COMPUTATIONS ON THE QUASI-2D LEE-HUANG-YANG ENERGY FORMULA

KELVIN NGUYEN
PROJECT ADVISOR: XUWEN CHEN

Abstract. This paper studies numerical aspects of the quasi-2D Lee–Huang–Yang correction in the periodic-box setting recently computed by Chen, Wu, and Zhang. In three dimensions, the Lee–Huang–Yang formula gives the first universal correction beyond mean-field theory for the ground-state energy of a dilute Bose gas, with the classical coefficient $\frac{128}{15\sqrt{\pi}}$. Our goal is to examine how the corresponding second-order correction behaves when the geometry is no longer fully three-dimensional, but instead is strongly confined in one direction.

We work with the Bogoliubov lattice sum $E^{(d)}_{\mathrm{Bog}}$ where the anisotropy is encoded by the confinement parameter d. After reviewing the physical background from Bose–Einstein condensation, Bogoliubov theory, and the Lee–Huang–Yang correction, we explain how this discrete sum arises as the finite-volume second-order contribution in the quasi-2D Gross–Pitaevskii regime. We then compute $E^{(d)}_{\mathrm{Bog}}$ numerically under variation of a_0 and d, using a truncated lattice-sum algorithm implemented in Python.

Our computations recover the expected $a_0^{5/2}$ scaling in the isotropic case and show that, for the parameter range considered, the dependence on d is well approximated by an exponential factor. Combining these observations, we obtain the empirical approximation

$$E^{(d)}_{\mathrm{Bog}} \approx 8.88\, e^{1.25d}\, a_0^{5/2}.$$

These results provide computational evidence for how the second-order Lee–Huang–Yang-type correction changes across the 3D-to-quasi-2D crossover, and they illustrate how confinement alters the Bogoliubov contribution beyond the classical three-dimensional formula.

Contents

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1. Introduction

Bose–Einstein condensation (BEC) was predicted in the 1920s as a quantum-statistical effect in an ideal Bose gas, and it became experimentally accessible in dilute alkali gases with the development of laser cooling and trapping. A Bose–Einstein condensate is a state of matter formed in a dilute gas of bosons cooled to extremely low temperature, in which a macroscopic fraction of the particles occupies the same lowest quantum state. In this regime, the particles' wave functions overlap strongly, so quantum-mechanical behavior becomes visible on a macroscopic scale. [11, 6] The first observations of gaseous BEC in 1995 initiated a large experimental and theoretical program on interacting quantum fluids in controlled settings. For these achievements and early studies of condensate properties, Cornell, Wieman, and Ketterle were awarded the 2001 Nobel Prize in Physics [11, 6]. Since then, cold-atom platforms have enabled precise tests of many-body theory, including beyond-mean-field corrections to the equation of state in regimes where interactions are tunable [10].

In three dimensions, the leading-order ground-state energy density is described by mean-field theory, while the first universal correction is the Lee–Huang–Yang (LHY) term. For a homogeneous dilute 3D Bose gas of density ρ and s-wave scattering length a, the LHY expansion has the form

$$e(\rho) = 4\pi a\, \rho^2 \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\Big(\sqrt{\rho a^3}\Big)\right), \tag{1.1}$$

where the coefficient $\frac{128}{15\sqrt{\pi}}$ is the characteristic signature of quantum-fluctuation (beyond-mean-field) physics [9, 1]. Historically, this correction can be interpreted as the contribution of the zero-point energy of Bogoliubov quasiparticles: Bogoliubov theory yields the excitation spectrum and the leading mean-field energy, while Lee–Huang–Yang (1957) compute the next-order correction arising from quantum fluctuations [1, 9]. More concretely, after expanding the Hamiltonian around the macroscopically occupied condensate mode and keeping the quadratic terms, one obtains a family of independent momentum modes that can be diagonalized by a Bogoliubov transformation. This produces the quasiparticle dispersion

$$E_p = \sqrt{\varepsilon_p(\varepsilon_p + 2g\rho)}, \qquad \varepsilon_p = p^2,$$

with $g = 4\pi a$ in the units used here. The beyond-mean-field correction then comes from summing the renormalized zero-point energies of these modes. After subtracting the divergent leading pieces, one is left with a convergent fluctuation integral whose scaling is $(g\rho)^{5/2}$; rewriting this in terms of ρ and a gives the factor $\rho^2\sqrt{\rho a^3}$, and the remaining dimensionless integral evaluates to the constant $\frac{128}{15\sqrt{\pi}}$ [9, 1]. After about half a century of posted in physics, the formula (1.1) is proved in mathematics by [2, 7].

The dilute Bose gas is a canonical setting where microscopic quantum mechanics produces macroscopic phenomena such as superfluidity and quantized vortices. A central quantitative problem is to understand the ground-state energy beyond mean-field theory, and to track how this energy changes when the geometry of the confining region interpolates between different effective dimensions. This paper focuses on the quasi-two-dimensional (quasi-2D) regime: a three-dimensional gas that is strongly confined in one direction so that the domain is thin, but not strictly two-dimensional.

The quasi-2D setting introduces an additional difficulty: the effective interaction and the relevant small parameter depend on the confinement length scale. A key step is that tight confinement modifies scattering, leading to an effective two-dimensional description in appropriate regimes [12, 13]. Physically, quasi-2D means that the gas still lives in three spatial dimensions, but motion in one direction is so strongly confined that particles remain almost entirely in the lowest transverse mode, while the low-energy dynamics take place mainly in the remaining two directions. Thus the system is not literally two-dimensional, but it behaves effectively two-dimensionally at low energies, with the confinement length entering the effective interaction law. In particular, the dimensional crossover is not captured by simply inserting "2D formulas" into a 3D model; instead, one must understand how correlation energy and renormalization depend simultaneously on the particle number, scattering length, and thickness. Recent beyond-mean-field analyses of dimensional crossover highlight that confinement-induced effects can enter precisely at beyond-mean-field order [8]. Recently, the Lee-Huang-Yang correction for such quasi-2D setting has been computed and proved mathematically in [5]. Away from following [2, 7], [5] can be interpreted as continuation of the first-order dynamical dimension reduction results [3, 4]. This paper is the computation of the asymptotics of the exact and long formulas given in [5].

To make the ground-state energy expansion precise, we briefly recall the many-body Hamiltonian and the meaning of the scattering length. Following [5], we consider a dilute gas of N bosons confined to the anisotropic torus

$$\Lambda_d = [-1/2, 1/2]^2 \times [-d/2, d/2],$$

with $d \ll 1$, and governed by the Hamiltonian

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{1 \leqslant i < j \leqslant N} v_a(x_i - x_j) \qquad \text{on } L^2_s(\Lambda_d^N),$$

where $L^2_s(\Lambda_d^N)$ is the bosonic subspace of symmetric wave functions and v_a is a repulsive, radially symmetric, short-range interaction potential. The corresponding ground-state energy is

$$E_N := \inf \sigma(H_N).$$

A Bose–Einstein condensate may be viewed physically as a state of a dilute bosonic gas at very low temperature in which a macroscopic fraction of the particles occupies the same lowest quantum state, so that quantum effects become visible on macroscopic scales [11, 6]. The parameter a_0 denotes the scattering length of the reference interaction v, defined through the zero-energy scattering equation

$$-\Delta f(x) + \frac{1}{2} v(x) f(x) = 0, \qquad f(x) \to 1 \text{ as } |x| \to \infty,$$

for which $f(x) = 1 - \frac{a_0}{|x|}$ outside the support of v; equivalently,

$$\int_{\mathbb{R}^3} v(x) f(x)\, dx = 8\pi a_0.$$

Thus a_0 is the effective low-energy parameter measuring the strength of the two-body interaction in the dilute regime.

The interplay among N, a, and d leads Chen–Wu–Zhang to divide the problem into three parameter regions:

$$\text{Region I: } \frac{d}{a} \gg |\ln(Nd^2)|, \qquad Nd^2 \gg 1,$$
$$\text{Region II: } \frac{d}{a} \gg |\ln(Nd^2)|, \qquad Nd^2 \lesssim 1,$$
$$\text{Region III: } \frac{d}{a} \sim |\ln(Nd^2)|.$$

They refer to Region I as the 3D region, Region II as an intermediate region, and Region III as the true 2D region [5]. In the Gross–Pitaevskii regime, one assumes $N \to \infty$, $a \to 0$, $d \to 0$, and $a/d \to 0$, together with the normalization $\frac{Na}{d} = 1$ in Regions I and II, while in Region III the effective coupling is normalized by $Ng \sim a_0$ [5]. In particular, Theorem 1.1 of [5] shows that in Regions I and III, under the additional lower bound $d \gtrsim e^{-CN^{t_1}}$ with $t_1 = \frac{1}{72}$, the ground-state energy admits the second-order expansion

$$E_N = 4\pi(N-1)N\frac{a}{d}a_0 + e_d + E_{\mathrm{Bog}}^{(d)} + O\left(d^{1/4}\ln d^{-1} + N^{-1/8+t_1}\right),$$

so that the quantity $E_{\mathrm{Bog}}^{(d)}$ introduced below is the explicit Bogoliubov correction in precisely this parameter regime [5]. The paper [5] can be viewed as continuing two earlier lines of work. On the one hand, it extends the dimension-reduction program of Chen and Holmer [3, 4] from dynamical limits to second-order ground-state energy asymptotics. On the other hand, it brings rigorous three-dimensional beyond-mean-field results, namely the proof of the Lee–Huang–Yang energy density formula by Fournais and Solovej [7] and the Gross–Pitaevskii Bogoliubov theory of Boccato, Brennecke, Cenatiempo, and Schlein [2] into the quasi-2D dimensional-crossover setting.

Working in the periodic-box geometry used by Chen–Wu–Zhang, the second-order correction to the ground-state energy can be expressed in terms of a Bogoliubov lattice sum over discrete momenta $p \in 2\pi\mathbb{Z}^3\backslash\{0\}$, where anisotropy from confinement enters through the scaled dispersion

$$|M_d p|^2 = p_1^2 + p_2^2 + \frac{p_3^2}{d^2}, \qquad M_d = \mathrm{diag}\left(1, 1, \frac{1}{d}\right),$$

[5]. To describe the summand appearing in this lattice sum, set

$$s := |M_d p|^2,$$

and define, for each $p \neq 0$, the corresponding mode contribution

$$e_p^{(d)} := -s - 8\pi a_0 + \sqrt{s^2 + 16\pi a_0\, s} + \frac{(8\pi a_0)^2}{2s}, \qquad s = |M_d p|^2, \tag{1.2}$$

as in [5]. Physically, $e_p^{(d)}$ represents the (renormalized) zero-point energy shift contributed by the Bogoliubov mode at momentum p after diagonalizing the quadratic Hamiltonian; mathematically, it is arranged so that the large-momentum behavior is sufficiently decaying for the lattice sum to be well-defined [5]. With this notation, the Bogoliubov correction is

$$E_{\mathrm{Bog}}^{(d)} = \frac{1}{2} \sum_{p \in 2\pi\mathbb{Z}^3\backslash\{0\}} e_p^{(d)}. \tag{1.3}$$

Physically, this lattice sum represents the aggregate zero-point energy shift obtained after diagonalizing the quadratic (Bogoliubov) Hamiltonian; mathematically, it is the finite-volume, anisotropic analogue of the continuum integral whose asymptotics produce the classical LHY coefficient in 3D. In the thin-direction limit $d \to 0$, the same object becomes sensitive to quasi-2D physics and encodes the crossover between three- and two-dimensional correlation effects [5].

We study the asymptotic behavior of this Bogoliubov lattice sum as the confinement parameter d varies and as selected parameters are scaled, and we complement the asymptotic analysis with numerical evaluation under parameter changes. Our computations aim to clarify how the second-order (LHY-type) correction evolves across the 3D-to-quasi-2D crossover in a concrete lattice-sum representation.

2. Physics background and historical context

A central quantity in the weakly interacting Bose gas is the ground-state energy density as a function of density and interaction strength. Bogoliubov theory provides a quasiparticle description of low-energy excitations and yields the leading-order (mean-field) ground-state energy in the dilute limit. The first universal correction beyond mean field is the Lee–Huang–Yang (LHY) term, which arises from quantum fluctuations, i.e., the zero-point energy of Bogoliubov quasiparticles. For a homogeneous 3D Bose gas with number density ρ and s-wave scattering length a, the LHY expansion takes the form

$$e(\rho) = 4\pi a\,\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\Big(\sqrt{\rho a^3}\Big)\right),$$

where the coefficient $\frac{128}{15\sqrt{\pi}}$ is universal in the dilute regime [9, 1]. Modern presentations emphasize that the expansion is controlled by the gas parameter $\sqrt{\rho a^3}$ and that the LHY contribution is the leading quantum correction in that parameter [1].

A useful way to see where the coefficient $\frac{128}{15\sqrt{\pi}}$ comes from is through Bogoliubov's diagonalization of the quadratic Hamiltonian around the condensate. In the weakly interacting regime one replaces the interaction by a contact coupling $g = 4\pi a$ (in units $\hbar = 2m = 1$), and after expanding around the macroscopically occupied zero mode, the Hamiltonian becomes approximately a sum of independent quadratic pieces indexed by momenta $p \neq 0$. A Bogoliubov transformation then diagonalizes each mode and produces the quasiparticle dispersion

$$E_p = \sqrt{\varepsilon_p\big(\varepsilon_p + 2g\rho\big)}, \qquad \varepsilon_p = p^2,$$

together with a shift in the ground-state energy coming from the zero-point energy of these modes [1]. Formally, this fluctuation contribution has the continuum form

$$\Delta e = \frac{1}{2}\int_{\mathbb{R}^3} \frac{d^3p}{(2\pi)^3}\left(E_p - \varepsilon_p - g\rho + \frac{(g\rho)^2}{2\varepsilon_p}\right),$$

where the subtractions remove the ultraviolet divergence and isolate the genuine second-order (beyond-mean-field) correction [1, 9]. Evaluating this integral by scaling $p = \sqrt{g\rho}\,q$ shows that Δe is proportional to $(g\rho)^{5/2}$, i.e. proportional to $\rho^2\sqrt{\rho a^3}$, and the remaining dimensionless integral is exactly what produces the numerical constant $\frac{128}{15\sqrt{\pi}}$ in the LHY term [9, 1]. Thus, the LHY coefficient is a direct quantitative imprint of Bogoliubov quantum fluctuations in three dimensions.

Dimensional reduction is not merely a geometric limit of a 3D theory. When a Bose gas is tightly confined in one direction, the scattering processes responsible for effective interactions change, producing confinement-dependent effective couplings and new small parameters. Early analyses of trapped quasi-2D gases clarified that the mean-field interaction in quasi-2D depends sensitively on the confinement length scale and that quasi-condensate physics can appear in experimentally relevant temperature ranges [12]. Related work on interatomic collisions in tight confinement provides a systematic way to derive effective low-dimensional interactions starting from a 3D short-range potential [13].

Physically, the term quasi-2D means that the gas still lives in three spatial dimensions, but motion in one direction (say z) is frozen into the lowest transverse mode of the confining potential. Equivalently, the confinement length (or thickness) ℓ_z is so small that the energy spacing of transverse excitations is large compared to the energy scales of interest (temperature and typical interaction/chemical-potential scales), so particles rarely populate excited z-modes. The system then behaves effectively two-dimensionally in the (x, y) directions while retaining a 3D short-range interaction that has been renormalized by the confinement [12, 13]. From the Bogoliubov point of view, the excitation spectrum becomes highly anisotropic: modes carrying nonzero transverse momentum are pushed to high energy, and the low-energy fluctuations are dominated by in-plane momenta. This is the mechanism behind the dimensional crossover, and it is precisely why a confinement parameter (thickness) enters the beyond-mean-field correction.

Beyond mean field, the crossover becomes even more delicate: confinement-induced effects can enter precisely at the order of the LHY correction. In particular, analyses of the dimensional crossover show that the leading contribution of a confinement-induced resonance may appear at beyond-mean-field order, and they provide explicit asymptotics in the 3D and low-dimensional limits [8]. This makes the quasi-2D regime a natural setting to ask how the LHY-type correction evolves as one interpolates between effective dimensions.

In this paper we work in the periodic-box (torus) geometry used by Chen–Wu–Zhang [5]. In that setting, the confinement is represented by an anisotropic box of thickness $d \ll 1$ in the strongly confined direction. The second-order correction to the ground-state energy can be written in terms of a discrete momentum sum (a Bogoliubov lattice sum) over $p \in 2\pi\mathbb{Z}^3 \backslash \{0\}$, with anisotropy entering through the scaled dispersion $|M_d p|^2 = p_1^2 + p_2^2 + p_3^2/d^2$ [5]. Conceptually, this sum is the finite-volume analogue of the continuum fluctuation integral that yields the 3D LHY coefficient, but it remains sensitive to the crossover as $d \to 0$. Our goal is to compute and analyze this lattice-sum representation under parameter variation, and to compare numerical evaluations with asymptotic predictions in the quasi-2D regimes described in [5].

The dimensional-reduction problem is substantially newer. When the gas is tightly confined in one direction, two-body scattering changes qualitatively and an effective 2D description emerges in appropriate limits because confinement affects the interaction at the same order as quantum fluctuations, the crossover can modify the beyond-mean-field term itself, motivating explicit crossover analyses and computations.

3. Computation of Main Result

We now present the main result.

Theorem 3.1 (Empirical scaling law for the Bogoliubov correction)**.** *Let $E_{\mathrm{Bog}}^{(d)}$ denote the Bogoliubov (second-order) correction term defined by the discrete momentum sum in the quasi-2D periodic-box setting of* [5]*. Fix a parameter window*

$$a_0 \in [a_{0,\min}, a_{0,\max}], \qquad d \in [d_{\min}, d_{\max}],$$

and let $\widehat{E}_{\mathrm{Bog}}^{(d)}(a_0)$ be the numerical value obtained by evaluating the lattice sum with the same truncation and numerical protocol used throughout this paper.

Then the data are well-approximated by the model

$$\widehat{E}_{\mathrm{Bog}}^{(d)}(a_0) \;\approx\; C\, e^{\kappa d}\, a_0^{5/2}, \tag{3.1}$$

with fitted constants

$$C = 8.88, \qquad \kappa = 1.25.$$

Equivalently, there exists an relative error function $\varepsilon(a_0, d)$ such that

$$\widehat{E}_{\mathrm{Bog}}^{(d)}(a_0) = 8.88\, e^{1.25d}\, a_0^{5/2} \left(1 + \varepsilon(a_0, d)\right), \qquad (a_0, d) \in [a_{0,\min}, a_{0,\max}] \times [d_{\min}, d_{\max}],$$

where $\sup |\varepsilon(a_0, d)|$ is small on the parameter window above.

We now derive the algebraic steps leading to a computable expression for (1.3). For definiteness we specialize to $d = 1$.

First, recall the one–mode energy

$$e_p^{(d)} = -|M_d p|^2 - 8\pi a_0 + \sqrt{|M_d p|^4 + 16\pi a_0\, |M_d p|^2} + \frac{(8\pi a_0)^2}{2\, |M_d p|^2}\,. \tag{3.2}$$

In the case $d = 1$ we have $M_1 = \mathrm{diag}(1, 1, 1)$ and therefore

$$|M_1 p|^2 = \|p\|^2 = p_1^2 + p_2^2 + p_3^2.$$

Consequently,

$$e_p^{(1)} = -\|p\|^2 - 8\pi a_0 + \sqrt{\|p\|^4 + 16\pi a_0\, \|p\|^2} + \frac{(8\pi a_0)^2}{2\, \|p\|^2}\,. \tag{3.3}$$

With this in hand,

$$E_{\mathrm{Bog}}^{(1)} = \frac{1}{2} \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} e_p^{(1)}. \tag{3.4}$$

Passing from the Riemann sum to an integral by the standard lattice–to–continuum approximation, we are led to

$$E_{\mathrm{Bog}}^{(1)} \approx -\frac{\hat{p}^{\frac{5}{2}}}{2(2\pi)^3} \int_{\mathbb{R}^3} \left(p^2 + 8\pi a_0 - \sqrt{p^4 + 16\pi a_0\, p^2} - \tfrac{(8\pi a_0)^2}{2\, p^2}\right) d^3p. \tag{3.5}$$

To proceed in an orderly way, we pass to spherical coordinates. Writing $d^3p = r^2 \sin\phi \, dr \, d\phi \, d\theta$ and integrating over the angles produces a factor 4π. Thus,

$$E^{(1)}_{\mathrm{Bog}} \approx -\frac{\hat{p}^{\frac{5}{2}}}{2(2\pi)^3} \cdot 4\pi \int_0^\infty \left(r^2 + 8\pi a_0 - \sqrt{r^4 + 16\pi a_0 \, r^2} - \tfrac{(8\pi a_0)^2}{2\, r^2} \right) r^2 \, dr. \tag{3.6}$$

For compactness, set

$$I := \int_0^\infty \left(r^4 + 8\pi a_0 \, r^2 - r^2\sqrt{r^4 + 16\pi a_0 \, r^2} - \tfrac{(8\pi a_0)^2}{2} \right) dr. \tag{3.7}$$

Then (3.6) may be rewritten succinctly as

$$E^{(1)}_{\mathrm{Bog}} \approx -\frac{\hat{p}^{\frac{5}{2}}}{2(2\pi)^3} \, 4\pi \, I = -\frac{\hat{p}^{\frac{5}{2}}}{4\pi^2} \, I. \tag{3.8}$$

At this stage, it is natural to nondimensionalize the radius. Let

$$r = \sqrt{8\pi a_0} \, x, \qquad dr = \sqrt{8\pi a_0} \, dx,$$

so that

$$r^4 = (8\pi a_0)^2 x^4, \quad 8\pi a_0 \, r^2 = (8\pi a_0)^2 x^2, \quad \sqrt{r^4 + 16\pi a_0 \, r^2} = (8\pi a_0)\sqrt{x^4 + 2x^2}.$$

Pulling out the common factor $(8\pi a_0)^2$ and remembering the Jacobian gives

$$I = (8\pi a_0)^{5/2} \int_0^\infty \left(x^4 + x^2 - x^2\sqrt{x^4 + 2x^2} - \tfrac{1}{2} \right) dx =: (8\pi a_0)^{5/2} J. \tag{3.9}$$

Numerical integration yields

$$J = -\frac{8\sqrt{2}}{15}. \tag{3.10}$$

Inserting (3.9)–(3.10) into (3.8), we carry the constants carefully:

$$\begin{aligned} E^{(1)}_{\mathrm{Bog}} &\approx -\frac{\hat{p}^{\frac{5}{2}}}{4\pi^2} \, (8\pi a_0)^{5/2} \, J \\ &= -\hat{p}^{\frac{5}{2}} a_0^{5/2} \left(\tfrac{(8\pi)^{5/2}}{4\pi^2} \right) J = -\hat{p}^{\frac{5}{2}} a_0^{5/2} \left(2^{11/2} \pi^{1/2} \right) J \\ &= -\hat{p}^{\frac{5}{2}} a_0^{5/2} \left(2^{11/2} \pi^{1/2} \right) \left(-\frac{8\sqrt{2}}{15} \right) = \hat{p}^{\frac{5}{2}} a_0^{5/2} \, \frac{2^{11/2} \cdot 8 \cdot \sqrt{2}}{15} \, \pi^{1/2} \\ &= \hat{p}^{\frac{5}{2}} a_0^{5/2} \, \frac{2^{11/2+3+1/2}}{15} \, \pi^{1/2} = \frac{512}{15} \sqrt{\pi} \, \hat{p}^{5/2} \, a_0^{5/2}. \end{aligned}$$

Hence, with the exact constants carried through,

$$E^{(1)}_{\mathrm{Bog}} \approx \frac{512}{15} \sqrt{\pi} \, \hat{p}^{5/2} \, a_0^{5/2} = 4\pi a_0 \frac{128}{15\sqrt{\pi}} a_0^{\frac{3}{2}} \hat{p}^{\frac{5}{2}} \tag{3.11}$$

This matches the LHY formula. Now the goal of this paper is to look at when $d << 1$ and see how (1.3) behaves as we change the other variables, such as a_0. For these computations, we wrote a script in Python to produce graphs of the results.

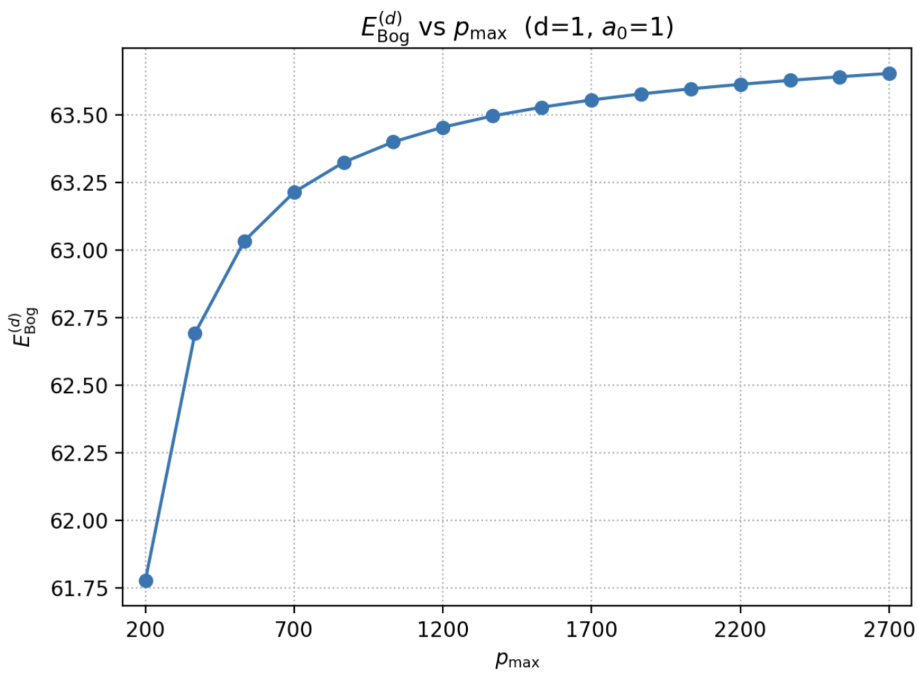

FIGURE 1. Base case when $d = 1$, p_{max} is as high as possible without memory overflow.

Figure 1 shows what we just computed. But using a Python Script. p_{max} here represents the vectors in $2\pi\mathbb{Z}^3\backslash\{0\}$, it was limited to $2,700$ because of memory overflow errors, but it was high enough to start to see a convergence.

Now the real goal of this project is when $d << 1$. When this happens, the formula loses its spherical symmetry, we will show graphs for when the value of d is varying and also a_0 so there can be a closed formula for general d and a_0.

3.1. E_{Bog} **in relation to** a_0**.** In this section, we still provide graphs showing the scaling of (1.3) in relation to a_0. Here, we keep p_{max} fixed at $p_{max} = 2,700$ and we will very d. We will also provide a best fit line to get how a_0 scales exponentially and provide the coefficient of determination.

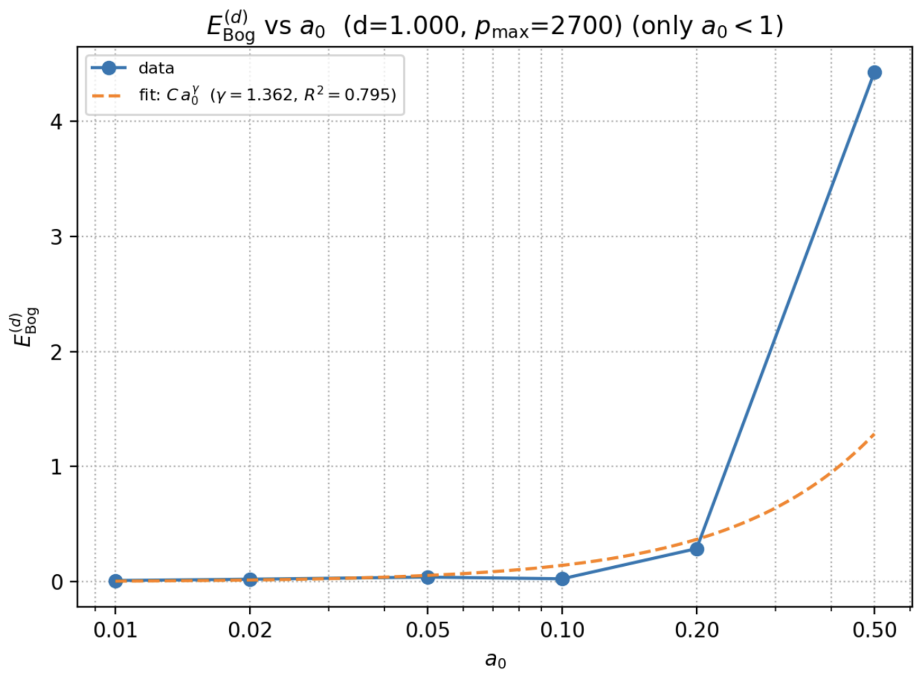

FIGURE 2. Plot of $E_{\mathrm{Bog}}^{(d)}$ versus a_0 for $d = 1$, $p_{\max} = 2700$, and $a_0 < 1$, with a power-law fit. The fit is weaker in this small-a_0 regime.

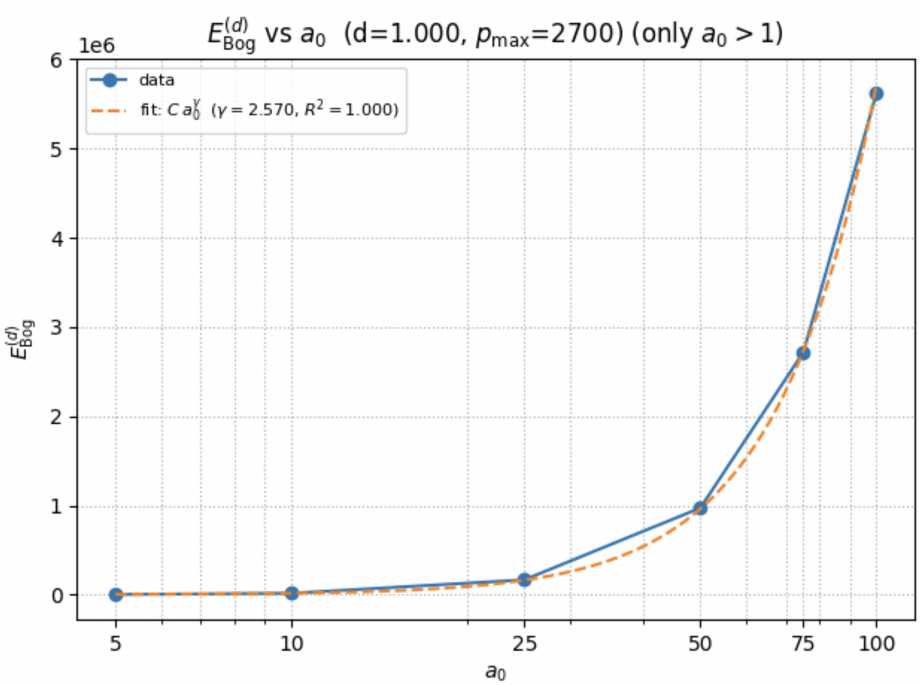

FIGURE 3. Plot of $E_{\mathrm{Bog}}^{(d)}$ versus a_0 for $d = 1$, $p_{\max} = 2700$, and $a_0 > 1$, with a power-law fit. The fitted exponent is close to the expected $\frac{5}{2}$ scaling.

In Figure (2) and (3) we have that when $d = 1$, we see figure (3) is going to better fit the scale of $a_0^{\frac{5}{2}}$.

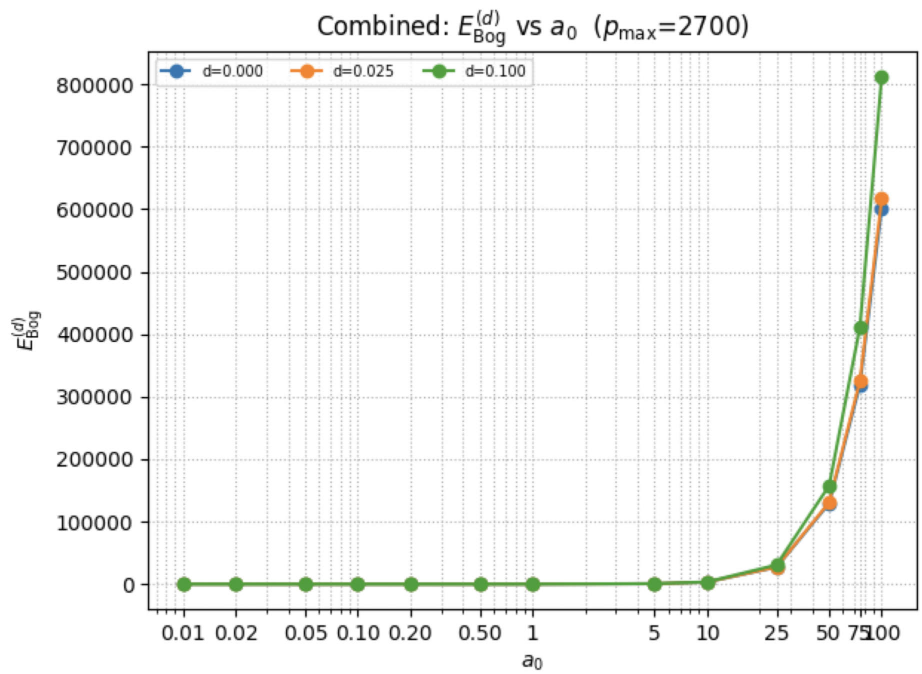

FIGURE 4. Combined plot of $E^{(d)}_{\text{Bog}}$ versus a_0 for three small values of d with $p_{\max} = 2700$. We still observe the same overall power-scaling behavior in a_0 as in the case $d = 1$.

Then for Figure (4), we have 3 smaller values of d, and we still see a trend of a_0 following the same power-scaling.

3.2. E_{Bog} **in relation to** d**.** In this section, we still provide a graph showing the scaling of (1.3) in relation to d. Here, we keep p_{max} fixed at $p_{max} = 2,700$ and we will very a_0. We will also provide a best fit line to get how d scales exponentially and provide the coefficient of determination.

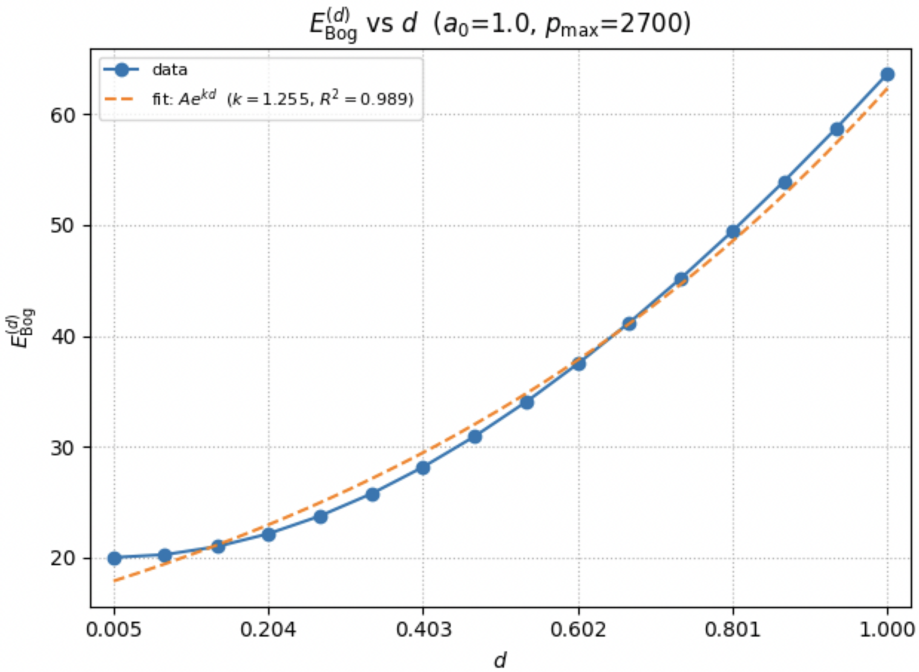

FIGURE 5. Plot of $E_{\mathrm{Bog}}^{(d)}$ versus d for $a_0 = 1$ and $p_{\max} = 2700$. The exponential fit matches the data well and suggests a scaling of about $8.88e^{1.25d}$.

In the above graph, we see that using an exponential fit, we get that we have a strong correlation between (1.3) and d, with the numerical value of the scaling being about $8.88e^{1.25d}$.

Combining the results of both sections, we can estimate that in general, we can estimate (1.3) with $a_0^{\frac{5}{2}}$ and $8.88e^{1.25d}$.

4. Description of the Algorithms

The following is the Algorithm for computing (1.3)

```
def e_p_term(s, a0):
    # Mode contribution e_p^{(d)} as a function of s = |M_d p|^2 and a0
    return (-s - 8.0 * pi * a0
            + np.sqrt(s * s + 16.0 * pi * a0 * s)
            + (8.0 * pi * a0) ** 2 / (2.0 * s))


def E_bog_for_fixed_a0(d, a0, Rmax, chunk=128, dtype=np.float64):
    # Sum E_Bog^{(d)} = (1/2) * _{p2Z^3\{0}} e_p^{(d)} with cutoff s=|M_d p|^2  Rmax^2,
    # where |M_d p|^2 = p1^2 + p2^2 + (p3^2)/(d^2), and p = 2(n1,n2,n3).

    two_pi = 2.0 * pi
    two_pi_sq = (2.0 * pi) ** 2
    R2 = Rmax * Rmax

    # Index bounds implied by the cutoff in the anisotropic metric
```

```
    n_max_xy = int(np.floor(Rmax / two_pi))
    n_max_z = int(np.floor(d * Rmax / two_pi))

    nx = 2 * n_max_xy + 1
    nz = 2 * n_max_z + 1
    nblocks_1d = (nx + chunk - 1) // chunk
    total_blocks = nblocks_1d * nblocks_1d * nz

    a0 = float(a0)
    E_sum = dtype(0.0)
    ## Use a progress bar in the console to track progression.
    with tqdm(total=total_blocks, desc=f"Summing (d={d:.4f})", unit="blk") as pbar:
        for i_start in range(-n_max_xy, n_max_xy + 1, chunk):
            i_end = min(i_start + chunk, n_max_xy + 1)
            n1_block = np.arange(i_start, i_end, dtype=np.int32)

            for j_start in range(-n_max_xy, n_max_xy + 1, chunk):
                j_end = min(j_start + chunk, n_max_xy + 1)
                n2_block = np.arange(j_start, j_end, dtype=np.int32)

                n1g, n2g = np.meshgrid(n1_block, n2_block, indexing="ij")
                base_xy = two_pi_sq * (n1g.astype(dtype) ** 2 + n2g.astype(dtype) ** 2)
                at_origin_xy = (n1g == 0) & (n2g == 0)

                for n3 in range(-n_max_z, n_max_z + 1):
                    p3 = two_pi * n3
                    c_n3 = (p3 * p3) / (d * d)
                    s = base_xy + c_n3

                    # Exclude the zero mode (n1,n2,n3)=(0,0,0) and enforce cutoff s
    Rmax^2
                    zero_mask = at_origin_xy if (n3 == 0) else np.zeros_like(s,
    dtype=bool)
                    mask = (s <= R2) & (~zero_mask)

                    if np.any(mask):
                        s_sel = s[mask].astype(dtype, copy=False)
                        E_sum += 0.5 * np.sum(e_p_term(s_sel, a0))

                    pbar.update(1)

    return float(E_sum)
## Complexity is Theta(dR^3) where R=R_Max
```

The following code is a general skeleton for creating the graphs and labels.

```
if __name__ == "__main__":

    # Fixed cutoff and parameter grids
    p_max_fixed = 2700.0
    a0_values = piecewise_a0_values()
    print("a0 values:", ", ".join(f"{a0:.2f}" if a0 < 1 else f"{int(a0)}" for a0 in
    a0_values))
```

```
d_values = nice_d_values_up_to_one()
print("d values:", ", ".join(f"{d:.3f}" for d in d_values))

# Output folder (timestamped)
timestamp = datetime.now().strftime("%Y%m%d_%H%M%S")
out_dir = f"ebog_a0_piecewise_with_fit_outputs_{timestamp}"
os.makedirs(out_dir, exist_ok=True)

# Collect results for CSV summaries
combined_rows = []      # (d, a0, E_bog)
fit_rows = []           # (d, C, gamma, R2, n_used)

for d in d_values:

    # Compute E_bog for all a0 at this d
    E_vals = sum_E_over_s_for_many_a0(d, a0_values, Rmax=p_max_fixed, chunk=128)

    # Save per-d plot and compute power-law fit parameters
    png_path = os.path.join(out_dir, f"Ebog_vs_a0_d={d:.3f}.png")
    C, gamma, R2 = plot_and_save_with_fit(a0_values, E_vals, d, p_max_fixed,
png_path)

    # Print and save per-d table
    print_table_to_console(d, p_max_fixed, a0_values, E_vals, C, gamma, R2)
    csv_path = os.path.join(out_dir, f"Ebog_vs_a0_d={d:.3f}.csv")
    save_table_csv(csv_path, a0_values, E_vals, x_name="a0", y_name="E_bog")

    # Append long-form rows (all d, all a0)
    for a0, E in zip(a0_values, E_vals):
        combined_rows.append((float(d), float(a0), float(E)))

    # Record fit summary for this d
    n_used = int(np.count_nonzero((np.array(E_vals) > 0) & np.isfinite(E_vals)))
    fit_rows.append((float(d), float(C) if np.isfinite(C) else np.nan,
                     float(gamma) if np.isfinite(gamma) else np.nan,
                     float(R2) if np.isfinite(R2) else np.nan,
                     n_used))

# Write combined long-form CSV
combined_csv_path = os.path.join(out_dir, "Ebog_a0_piecewise_long.csv")
with open(combined_csv_path, "w", newline="") as f:
    writer = csv.writer(f)
    writer.writerow(["d", "a0", "E_bog"])
    writer.writerows(combined_rows)

# Write per-d fit summary CSV
fits_csv_path = os.path.join(out_dir, "Ebog_powerlaw_fits_by_d.csv")
with open(fits_csv_path, "w", newline="") as f:
    writer = csv.writer(f)
    writer.writerow(["d", "C", "gamma", "R2", "n_points_used"])
    writer.writerows(fit_rows)

# Combined plot: E_bog vs a0 for all d on one figure
plt.figure()
```

```
for d in d_values:
    rows_for_d = [(a0, E) for (dd, a0, E) in combined_rows if abs(dd - float(d)) <
1e-12]
    rows_for_d.sort(key=lambda t: t[0])
    a0s = [x for x, _ in rows_for_d]
    Es  = [y for _, y in rows_for_d]
    plt.plot(a0s, Es, marker='o', label=f"d={d:.3f}")

plt.xscale('log')
plt.xlabel(r"$a_{0}$")
plt.ylabel(r"$E_{\mathrm{Bog}}^{(d)}$")
plt.title(fr"Combined: $E_{{\mathrm{{Bog}}}}^{{(d)}}$ vs $a_0$
($p_{{\max}}$={int(p_max_fixed)})")
plt.grid(True, which='both', linestyle=':')
plt.xticks(a0_values, [f"{a0:.2f}" if a0 < 1 else f"{int(a0)}" for a0 in a0_values],
rotation=0)
plt.legend(ncol=3, fontsize=7)
plt.tight_layout()
combined_png_path = os.path.join(out_dir, "Ebog_vs_a0_all_d.png")
plt.savefig(combined_png_path, dpi=200)
plt.show()

# Final paths for convenience
print("\nSaved outputs to:", out_dir)
print(" - Per-d CSVs and PNGs (each with power-law fit overlay)")
print(" - Long-form E table:   ", combined_csv_path)
print(" - Fit summary table:   ", fits_csv_path)
print(" - Combined plot PNG:   ", combined_png_path)
```

This next section will be the code the is reuqired to show the relationship between (1.3) and a_0.

```
def power_law_fit(a0_vals, E_vals):
 # Fit E  C * a0^gamma by linear regression in log-log space.
 # Returns (C, gamma, R^2, mask) where mask selects the points used in the fit.

 a0_vals = np.asarray(a0_vals, dtype=float)
 E_vals  = np.asarray(E_vals, dtype=float)
 mask = np.isfinite(a0_vals) & np.isfinite(E_vals) & (a0_vals > 0) & (E_vals > 0)
 if np.count_nonzero(mask) < 2:
     return np.nan, np.nan, np.nan, mask

 x = np.log(a0_vals[mask])
 y = np.log(E_vals[mask])
 m, b = np.polyfit(x, y, 1)          # y  m x + b  =>  E  exp(b) * a0^m
 yhat = m * x + b

 # R^2 in log-space (measures goodness-of-fit for the log-log regression)
 ss_res = np.sum((y - yhat) ** 2)
 ss_tot = np.sum((y - np.mean(y)) ** 2)
 R2 = 1.0 - (ss_res / ss_tot if ss_tot > 0 else np.inf)

 C = float(np.exp(b))
 gamma = float(m)
```

```
    return C, gamma, float(R2), mask


def plot_and_save_with_fit(a0_values, E_vals, d, p_max_fixed, out_path_png):
    # Plot E_bog vs a0 (log x-axis), overlay power-law fit, save to PNG.

    C, gamma, R2, mask = power_law_fit(a0_values, E_vals)

    plt.figure()
    plt.plot(a0_values, E_vals, marker='o', label="data")
    plt.xscale('log')

    if np.isfinite(gamma):
        # Smooth fit curve across the a0 range that was actually used in the fit
        x_fit = np.logspace(np.log10(np.min(a0_values[mask])),
                            np.log10(np.max(a0_values[mask])),
                            300)
        y_fit = C * (x_fit ** gamma)
        plt.plot(x_fit, y_fit, linestyle='--',
                 label=fr"fit: $C\,a_0^{{\gamma}}$  ($\gamma={gamma:.3f}$,
    $R^2={R2:.3f}$)")

    xtick_labels = [f"{a0:.2f}" if a0 < 1 else f"{int(a0)}" for a0 in a0_values]
    plt.xticks(a0_values, xtick_labels, rotation=0)

    plt.xlabel(r"$a_{0}$")
    plt.ylabel(r"$E_{\mathrm{Bog}}^{(d)}$")
    plt.title(fr"$E_{{\mathrm{{Bog}}}}^{{(d)}}$ vs $a_0$  (d={d:.3f},
    $p_{{\max}}$={int(p_max_fixed)})")
    plt.grid(True, which='both', linestyle=':')
    plt.legend(fontsize=8)
    plt.tight_layout()
    plt.savefig(out_path_png, dpi=200)
    plt.close()

    return C, gamma, R2


def save_table_csv(path, x_vals, y_vals, x_name, y_name):
    # Save two columns (x, y) to CSV with a header line.
    arr = np.column_stack([x_vals, y_vals])
    header = f"{x_name},{y_name}"
    np.savetxt(path, arr, delimiter=",", header=header, comments="", fmt="%.8f")


def print_table_to_console(d, p_max_fixed, a0_values, E_vals, C, gamma, R2):
    # Print the (a0, E) table and the power-law fit summary to the terminal.
    print(fr"E_Bog^(d) vs a0  (d={d:.3f}, p_max={p_max_fixed})")
    for a0, E in zip(a0_values, E_vals):
        a0_disp = f"{a0:.2f}" if a0 < 1 else f"{int(a0)}"
        print(f"{a0_disp:>6}  ->  {E:.8f}")
    if np.isfinite(gamma):
        print(f"  Power-law fit (E  C * a0^):  C={C:.6g},  ={gamma:.6f},  R^2={R2:.4f}")
    else:
```

```
        print("  Power-law fit skipped (need at least two positive E points).")


def piecewise_a0_values():
    # Hand-picked a0 grid: dense at small a0, then larger values.
    small = [0.01, 0.02, 0.05, 0.10, 0.20, 0.50, 1.00]
    large = [5.0, 10.0, 25.0, 50.0, 75.0, 100.0]
    return np.array(small + large, dtype=np.float64)


def nice_d_values_up_to_one():
    # Small set of d values for quick runs / plots.
    return np.array([0.0001, 0.025, 0.1], dtype=float)
## O(n) for complexity
```

The following is the code needed for (1.3) vs d with the expondential fit.

```
   def nice_evenly_spaced_ds(d_min=0.005, d_max=1.0, n=16):
    # Generate n evenly spaced d values in [d_min, d_max], rounded for nicer
    printing/filenames.
    raw = np.linspace(d_min, d_max, n)
    d_vals = np.round(raw, 3)
    if len(np.unique(d_vals)) != n:
        d_vals = np.round(raw, 4)
        if len(np.unique(d_vals)) != n:
            d_vals = raw
    return np.array(d_vals, dtype=float)


def exponential_fit(d_vals, E_vals):
    # Fit E  A * exp(k d) by linear regression on log(E): log(E)  k d + b.
    # Returns (A, k, R^2, mask) where mask selects the points used in the fit.

    d_vals = np.asarray(d_vals, dtype=float)
    E_vals = np.asarray(E_vals, dtype=float)

    mask = np.isfinite(d_vals) & np.isfinite(E_vals) & (E_vals > 0)
    if np.count_nonzero(mask) < 2:
        return np.nan, np.nan, np.nan, mask

    x = d_vals[mask]
    y = np.log(E_vals[mask])

    k, b = np.polyfit(x, y, 1)  # y = k x + b
    yhat = k * x + b

    # R^2 in log-space (goodness-of-fit for the log(E) vs d regression)
    ss_res = np.sum((y - yhat) ** 2)
    ss_tot = np.sum((y - np.mean(y)) ** 2)
    R2 = 1.0 - (ss_res / ss_tot if ss_tot > 0 else np.inf)

    A = float(np.exp(b))
    return A, float(k), float(R2), mask
```

```
## O(n) for complexity.
```


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Department of Mathematics, University of Rochester, Rochester, NY, USA

Email address: knguy43@u.rochester.edu