exp\left\{-\sum_{j=2}^n V_{1j}\right\} \exp\left\{-\sum_{2 \leq k < l \leq n} V_{kl}\right\} \\ & \geq \left[1 - \sum_{j=2}^n (1 - e^{-V_{1j}})\right] \exp\left\{-\sum_{2 \leq k < l \leq n} V_{kl}\right\}. \end{aligned} \quad (19)$$

We use this lower bound in Eq. (18). The first term (the 1 in square brackets in (19)) is then $|\Lambda|^{-1} \int d\mu(\omega_1) k_1$, since the integration over ω_j with $j \geq 2$ yields exactly Z . For the remaining terms (the sum over j), we also use the fact that the potential is repulsive so as to drop the interactions between ω_j and the other loops in the last term in (19) for a lower bound. We conclude that

$$\begin{aligned} \rho(z) & \geq \frac{1}{|\Lambda|} \int d\mu(\omega) k \\ & \quad - \frac{1}{|\Lambda|} \int d\mu(\omega_1) k_1 \int d\mu(\omega_2) (1 - e^{-V_{12}}). \end{aligned} \quad (20)$$

In a similar fashion to (19), we have

$$\begin{aligned} e^{-V(\omega)} & \geq 1 - \sum_{0 \leq \ell < m \leq k-1} \left(1 - e^{-\bar{U}(\omega_\ell, \omega_m)}\right), \\ e^{-V(\omega_1, \omega_2)} & \geq 1 - \sum_{\ell_1=0}^{k_1-1} \sum_{\ell_2=0}^{k_2-1} \left(1 - e^{-\bar{U}(\omega_{\ell_1}, \omega_{\ell_2})}\right). \end{aligned}$$

Here, $\omega_{i,\ell}$ denotes the ℓ -th leg of the path ω_i . We insert these inequalities into (20), and obtain

$$\rho(z) \geq \rho^{(0)}(z) - A - B,$$

with

$$\begin{aligned} A & = \frac{1}{|\Lambda|} \sum_{k \geq 2} z^k \int_{\Lambda} dx \int dW_{x,x}^{2\beta k}(\omega) \\ & \quad \times \sum_{0 \leq \ell < m \leq k-1} \left(1 - e^{-\bar{U}(\omega_\ell, \omega_m)}\right), \\ B & = \frac{1}{|\Lambda|} \int d\mu(\omega_1) k_1^2 \int d\mu(\omega_2) k_2 \left(1 - e^{-\bar{U}(\omega_{1,1}, \omega_{2,1})}\right). \end{aligned}$$

We also used $\chi_\Lambda \leq 1$ to drop the restriction that paths stay inside Λ . Notice that only the first legs of ω_1 and ω_2 interact in B ; this is correct because we multiplied by $k_1 k_2$.

We decompose the terms in A as $A_1 + A_2 + A_3$ according to the distance between interacting legs. Namely, the term $k = 2$ in A is equal to

$$\begin{aligned} A_1 & = \frac{z^2}{|\Lambda|} \int_{\Lambda^2} dx_1 dx_2 \int dW_{x_1, x_2}^{2\beta}(\omega_1) \\ & \quad \times \int dW_{x_2, x_1}^{2\beta}(\omega_2) \left(1 - e^{-\bar{U}(\omega_{1,1}, \omega_{2,1}(s))}\right). \end{aligned}$$

Using Lemma IV.1, we get

$$A_1 \leq \frac{z^2}{(2\pi\beta)^{d/2}} \int K(x, -x) dx.$$

The terms with $k \geq 3$ and two consecutive interacting legs are

$$\begin{aligned} A_2 & = \frac{1}{|\Lambda|} \int_{\Lambda^3} dx_1 dx_2 dx_3 \int dW_{x_1, x_2}^{2\beta}(\omega_1) dW_{x_2, x_3}^{2\beta}(\omega_2) \\ & \quad \left(1 - e^{-\bar{U}(\omega_{1,1}, \omega_{2,1})}\right) \sum_{k \geq 1} \frac{(k+2)z^{k+2}}{(4\pi\beta k)^{d/2}} e^{-\frac{|x_1 - x_3|^2}{4\beta k}}. \end{aligned}$$

Using Lemma IV.1 and bounding the exponentials by 1, we get

$$A_2 \leq \frac{2^{d/2} z^2}{(4\pi\beta)^d} \left[g_{d/2-1}(z) + 2g_{d/2}(z) \right] \int K(x, y) dx dy.$$

The terms where no consecutive legs interact are

$$\begin{aligned} A_3 & = \frac{1}{2|\Lambda|} \int_{\Lambda^4} dx_1 dx_2 dx_3 dx_4 \\ & \quad \int dW_{x_1, x_2}^{2\beta}(\omega_1) \int dW_{x_3, x_4}^{2\beta}(\omega_2) \left(1 - e^{-\bar{U}(\omega_{1,1}, \omega_{2,1})}\right) \\ & \quad \sum_{k_1, k_2 \geq 1} \frac{(k_1 + k_2 + 2)z^{k_1 + k_2 + 2}}{(4\pi\beta k_1)^{d/2} (4\pi\beta k_2)^{d/2}} e^{-\frac{|x_2 - x_3|^2}{4\beta k_1} - \frac{|x_1 - x_4|^2}{4\beta k_2}}. \end{aligned}$$

Then

$$\begin{aligned} A_3 & \leq \frac{2^{d/2-1}}{(4\pi\beta)^{3d/2}} \int_{\mathbb{R}^{3d}} dx dy dz e^{-\frac{|x-y-2z|^2}{8\beta}} K(x, y) \\ & \quad \times \sum_{k_1, k_2 \geq 1} \frac{(k_1 + k_2 + 2)z^{k_1 + k_2 + 2}}{(k_1 k_2)^{d/2}} \\ & = \frac{z^2}{(4\pi\beta)^d} g_{\frac{d}{2}}(z) \left[g_{\frac{d}{2}-1}(z) + g_{\frac{d}{2}}(z) \right] \int K(x, y) dx dy. \end{aligned}$$

We now decompose the terms in B as $B_1 + B_2 + B_3$ according to the winding numbers of ω_1 and ω_2 . The term B_1 involves two paths of winding numbers 1, and with the aid of Lemma IV.1 we find

$$B_1 \leq \frac{z^2}{(2\pi\beta)^{d/2}} \int_{\mathbb{R}^d} K(x, x) dx.$$

Next, B_2 involves a path of winding number 1 and another path of higher winding number. Dropping the self-interaction terms yields the upper bound

$$\begin{aligned} B_2 & \leq \frac{2^{d/2}}{(4\pi\beta)^d} \int_{\mathbb{R}^{2d}} dx dy e^{-\frac{|x-y|^2}{8\beta}} K(x, y) \\ & \quad \times \sum_{k \geq 1} \frac{(k+2)z^{k+2}}{k^{d/2}} \\ & \leq \frac{2^{d/2} z^2}{(4\pi\beta)^d} \left[g_{d/2-1}(z) + 2g_{d/2}(z) \right] \int K(x, y) dx dy. \end{aligned}$$

Finally, B_3 involves paths with winding numbers higher than 2. We have

$$\begin{aligned} B_3 &\leq \frac{2^{d/2}}{(4\pi\beta)^{\frac{3d}{2}}} \int_{\mathbb{R}^{3d}} dx dy dz e^{-\frac{|x-y-2z|^2}{8\beta}} K(x, y) \\ &\quad \times \sum_{k_1, k_2 \geq 1} \frac{(k_1 + 1)z^{k_1+k_2+2}}{(k_1 k_2)^{d/2}} \\ &= \frac{z^2}{(4\pi\beta)^d} g_{\frac{d}{2}}(z) [g_{\frac{d}{2}-1}(z) + g_{\frac{d}{2}}(z)] \int K(x, y) dx dy. \end{aligned}$$

Collecting the bounds on $A_1, A_2, A_3, B_1, B_2, B_3$, we get the lower bound of Proposition IV.2. \square

V. SCATTERING ESTIMATES

As before, let $U(x) \geq 0$ be radial and supported on the set $\{x : |x| \leq R_0\}$. Let a be the scattering length of U . We consider the Hilbert space $L^2(\mathbb{R}^d)$ and the integral kernel $K(x, y)$ of the operator $e^{2\beta\Delta} - e^{\beta(2\Delta-U)}$. It follows from the Feynman-Kac representation that $K(x, y) \geq 0$, see Eq. (15) in the previous section.

We introduce

$$a(\beta) = \frac{1}{8\pi\beta} \int K(x, y) dx dy. \quad (21)$$

We shall see below that, for $d = 3$, $a(\beta)$ is a good approximation to the scattering length. In fact, $a \leq a(\beta) \leq a_0$, with a_0 the first order Born approximation to a . In two dimensions $a(\beta)$ is dimensionless and its relation to the scattering length is $a(\beta) \approx |\ln(a^2/\beta)|^{-1}$ for large β . For $t > 0$, we also introduce the function

$$f(t) = t \frac{1 - e^{-t}}{t - 1 + e^{-t}}.$$

Lemma V.1. *We have*

$$a(\beta) = \frac{1}{8\pi} \inf_{\psi \in H^1(\mathbb{R}^d)} \mathcal{E}_\beta(\psi), \quad (22)$$

where

$$\begin{aligned} \mathcal{E}_\beta(\psi) &= \int_{\mathbb{R}^d} (2|\nabla\psi(x)|^2 + U(x)|1 - \psi(x)|^2) dx \\ &\quad + \frac{1}{\beta} \langle \psi | f(\beta(-2\Delta + U)) | \psi \rangle. \end{aligned}$$

Note that f is monotone decreasing, with $1 \leq f(t) \leq 2$ for all $t > 0$. From monotonicity it follows immediately that $a(\beta)$ is monotone decreasing in β . Moreover, for $d = 3$ it is not hard to see that $\lim_{\beta \rightarrow \infty} a(\beta) = a$. For any d , $\lim_{\beta \rightarrow 0} a(\beta) = (8\pi)^{-1} \int U(x) dx$. (This is also true when $\int U(x) dx = \infty$.)

Proof. We first consider the case when U is bounded.

With the aid of the Duhamel formula we have

$$\begin{aligned} e^{2\beta\Delta} - e^{\beta(2\Delta-U)} &= \int_0^\beta e^{2(\beta-t)\Delta} U e^{t(2\Delta-U)} dt \\ &= \int_0^\beta e^{2(\beta-t)\Delta} U e^{2t\Delta} dt \\ &\quad - \int_0^\beta \int_0^t e^{2(\beta-t)\Delta} U e^{s(2\Delta-U)} U e^{2(t-s)\Delta} ds dt. \end{aligned}$$

Hence

$$a(\beta) = \frac{1}{8\pi} \int U(x) (1 - \psi_\beta(x)) dx, \quad (23)$$

where $\psi_\beta(x) = (L_\beta U)(x)$, with

$$L_\beta = \int_0^\beta (1 - s/\beta) e^{s(2\Delta-U)} ds.$$

The functional $\mathcal{E}_\beta(\psi)$ has a quadratic and a linear part in ψ , and it is not hard to see that the unique minimizer satisfies

$$[-2\Delta + U + \frac{1}{\beta} f(\beta(-2\Delta + U))] \psi = U. \quad (24)$$

Since

$$\frac{1}{t + f(t)} = \int_0^1 (1 - s) e^{-st} ds$$

it follows that $\psi = \psi_\beta$, i.e. $\psi_\beta = L_\beta U$ is the unique minimizer of \mathcal{E}_β . After multiplying (24) by ψ_β and integrating we see that $\mathcal{E}_\beta(\psi_\beta) = \int U(x)(1 - \psi_\beta(x)) dx$ which, because of (23), implies (22).

Finally, the case of unbounded U can be dealt with using monotone convergence. If we replace U by $U_s(x) = \min\{U(x), s\}$ then the kernel $K(x, y)$ corresponding to U_s is monotone increasing in s . We can apply the argument above to U_s and take the limit $s \rightarrow \infty$ at the end. The convergence of $a(\beta)$ is guaranteed by monotonicity. \square

The variational principle of Lemma V.1 is convenient for obtaining an upper bound on $a(\beta)$.

Lemma V.2. *For $d = 2$ and $\sqrt{\beta} |\ln(a/\sqrt{\beta})|^{-1} > R_0$,*

$$a(\beta) \leq \frac{1}{|\ln(a^2/\beta)| - 2 \ln |\ln(a/\sqrt{\beta})|} + \frac{1}{|\ln(a^2/\beta)|^2}. \quad (25)$$

For $d \geq 3$ and $a\sqrt{\beta} > R_0^{d-1}$,

$$\begin{aligned} a(\beta) &\leq \frac{\pi^{d/2-1}}{2\Gamma(d/2)} a \left(\left[1 - (a\beta^{1-d/2})^{1/(d-1)} \right]^{-1} \right. \\ &\quad \left. + \frac{1}{d} (a\beta^{1-d/2})^{1/(d-1)} \right). \quad (26) \end{aligned}$$

Note that the prefactor in (26) is equal to 1 for $d = 3$. Lemma V.2 is the only place where the finiteness of the range R_0 of U is being used. Appropriate upper bounds on $a(\beta)$ can also be obtained without this assumption,

and hence our main results generalize to repulsive interaction potentials with infinite range (but finite scattering length). For simplicity, we shall not pursue this generalization here.

Proof. Let $R > R_0$, and let ψ_∞ be the minimizer of

$$\int_{|x| \leq R} (2|\nabla\psi|^2 + U|1 - \psi|^2) dx \quad (27)$$

subject to the boundary condition $\psi(x) = 0$ for $|x| = R$. It can be shown^{30,31} that there exists a unique minimizer for this problem, which satisfies $0 \leq \psi_\infty \leq 1$ and

$$\psi_\infty(x) = \begin{cases} 1 - \frac{\ln(|x|/a)}{\ln(R/a)} & \text{for } d = 2 \\ 1 - \frac{1 - a|x|^{2-d}}{1 - aR^{2-d}} & \text{for } d \geq 3 \end{cases}$$

in the region $R_0 \leq |x| \leq R$. Moreover, the minimum of (27) is given by

$$E_R = \begin{cases} \frac{4\pi}{\ln(R/a)} & \text{for } d = 2 \\ \frac{4\pi^{d/2} a}{\Gamma(d/2)(1 - aR^{2-d})} & \text{for } d \geq 3. \end{cases}$$

To obtain an upper bound on $a(\beta)$, we use the variational principle (22) with $\psi(x) = \psi_\infty(x)$ for $|x| \leq R$, and $\psi(x) = 0$ for $|x| \geq R$. Using $|\psi_\infty| \leq 1$ and $f \leq 2$, we obtain the bound

$$a(\beta) \leq \frac{E_R}{8\pi} + \frac{\sigma_d R^d}{4\pi\beta},$$

where $\sigma_d = \pi^{d/2}/\Gamma(1 + d/2)$ denotes the volume of the unit ball in \mathbb{R}^d . The choice $R = \sqrt{\beta} [\ln(\sqrt{\beta}/a)]^{-1}$ for $d = 2$ and $R = (a\sqrt{\beta})^{1/(d-1)}$ for $d \geq 3$ yields (25) and (26). \square

For our lower bound on the density in Proposition IV.2, we need a bound on two more integrals of the kernel K . Since they appear only in terms of higher order, a rough bound will do.

Lemma V.3. *Let*

$$\begin{aligned} a'(\beta) &= (8\pi\beta)^{d/2-1} \int K(x, x) dx, \\ a''(\beta) &= (8\pi\beta)^{d/2-1} \int K(x, -x) dx. \end{aligned} \quad (28)$$

Then

$$\max\{a'(\beta), a''(\beta)\} \leq 2^{d/2} a(\beta/2).$$

For $d = 3$, it can be shown that both $a'(\beta)$ and $a''(\beta)$ converge to a as $\beta \rightarrow \infty$, but we do not need this here.

Proof. Using the semi-group property of the heat kernel we can write

$$K(x, z) = \int_{\mathbb{R}^d} \left(e^{\beta\Delta}(x, y) e^{\beta\Delta}(y, z) - e^{\beta(\Delta - \frac{1}{2}U)}(x, y) e^{\beta(\Delta - \frac{1}{2}U)}(y, z) \right) dy.$$

Since $ab - cd \leq a(b-d) + b(a-c)$ for $a \geq c$ and $b \geq d$, $K(x, z)$ is bounded above by

$$\begin{aligned} & \int_{\mathbb{R}^d} e^{\beta\Delta}(x, y) \left(e^{\beta\Delta}(y, z) - e^{\beta(\Delta - \frac{1}{2}U)}(y, z) \right) dy \\ & + \int_{\mathbb{R}^d} e^{\beta\Delta}(y, z) \left(e^{\beta\Delta}(x, y) - e^{\beta(\Delta - \frac{1}{2}U)}(x, y) \right) dy. \end{aligned}$$

Using the bound $e^{\beta\Delta}(x, y) \leq (4\pi\beta)^{-d/2}$ the claim follows easily. \square

VI. CONCLUSION

We have given rigorous upper bounds on the critical temperature for two- and three-dimensional Bose gases with repulsive two-body interactions. In two dimensions, our bound agrees to leading order in $a^2\rho$ with the expected critical temperature for superfluidity. In three dimensions, our bound shows that the critical temperature is not greater than the one for the ideal gas plus a constant times $\sqrt{a\rho^{1/3}}$.

Our bounds are based on the observation that the one-particle reduced density matrix decays exponentially if the fugacity z satisfies $z < 1$. What is needed are lower bounds on the particle density in the grand canonical ensemble. The Feynman-Kac path integral representation allows us to get bounds in terms of certain integral kernels which, in turn, can be estimated by the scattering length of the interaction potential using a suitable variational principle.

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