Constructive Approximation
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CONSTRUCTIVE APPROXIMATION

Expected Energy of Zeros of Elliptic Polynomials

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Abstract
In 2011, Armentano, Beltrán and Shub obtained a closed expression for the expected logarithmic energy of the random point process on the sphere given by the roots of random elliptic polynomials. We consider a different approach which allows us to extend the study to the Riesz energies and to compute the expected separation distance.

Keywords Riesz energy · Elliptic polynomials · Asymptotics for energy minimizing Configurations · Random polynomials · Point processes on the sphere

Mathematics Subject Classification 31C20 · 52A40 · 60J45

1 Introduction and Main Results

Elliptic polynomials, also called Kostlan–Shub–Smale or $SU(2)$ polynomials, are defined by

$$\sum_{n=0}^{N} a_n \sqrt{\binom{N}{n}} z^n,$$

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where a_n are i.i.d. random variables with standard complex Gaussian distribution. These polynomials appeared first in the mathematical physics literature [17, 18, 28] and were readily studied from a mathematical point of view [31, 38]. One reason for the interest in these polynomials is that the random point process on $\mathbb{S}^2$ given by the stereographic projection of the roots of elliptic polynomials is invariant through rotations. Moreover, it is the unique point process given by zeros of random analytic functions with this property [40]. Among its many interesting properties, especially relevant are the connections, studied in [38], with well conditioned polynomials and with minimal logarithmic energy points.

The Riesz or logarithmic energy of a set of N different points $x_1, \ldots, x_N$ on the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ is

$$E_s(x_1, \ldots, x_N) = \sum_{i \neq j} f_s(|x_i - x_j|),$$

where $f_s(r) = r^{-s}$ for $s \neq 0$ and $f_0(r) = -\log r$ are, respectively, the Riesz and logarithmic potentials. We denote the extremal (minimal or maximal) energy attained by a set of N points on the sphere by

$$\mathcal{E}_s(N) = \begin{cases} \min_{x_1,\ldots,x_N \in \mathbb{S}^2} E_s(x_1, \ldots, x_N) & \text{if } s \geq 0, \\ \max_{x_1,\ldots,x_N \in \mathbb{S}^2} E_s(x_1, \ldots, x_N) & \text{if } s < 0. \end{cases}$$

The condition number of a univariate polynomial, defined by Shub and Smale, is a measure of how much the roots of a polynomial change when perturbing the coefficients. It was shown in [39] that points of almost minimal logarithmic energy, $s = 0$, are the roots of well conditioned polynomials. In [38], the authors also proved that, with high probability, elliptic polynomials are well conditioned, see [7, 9] for a deterministic example. It was therefore natural to study the expected energy of the zeros of elliptic polynomials. This was done in [3] where the authors obtained the following closed expression for the expected logarithmic energy of random points $x_1, \ldots, x_N \in \mathbb{S}^2$, images by the stereographic projection of zeros of elliptic polynomials,

$$\mathbb{E}[E_0(x_1, \ldots, x_N)] = \left(\frac{1}{2} - \log 2\right) N^2 - \frac{1}{2} N \log N - \left(\frac{1}{2} - \log 2\right) N. \qquad (1)$$

The asymptotic expression above is indeed very close to the minimal logarithmic energy of N points on the sphere, see Sect. 4. Working in a more general setting in [43–45] and [25] for the geodesic distance, the same expression (1) was obtained but with a $o(N)$ remainder. See also the recent [35] where the authors study fluctuations of the logarithmic energy. Our main result is an extension of the above result (1) to the Riesz s-energies for $s < 4$.

Theorem 1.1 *Let $x_1, \ldots, x_N \in \mathbb{S}^2$ be the image by the stereographic projection of N points drawn from zeros of elliptic polynomials. Then,*

(i) *for $s < 4$, $s \neq 0, 2$ and a fixed $m \geq 1$,*

$$\mathbb{E}[E_s(x_1, \ldots, x_N)]$$

$$
\begin{aligned}
&= \frac{2^{1-s}}{2-s}N^2 + \frac{\Gamma\left(1-\frac{s}{2}\right)}{2^{s+1}}\Bigg[s\left(1+\frac{s}{2}\right)\sum_{j=0}^{m-1}\frac{B_{2j}^{(\frac{s}{2})}(\frac{s}{4})(1-\frac{s}{2})_{2j}}{(2j)!}N^{\frac{s}{2}+1-2j} \\
&\zeta\left(1-\frac{s}{2}+2j, 1+\frac{4-s}{4N}\right) + s\left(1-\frac{s}{2}\right) \\
&\times \sum_{j=0}^{m-1}\frac{B_{2j}^{(\frac{s}{2}-1)}(\frac{s-2}{4})(2-\frac{s}{2})_{2j}}{(2j)!}N^{\frac{s}{2}-2j}\zeta\left(2-\frac{s}{2}+2j, 1+\frac{2-s}{4N}\right)\Bigg] \\
&+O\left(N^{\frac{s}{2}+1-2m}\right) \qquad (2)
\end{aligned}
$$

as $N \to +\infty$.

(ii) *Moreover, the energies with $s = -2n$ for integer $n \geq -1$, can be computed exactly: For $s = 0$,*

$$
\mathbb{E}[E_0(x_1,\ldots,x_N)] = \left(\frac{1}{2}-\log 2\right)N^2 - \frac{N\log N}{2} - \left(\frac{1}{2}-\log 2\right)N. \qquad (3)
$$

For $s = 2$,

$$
\mathbb{E}[E_2(x_1,\ldots,x_N)] = -\frac{N\pi}{4}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}. \qquad (4)
$$

For $s = -2n$, $n \geq 1$,

$$
\begin{aligned}
&\mathbb{E}[E_{-2n}(x_1,\ldots,x_N)] \\
&\quad = 2^{2n}N^2\left(1-n-n\sum_{m=1}^{n}\frac{1}{m}\right) \\
&\quad + 2^{2n}nN\left(-\gamma + \sum_{m=1}^{n+1}\binom{n+1}{m}(-1)^m\psi\left(\frac{m}{N}\right)\left(\frac{n-1}{n+1}m+1\right)\right). \qquad (5)
\end{aligned}
$$

In the above result, γ is the Euler–Mascheroni constant, $B_{2j}^{(2\rho)}(\rho)$ are the generalized Bernoulli polynomials defined by

$$
\left(\frac{t}{e^t-1}\right)^{2\rho}e^{\rho t} = \sum_{j=0}^{\infty}\frac{t^{2j}}{(2j)!}B_{2j}^{(2\rho)}(\rho)
$$

for $|t| < 2\pi$, with $B_0^{(2\rho)}(\rho) = 1$,

$$
\zeta(s,a) = \sum_{j=0}^{\infty}\frac{1}{(j+a)^s}, \quad \Re s > 1, \ a \notin \mathbb{Z}_{\leq 0}
$$

is the Hurwitz Zeta function and $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function.

By considering two terms of the asymptotic expansion of the Hurwitz Zeta function

$$\zeta(s, 1+a) = \sum_{k=0}^{\infty} \frac{(-1)^k (s)_k \zeta(s+k)}{k!} a^k,$$

for $|a| < 1$ and $s \neq 1$ [36, 25.11.10] and taking $m = 1$ in (2) we get, for $0, 2 \neq s < 4$,

$$\begin{aligned}\mathbb{E}[E_s(x_1, \ldots, x_N)] = \frac{2^{1-s}}{2-s} N^2 + C(s) N^{1+s/2} + \frac{s}{16} C(s-2) N^{s/2} \\ + O(N^{-1+s/2}),\end{aligned} \tag{6}$$

when $N \to \infty$, where

$$C(s) = \frac{1}{2^s} \frac{s}{2} \left(1 + \frac{s}{2}\right) \Gamma\left(1 - \frac{s}{2}\right) \zeta\left(1 - \frac{s}{2}\right). \tag{7}$$

Remark 1 The result above for the expected Riesz energy allow us to compare the zeros of elliptic polynomials with other point processes, for example in terms of expected p-moments of averages. Indeed, from Khintchine's inequality [30, Theorem 3], it follows that

$$\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^p\right] \sim N^{p/2}$$

when $x_1, \ldots, x_N$ are uniform i.i.d. points on the sphere $\mathbb{S}^2$ and $1 \leq p < \infty$. For points drawn from the spherical ensemble, for which there is repulsion between points, it follows from

$$\sum_{i,j=1}^{N} |x_i - x_j|^2 = 2N^2 - 2\left|\sum_{i=1}^{N} x_i\right|^2, \tag{8}$$

and the results about the expected Riesz energy $s = -2$ in [1], that the expected 2-moment is bounded. Therefore for the spherical ensemble $\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^p\right]$ is bounded for $1 \leq p \leq 2$, and numerical simulations suggest that the same holds for $p > 2$. In our case, for zeros of elliptic polynomials mapped to the sphere by the stereographic projection, it follows from (5) and the asymptotic expansion of the digamma function that

$$\mathbb{E}\left[\left|\sum_{i=1}^{N} x_i\right|^2\right] = 4\frac{\zeta(3)}{N} + o(N^{-1}) \tag{9}$$

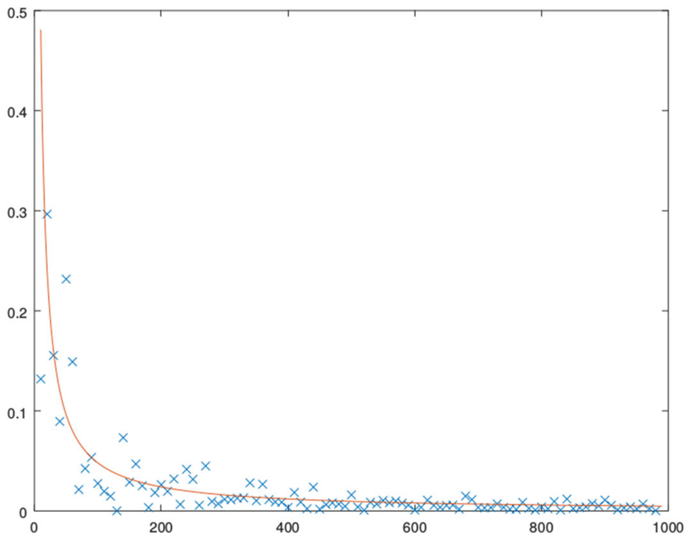

Fig. 1 Plot of $4\zeta(3)/N$ and realizations of $|\sum_{i=1}^N x_i|^2$ for natural N up to 1000

as $N \to +\infty$, and the average p-moments for $1 \le p \le 2$ converge to zero (Fig. 1). Again, numerical simulations suggest the same behavior for $p > 2$. It is well known that minimal logarithmic points have center of mass in the center of the sphere, i.e. have zero dipole, [19, Corollary 6.7.5], [12]. Therefore, the behavior of the expected p-moments matches the particularly low logarithmic energy of zeros of elliptic polynomials. For the comparison with minimal and expected energies of other point processes, see discussion in Sect. 4.

In our last result, we compute a closed expression for the expected separation distance between points drawn from zeros of elliptic polynomials mapped to the sphere. The separation distance of $X_N = \{x_1, \dots, x_N\}$ is defined by

$$\operatorname{sep}(X_N) = \min_{i \neq j} |x_i - x_j|,$$

and its counting version by $G(t, X_N) = \sharp\{i < j : |x_i - x_j| \le t\}$. Recall that energy minimizers have a separation distance of order $N^{-1/2}$, [19, Section 6.9].

Theorem 1.2 *Let X_N be a set of $N-$points drawn from zeros of elliptic polynomials mapped to the sphere by the stereographic projection. Then*

$$\mathbb{E}[G(t, X_N)] = \frac{t^2N^2}{8} - \frac{N}{2} + \frac{t^2N^2}{8(4-t^2)\left(\left(\frac{4}{4-t^2}\right)^N - 1\right)} \times \left[8 - t^2 - t^2N - \frac{t^2N}{\left(\frac{4}{4-t^2}\right)^N - 1}\right]. \tag{10}$$

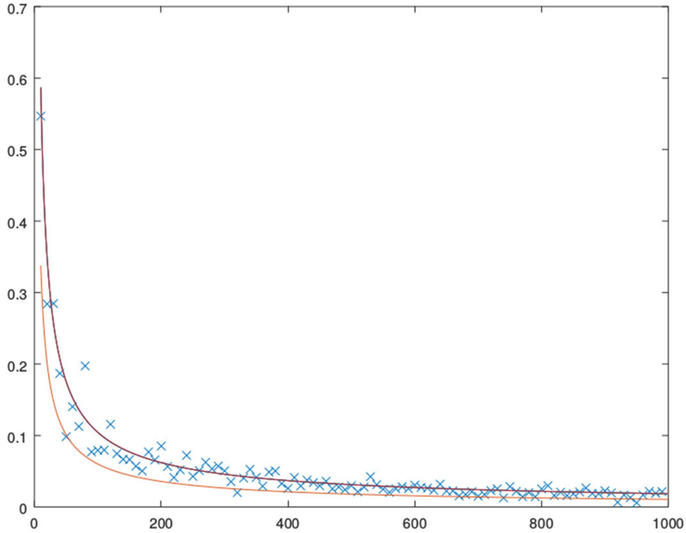

Fig. 2 x marks correspond to the values of the minimal separation for realizations of N elliptic zeros for natural N from 10 up to 1000. The continuous graph are $cN^{-3/4}$ for $c = 1.89$ (yellow) and 3.27 (brown): using Chebyshev's inequality at least 90% of the realizations are above yellow and at least 10% above brown (Color figure online)

Therefore,

$$\mathbb{E}[G(t, X_N)] = \frac{N^3 t^4}{128}(1 + o(1)), \tag{11}$$

if $t = o(1/\sqrt{N})$*, and moreover*

$$\mathbb{E}[G(t, X_N)] \leq \frac{N^3 t^4}{128}, \tag{12}$$

for $t \leq 2$.

Note that $\operatorname{sep}(X_N) \leq t$ implies $G(t, X_N) \geq 1$, hence $\mathbb{P}(\operatorname{sep}(X_N) \leq t) \leq \mathbb{P}(G(t, X_N) \geq 1) \leq \mathbb{E}(G(t, X_N))$ and therefore, as in the harmonic case, see [11], an N-tuple drawn from the zeros of elliptic polynomials likely satisfies $\operatorname{sep}(X_N) = \Omega(N^{-3/4})$, cf. Figure 2. See also [1, Corollary 1.6] for the analogue result for the spherical ensemble.

1.1 Organization of the Paper

In Sect. 2 we compute the 2-point intensity function of our point process and explain how to compute the expected energy. Section 3 contains the proof of our main result, Theorem 1.1. In Sect. 4 we deduce some bounds for the extremal energy and compare our bounds with previous results. Finally, in Sect. 5 we prove Theorem 1.2 about separation.

2 Intensity Function and Expected Riesz Energy

In this section we compute the 2-point intensity function of the random point process on $\mathbb{S}^2$ corresponding to the stereographic projection of the roots of random elliptic polynomials

$$P_N(z) = \sum_{n=0}^{N} a_n \sqrt{\binom{N}{n}} z^n,$$

where a_n are i.i.d. random variables with standard complex Gaussian distribution. Let $F(x, y)$ be a measurable function defined on $\mathbb{S}^2 \times \mathbb{S}^2$ whose variables will be considered in $\mathbb{C}$ through the stereographic projection, i.e. $F(z, w) = F(x(z), y(w))$, with the points $x, y \in \mathbb{S}^2$ corresponding to $z, w \in \mathbb{C}$. By Campbell's formula [24, (1.6)], if $x_1, \ldots x_N \in \mathbb{S}^2$ are the images of the zeros $z_1, \ldots, z_N$ of elliptic polynomials, then

$$\mathbb{E}\left[\sum_{i \neq j} F(x_i, x_j)\right] = \mathbb{E}\left[\sum_{i \neq j} F(z_i, z_j)\right] = \int_{\mathbb{C}} \int_{\mathbb{C}} F(z, w) \rho_2(z, w) dz dw, \tag{13}$$

with $\rho_2(z, w)$ the 2-point intensity function. Following [29, Corollary 3.4.2], the intensity function can be computed as the quotient of the permanent and the determinant of some matrices

$$\rho_2(z_1, z_2) = \frac{\operatorname{per}(C - BA^{-1}B^*)}{\det(\pi A)}, \tag{14}$$

where A, B, C are the 2×2 matrices with entries

$$\begin{aligned} A(i, j) &= \mathbb{E}[P_N(z_i)\overline{P_N}(z_j)], \\ B(i, j) &= \mathbb{E}[P'_N(z_i)\overline{P_N}(z_j)], \\ C(i, j) &= \mathbb{E}[P'_N(z_i)\overline{P'_N}(z_j)]. \end{aligned}$$

It is easy to see that when F is rotational invariant we get

$$\mathbb{E}\left[\sum_{i \neq j} F(x_i, x_j)\right] = \pi \int_{\mathbb{C}} F(z, 0) \rho_2(z, 0) dz. \tag{15}$$

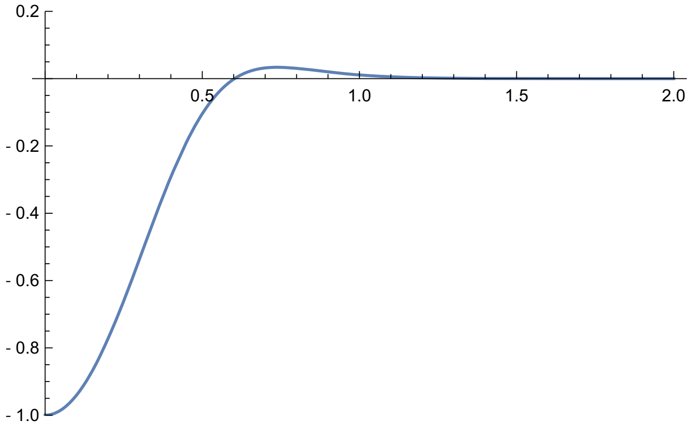

Fig. 3 $\frac{\pi^2}{N^2}(\rho_2(r,0)-\rho_1(r)\rho_1(0))$ for $r>0$ and $N=10$

Therefore, it is enough to compute $\rho_2(z_1, z_2)$ for $z_1 = z \in \mathbb{C}$ and $z_2 = 0$. The matrices in (14) are then

$$
\begin{aligned}
A &= \begin{pmatrix} (1+|z|^2)^N & 1 \\ 1 & 1 \end{pmatrix}, \\
B &= N \begin{pmatrix} \overline{z}(1+|z|^2)^{N-1} & 0 \\ \overline{z} & 0 \end{pmatrix}, \\
C &= N \begin{pmatrix} (1+|z|^2)^{N-2}(1+N|z|^2) & 1 \\ 1 & 1 \end{pmatrix},
\end{aligned}
$$

and we obtain

$$
\rho_2(z,0) = \frac{N^2\left[\left(1-\frac{N|z|^2}{(1+|z|^2)^N-1}\right)^2(1+|z|^2)^{N-2}+\left(1-\frac{N|z|^2(1+|z|^2)^{N-1}}{(1+|z|^2)^N-1}\right)^2\right]}{\pi^2[(1+|z|^2)^N-1]},
$$

see [28] and Fig. 3 where one can notice that this point process is not determinantal ([29, p.83]).

Using the relation with the chordal metric

$$
|x-y| = \frac{2|z-w|}{\sqrt{1+|z|^2}\sqrt{1+|w|^2}},
$$

we get

$$\mathbb{E}[E_0(x_1,\ldots x_N)] = \pi\int_{\mathbb{C}} f_0(z,0)\rho_2(z,0)dz = -\pi\int_{\mathbb{C}}\log\left(\frac{2|z|}{\sqrt{1+|z|^2}}\right)\rho_2(z,0)dz$$
$$= -2N^2\int_0^\infty r\log\left(\frac{2r}{\sqrt{1+r^2}}\right)\gamma(r)dr,$$

and for $s\neq 0$

$$\mathbb{E}[E_s(x_1,\ldots,x_N)] = \pi\int_{\mathbb{C}} f_s(z,0)\rho_2(z,0)dz = \pi\int_{\mathbb{C}}\left(\frac{2|z|}{\sqrt{1+|z|^2}}\right)^{-s}\rho_2(z,0)dz$$
$$= 2^{1-s}N^2\int_0^\infty r^{1-s}(1+r^2)^{s/2}\gamma(r)dr, \tag{16}$$

where

$$\gamma(r) = \frac{\left(1-\frac{Nr^2}{(1+r^2)^N-1}\right)^2(1+r^2)^{N-2} + \left(1-\frac{Nr^2(1+r^2)^{N-1}}{(1+r^2)^N-1}\right)^2}{(1+r^2)^N-1}. \tag{17}$$

In the logarithmic case, one can compute directly a primitive function that leads to the correct energy (1). However, we will compute the expected logarithmic energy as the limit of the Riesz case at $s=0$.

3 Proof of Theorem 1.1

In this section we prove first our general result (2) with the auxiliary Proposition 3.1. Then we prove the cases (4), (5) and finally (3).

Proof To simplify the notation we write $\mathbb{E}[E_s]$ instead of $\mathbb{E}[E_s(x_1,\ldots,x_N)]$. The change of variables $r=\sqrt{x}$ in (16) yields

$$\mathbb{E}[E_s] = \frac{N^2}{2^s}\int_0^\infty \frac{x^{-s/2}(1+x)^{s/2}}{[(1+x)^N-1]^3}\left[\left((1+x)^N-1-Nx\right)^2(1+x)^{N-2}\right.$$
$$\left.+\left((1+x)^N-1-Nx(1+x)^{N-1}\right)^2\right]dx.$$

The integrand is equivalent to x^{-2} at infinity, which is integrable, and to $x^{1-s/2}$ at $x=0$, which is integrable iff $1-s/2>-1$. Then, the energy will be finite iff $s<4$.

Now let us compute the integral. We take $r=s/2$ for simplicity, so we will be assuming $r<2$ throughout the proof. Using that $\frac{1}{(x-1)^3}=\frac{1}{2}\sum_{k=2}^\infty k(k-1)x^{-(k+1)}$ for $x>1$ and the fact that all the terms are positive we get

$$
\begin{aligned}
&\mathbb{E}[E_{2r}]\\
&= \frac{N^2}{2^{2r+1}} \sum_{k=2}^{\infty} k(k-1) \int_0^{\infty} \frac{(1+x)^{r-N(k+1)}}{x^r}\\
&\quad \times \left[\left((1+x)^N - 1 - Nx\right)^2 (1+x)^{N-2} + \left((1+x)^N - 1 - Nx(1+x)^{N-1}\right)^2 \right] dx\\
&= \frac{N^2}{2^{2r+1}} \lim_{M\to\infty} \sum_{k=2}^{M} k(k-1)\\
&\quad \times \Bigg[\underbrace{\int_0^{\infty} \frac{\left[(1+x)^{r-2-Nk} + (1+x)^{r-N(k+1)}\right]\left((1+x)^N - 1\right)^2}{x^r} dx}_{A_k}\\
&\quad - 2N \underbrace{\int_0^{\infty} x^{1-r} \left[(1+x)^{r-2-Nk} + (1+x)^{r-1-Nk}\right] \left((1+x)^N - 1\right) dx}_{B_k}\\
&\quad + N^2 \underbrace{\int_0^{\infty} x^{2-r} \left[(1+x)^{r-2-Nk} + (1+x)^{r-2-N(k-1)}\right] dx}_{C_k} \Bigg]. \qquad (18)
\end{aligned}
$$

Using the following integral representation for the beta function (see [27, 8.380 (3)]),

$$
B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^{\infty} \frac{t^{x-1}}{(1+t)^{x+y}} dt \qquad x, y > 0,
$$

it is immediate to obtain B_k, C_k in (18)

$$
\begin{aligned}
B_k &= B(2-r, N(k-1)) - B(2-r, Nk)\\
&\qquad + B(2-r, N(k-1)-1) - B(2-r, Nk-1), \qquad (19)\\
C_k &= B(3-r, Nk-1) + B(3-r, N(k-1)-1), \qquad (20)
\end{aligned}
$$

so

$$
\begin{aligned}
&-2NB_k + N^2 C_k\\
&= \Gamma(2-r)\Bigg[-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+2-r)} - \frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1-r)}\right.\\
&\quad \left. - \frac{\Gamma(Nk-1)}{\Gamma(Nk+1-r)}\right) + N^2(2-r)\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+2-r)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+2-r)}\right)\Bigg].
\end{aligned}
$$

To compute A_k we integrate by parts. Let $\beta \in \{r-2-Nk, r-N(k+1)\}$ denote the exponent in $(1+x)$. If $r \neq 1$,

$$\begin{aligned}
\int_0^\infty \frac{(1+x)^\beta \left((1+x)^N-1\right)^2}{x^r}dx &= \frac{1}{1-r}x^{1-r}(1+x)^\beta\left((1+x)^N-1\right)^2\Big|_0^\infty \\
&\quad - \frac{1}{1-r}\int_0^\infty x^{1-r}\Big[\beta(1+x)^{\beta-1}\left((1+x)^N-1\right)^2+2N(1+x)^{\beta+N-1} \\
&\quad \times \left((1+x)^N-1\right)\Big]dx \\
&= \frac{-1}{1-r}\Big[\beta\int_0^\infty x^{1-r}(1+x)^{\beta-1}\left((1+x)^{2N}-2(1+x)^N+1\right)dx \\
&\quad + 2N\int_0^\infty x^{1-r}(1+x)^{\beta+N-1}\left((1+x)^N-1\right)dx\Big] \\
&= \frac{-1}{1-r}\left[\beta\left(B(2-r,-\beta-2N-1+r)\right.\right. \\
&\quad -2B(2-r,-\beta-N-1+r)+B(2-r,-\beta-1+r)) \\
&\quad + 2N\left(B(2-r,-\beta-2N-1+r)-B(2-r,-\beta-N-1+r)\right)] \\
&= B(1-r,-\beta-2N-1+r) \\
&\quad - 2B(1-r,-\beta-N-1+r)+B(1-r,-\beta-1+r).
\end{aligned}$$

Then

$$\begin{aligned}
A_k &= B(1-r,N(k-2)+1)-2B(1-r,N(k-1)+1)+B(1-r,Nk+1) \\
&\quad + B(1-r,N(k-1)-1)-2B(1-r,Nk-1)+B(1-r,N(k+1)-1),
\end{aligned} \tag{21}$$

or, in terms of the gamma function,

$$\begin{aligned}
A_k &= \Gamma(1-r)\left[\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+2-r)}-2\frac{\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+2-r)}+\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}\right. \\
&\quad \left.+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-r)}-2\frac{\Gamma(Nk-1)}{\Gamma(Nk-r)}+\frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-r)}\right],
\end{aligned}$$

provided that $r \neq 1$. The case $r=1$ will be studied as the limit $r \to 1$.

Therefore, for $r \neq 1$, writting all together

$$\begin{aligned}
\mathbb{E}[E_{2r}] = \frac{N^2}{2^{2r+1}}\lim_{M\to\infty}\Bigg[\sum_{k=2}^{M}k(k-1)\Gamma(1-r)\Bigg(&\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+2-r)} \\
&-2\frac{\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+2-r)}+\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} \\
&+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-r)}-2\frac{\Gamma(Nk-1)}{\Gamma(Nk-r)}+\frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-r)}\Bigg)
\end{aligned}$$

$$+\sum_{k=2}^{M} k(k-1)\Gamma(2-r)\left(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+2-r)}-\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}\right.\right.$$
$$\left.+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1-r)}-\frac{\Gamma(Nk-1)}{\Gamma(Nk+1-r)}\right)$$
$$\left.\left.+N^2(2-r)\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+2-r)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+2-r)}\right)\right)\right]. \tag{22}$$

The sums get simplified by using the property $\Gamma(z+1)=z\Gamma(z)$ and changing the indices in such a way that all quotients have the form $\Gamma(Nk+1)/\Gamma(Nk+2-r)$

$$\mathbb{E}[E_{2r}]$$
$$=\frac{\Gamma(1-r)N^2}{2^{2r+1}}\lim_{M\to\infty}\left[\frac{2}{\Gamma(2-r)}+\sum_{k=1}^{M}(1-r+Nk(1+r))\frac{2r\Gamma(Nk)}{\Gamma(Nk+2-r)}\right.$$
$$-(M+1)M\frac{\Gamma(N(M-1)+1)}{\Gamma(N(M-1)+2-r)}$$
$$-\frac{(M+1)\left(r\left(N\left(N(4M-3)-2M+2\right)-1\right)-2(N-1)N(M-1)+(N-1)^2r^2\right)}{N(NM-1)}$$
$$\times\frac{\Gamma(NM+1)}{\Gamma(NM+2-r)}+\frac{M(M-1)(N(M+1)-r)(N(M+1)+1-r)}{N(M+1)(N(M+1)-1)}$$
$$\left.\times\frac{\Gamma(N(M+1)+1)}{\Gamma(N(M+1)+2-r)}\right].$$

Taking the asymptotic expansion of the terms in M as $M\to\infty$, we get

$$\mathbb{E}[E_{2r}]=\frac{\Gamma(1-r)N^2}{2^{2r+1}}\lim_{M\to\infty}\left[\frac{2}{\Gamma(2-r)}+2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}\right.$$
$$+\,2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}-2(1+r)N^{r-1}M^{r}$$
$$\left.-\,r(N+r+Nr-r^2)N^{r-2}M^{r-1}\right]. \tag{23}$$

Applying Proposition 3.1 below we obtain the following expression for every $r\neq 0,1$ with $r<2$

$$\mathbb{E}[E_{2r}]$$
$$=\frac{\Gamma(1-r)N^2}{2^{2r+1}}\left[\frac{2}{\Gamma(2-r)}+2r(1+r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}\right.$$
$$\zeta\left(1-r+2j,1+\frac{2-r}{2N}\right)N^{r-1-2j}$$

$$+2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}\zeta\left(2-r+2j,1+\frac{1-r}{2N}\right)$$
$$\times\ N^{r-2-2j}+O\left(N^{r-1-2m}\right)\Big].$$

Writing the expression in terms of $s=2r$ yields the result (2).

Now we prove (4), i.e. $r=1$ from the case $r\neq 1$. By continuity, the evaluation of the integral at the beginning of (18) can be performed by taking the limit $r\to 1$ in A_k, B_k, C_k, that is, in both sums in (22). The only tricky limit is the first one. It can be computed using the asymptotic expansion

$$\frac{1}{\Gamma(a+\gamma)}=\frac{1}{\Gamma(a)}-\frac{\psi(a)}{\Gamma(a)}\gamma+o(\gamma),$$

for $\gamma\to 0$, where a will be a natural number. Considering $\gamma=1-r$,

$$\begin{aligned}\lim_{\gamma\to 0}\Gamma(\gamma)\Bigg[&\frac{\Gamma(N(k-2)+1)}{\Gamma(N(k-2)+1+\gamma)}-\frac{2\Gamma(N(k-1)+1)}{\Gamma(N(k-1)+1+\gamma)}\\ &+\frac{\Gamma(Nk+1)}{\Gamma(Nk+1+\gamma)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)-1+\gamma)}\\ &-2\frac{\Gamma(Nk-1)}{\Gamma(Nk-1+\gamma)}+\frac{\Gamma(N(k+1)-1)}{\Gamma(N(k+1)-1+\gamma)}\Bigg]\\ =&-\psi(N(k-2)+1)+2\psi(N(k-1)+1)\\ &-\psi(Nk+1)-\psi(N(k-1)-1)+2\psi(Nk-1)-\psi(N(k+1)-1),\end{aligned}$$

and we get from (22)

$$\begin{aligned}\mathbb{E}[E_2]=\frac{N^2}{2^3}\lim_{M\to\infty}\Bigg[&\sum_{k=2}^{M}k(k-1)(-\psi(N(k-2)+1)+2\psi(N(k-1)+1)\\ &-\psi(Nk+1)-\psi(N(k-1)-1)+2\psi(Nk-1)-\psi(N(k+1)-1))\\ &+\sum_{k=2}^{M}k(k-1)\left(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+1)}-\frac{\Gamma(Nk)}{\Gamma(Nk+1)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1))}\right.\right.\\ &\left.\left.-\frac{\Gamma(Nk-1)}{\Gamma(Nk)}\right)+N^2\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+1)}+\frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1)}\right)\right)\Bigg].\end{aligned}\tag{24}$$

The first sum in (24) can be rewritten as

$$\begin{aligned}\Sigma_1:=&\sum_{k=2}^{M}k(k-1)(-\psi(N(k-2)+1)+2\psi(N(k-1)+1)-\psi(Nk+1)\\ &-\psi(N(k-1)-1)+2\psi(Nk-1)-\psi(N(k+1)-1))\\ =&(M+2)(M+1)\psi(NM+1)+(M+1)M\psi(N(M-1)+1)\end{aligned}$$

$$- 2(M+1)M\psi(NM+1) - 2\sum_{k=0}^{M}\psi(Nk+1) + (M+1)M\psi(NM-1)$$
$$- M(M-1)\psi(N(M+1)-1) - 2\sum_{k=1}^{M}\psi(Nk-1),$$

while the second becomes

$$\begin{aligned}
\Sigma_2 :=& \sum_{k=2}^{M} k(k-1)\left(-2N\left(\frac{\Gamma(N(k-1))}{\Gamma(N(k-1)+1)} - \frac{\Gamma(Nk)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1))}\right.\right.\\
&\left.\left. - \frac{\Gamma(Nk-1)}{\Gamma(Nk)}\right) + N^2\left(\frac{\Gamma(Nk-1)}{\Gamma(Nk+1)} + \frac{\Gamma(N(k-1)-1)}{\Gamma(N(k-1)+1)}\right)\right)\\
=& \sum_{k=2}^{M} k(k-1)\left(-2N\left(\frac{1}{N(k-1)} - \frac{1}{Nk} + \frac{1}{N(k-1)-1} - \frac{1}{Nk-1}\right)\right.\\
&\left. + N^2\left(\frac{1}{Nk-1} - \frac{1}{Nk} + \frac{1}{N(k-1)-1} - \frac{1}{N(k-1)}\right)\right)\\
=& \sum_{k=2}^{M} k(k-1)\left(\frac{2N-N^2}{Nk} - \frac{2N+N^2}{N(k-1)} + \frac{(2N+N^2)}{Nk-1} - \frac{(2N-N^2)}{N(k-1)-1}\right)\\
=& -\sum_{k=1}^{M-1}\frac{2kN(2+kN)}{Nk} + \frac{M(M-1)}{NM}(2N-N^2) + \sum_{k=1}^{M-1}\frac{2kN(-2+kN)}{Nk-1}\\
&+ \frac{M(M-1)}{NM-1}(2N+N^2) = -(M-1)(4+N) - \frac{2}{N}\sum_{k=1}^{M-1}\frac{1}{k-\frac{1}{N}}\\
&+ \frac{M(M-1)N(2+N)}{NM-1}.
\end{aligned}$$

We will use the functional relation $\psi(x+1) = \psi(x) + \frac{1}{x}$ for the digamma function, which allows us to obtain, for instance,

$$\sum_{k=1}^{M-1}\frac{1}{k-\frac{1}{N}} = \psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right).$$

Using this we get

$$\begin{aligned}
\Sigma_2 =& -(M-1)(4+N) - \frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right)\\
&+ \frac{M(M-1)N(2+N)}{NM-1}.
\end{aligned}$$

We can simplify Σ_1 with the same property. Since

$$\sum_{k=1}^{M} \psi(Nk-1) = \sum_{k=1}^{M} \left(\psi(Nk+1) - \frac{1}{Nk-1} - \frac{1}{Nk} \right),$$

then

$$\begin{aligned}
&-2\sum_{k=0}^{M} \psi(Nk+1) - 2\sum_{k=1}^{M} \psi(Nk-1) \\
&= 2\gamma - 4\sum_{k=1}^{M} \psi(Nk+1) + 2\sum_{k=1}^{M} \frac{1}{Nk-1} + 2\sum_{k=1}^{M} \frac{1}{Nk} \\
&= 2\gamma - 4\sum_{k=1}^{M} \psi(Nk+1) + \frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right) \right. \\
&\quad \left. -\psi\left(1-\frac{1}{N}\right)\right) + \frac{2}{N}(\psi(M+1)+\gamma).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\Sigma_1 + \Sigma_2 = {} & (M+2)(M+1)\psi(NM+1) + (M+1)M\psi(N(M-1)+1) \\
& - 2(M+1)M\psi(NM+1) + (M+1)M\psi(NM-1) \\
& - M(M-1)\psi(N(M+1)-1) + 2\gamma + \frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right) \right. \\
& \left. - \psi\left(1-\frac{1}{N}\right)\right) + \frac{2}{N}(\psi(M+1)+\gamma) - (M-1)(4+N) \\
& - \frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right) - \psi\left(1-\frac{1}{N}\right)\right) + \frac{M(M-1)N(2+N)}{NM-1} \\
& - 4\sum_{k=1}^{M} \psi(Nk+1).
\end{aligned}$$

From the relation [27, 8.365 (6)],

$$\begin{aligned}
\sum_{k=1}^{M} \psi(Nk+1) &= \frac{1}{N}\sum_{k=1}^{M}\sum_{j=1}^{N} \psi\left(k+\frac{j}{N}\right) + M\log N \\
&= \frac{1}{N}\sum_{j=1}^{N}\sum_{k=1}^{M} \psi\left(k+\frac{j}{N}\right) + M\log N.
\end{aligned}$$

Summation by parts gives

$$
\begin{aligned}
\sum_{k=1}^{M}\psi\left(k+\frac{j}{N}\right) &= M\psi\left(M+\frac{j}{N}\right)-\sum_{l=1}^{M-1}\left(\psi\left(l+1+\frac{j}{N}\right)-\psi\left(l+\frac{j}{N}\right)\right)l \\
&= M\psi\left(M+\frac{j}{N}\right)-\sum_{l=1}^{M-1}\frac{l}{l+\frac{j}{N}} \\
&= M\psi\left(M+\frac{j}{N}\right)-(M-1)+\frac{j}{N}\sum_{l=1}^{M-1}\frac{1}{l+\frac{j}{N}} \\
&= M\psi\left(M+\frac{j}{N}\right)-(M-1)+\frac{j}{N}\left(\psi\left(M+\frac{j}{N}\right)-\psi\left(1+\frac{j}{N}\right)\right) \\
&= \left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right)-\frac{j}{N}\psi\left(1+\frac{j}{N}\right)-(M-1),
\end{aligned}
$$

for every $1 \le j \le N$ and then

$$
\begin{aligned}
\Sigma_1+\Sigma_2 &= (M+2)(M+1)\psi(NM+1)+(M+1)M\psi(N(M-1)+1) \\
&\quad -2(M+1)M\psi(NM+1)+(M+1)M\psi(NM-1) \\
&\quad -M(M-1)\psi(N(M+1)-1) \\
&\quad +2\gamma+\frac{2}{N}\left(\psi\left(M+1-\frac{1}{N}\right)-\psi\left(1-\frac{1}{N}\right)\right)+\frac{2}{N}(\psi(M+1)+\gamma) \\
&\quad -(M-1)(4+N)-\frac{2}{N}\left(\psi\left(M-\frac{1}{N}\right)-\psi\left(1-\frac{1}{N}\right)\right) \\
&\quad +\frac{M(M-1)N(2+N)}{NM-1}-\frac{4}{N}\sum_{j=1}^{N}\left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right) \\
&\quad +\frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right)+4(M-1)-4M\log N \\
&= -M(M-1)\psi(N(M+1)-1)+2(M+1)\psi(NM+1) \\
&\quad +(M+1)M\psi(N(M-1)+1)-\frac{M(M+1)}{NM} \\
&\quad +\frac{(M-1)\left(\left(N^2+2N-1\right)M-2\right)}{NM-1}+\frac{2}{N}\psi(M+1)-N(M-1) \\
&\quad -4M\log N-\frac{4}{N}\sum_{j=1}^{N}\left(M+\frac{j}{N}\right)\psi\left(M+\frac{j}{N}\right) \\
&\quad +\frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1+\frac{j}{N}\right)+2\gamma\left(1+\frac{1}{N}\right).
\end{aligned}
$$

Using the asymptotic expansion $\psi(z) = \log z - \frac{1}{2z} - \frac{1}{12z^2} + O\left(z^{-4}\right)$ as $z \to \infty$, we obtain

$$\Sigma_1 + \Sigma_2 = -1 - \frac{3}{N} + 2\log N + O\left(M^{-1}\right) + \frac{4}{N}\sum_{j=1}^{N} \frac{j}{N}\psi\left(1 + \frac{j}{N}\right) + 2\gamma\left(1 + \frac{1}{N}\right).$$

Then

$$\begin{aligned}
\mathbb{E}[E_2] &= \frac{N^2}{2^3} \lim_{M\to\infty} \left[\Sigma_1 + \Sigma_2\right] \\
&= \frac{N^2}{2^3}\left(-1 - \frac{3}{N} + 2\log N + \frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(1 + \frac{j}{N}\right) + 2\gamma\left(1 + \frac{1}{N}\right)\right) \\
&= \frac{N^2}{2^3}\left(-1 - \frac{3}{N} + 2\log N + \frac{4}{N}\underbrace{\sum_{j=1}^{N}\frac{j}{N}\frac{1}{j/N}}_{=N} + \frac{4}{N}\sum_{j=1}^{N}\frac{j}{N}\psi\left(\frac{j}{N}\right) + 2\gamma\left(1 + \frac{1}{N}\right)\right) \\
&= \frac{N}{2^3}\left(3N - 3 + 2N\log N + 4\sum_{j=1}^{N}\frac{j}{N}\psi\left(\frac{j}{N}\right) + 2\gamma\,(N+1)\right) \\
&= \frac{N}{2^3}\left(3N - 3 + 2N\log N + 4\sum_{j=1}^{N-1}\frac{j}{N}\psi\left(\frac{j}{N}\right) + 2\gamma(N-1)\right).
\end{aligned}$$

Finally, using

$$\sum_{j=1}^{N-1}\frac{j}{N}\psi\left(\frac{j}{N}\right) = -\frac{\gamma}{2}(N-1) - \frac{N}{2}\log N - \frac{\pi}{2}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right),$$

[16, (B.11)], we get (4)

$$\mathbb{E}[E_2] = -\frac{N\pi}{4}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}.$$

To compute $\mathbb{E}[E_{-2n}]$ and $\mathbb{E}[E_0]$, we start observing that for $r < 1$ formula (23) yields

$$\mathbb{E}[E_{2r}] = \frac{\Gamma(1-r)N^2}{2^{2r}}\left(\frac{1}{\Gamma(2-r)} + r(1+r)\sum_{k=1}^{\infty}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)} + r(1-r)\right.$$
$$\left.\times \sum_{k=1}^{\infty}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}\right),$$

since both sums are convergent in this case. Using the expression of the beta function in terms of gamma function and the monotone convergence theorem, we get

$$\mathbb{E}[E_{2r}] = \frac{N^2}{2^{2r}}\left(\frac{1}{1-r} + r(1+r)\int_0^1 (1-t)^{-r}\frac{t^N}{1-t^N}\,dt\right.$$
$$\left. + r\int_0^1 (1-t)^{1-r}\frac{t^{N-1}}{1-t^N}\,dt\right). \tag{25}$$

For $r = -n$, the energy is

$$\mathbb{E}[E_{-2n}] = 2^{2n}N^2\left(\frac{1}{n+1} - n(1-n)\underbrace{\int_0^1 (1-t)^n\frac{t^N}{1-t^N}\,dt}_{I_1} - n\right.$$
$$\left.\times \underbrace{\int_0^1 (1-t)^{1+n}\frac{t^{N-1}}{1-t^N}\,dt}_{I_2}\right). \tag{26}$$

To compute I_1 and I_2 we will use the following integral representation [27, 8.361 (7)] for the digamma function

$$\psi(z) = \int_0^1 \frac{t^{z-1}-1}{t-1}\,dt - \gamma, \qquad z > 0,$$

from which we get

$$\int_0^1 \frac{t^a-1}{1-t^N}\,dt = \frac{1}{N}\int_0^1 \frac{y^{(a+1)/N-1} - y^{1/N-1}}{1-y}\,dt$$
$$= -\frac{1}{N}\left(\psi\left(\frac{a+1}{N}\right) - \psi\left(\frac{1}{N}\right)\right), \tag{27}$$

for any $a > -1$. Then

$$
\begin{aligned}
I_1 &= \int_0^1 \sum_{m=0}^{n} \binom{n}{m} (-1)^m \frac{t^{N+m}}{1-t^N}\, dt = \int_0^1 \sum_{m=0}^{n} \binom{n}{m} (-1)^m \frac{t^{N+m}-1}{1-t^N}\, dt \\
&= -\frac{1}{N} \sum_{m=0}^{n} \binom{n}{m} (-1)^m \left(\psi\left(\frac{m+1}{N}+1\right) - \psi\left(\frac{1}{N}\right)\right) \\
&= -\frac{1}{N} \sum_{m=0}^{n} \binom{n}{m} (-1)^m \psi\left(\frac{m+1}{N}+1\right),
\end{aligned}
$$

where we have used $\sum_{m=0}^{n} \binom{n}{m}(-1)^m = 0$ in the second and last equality. Applying $\psi(x+1) = \psi(x) + 1/x$,

$$
I_1 = -\frac{1}{N} \sum_{m=0}^{n} \binom{n}{m} (-1)^m \psi\left(\frac{m+1}{N}\right) + \sum_{m=0}^{n} \binom{n}{m} (-1)^{m+1} \frac{1}{m+1}
$$

and it is trivial to check that the second sum equals $-1/(n+1)$.

The integral I_2 can be computed in a similar way

$$
\begin{aligned}
I_2 &= \int_0^1 \sum_{m=0}^{n+1} \binom{n+1}{m} (-1)^m \frac{t^{N-1+m}-1}{1-t^N}\, dt = -\frac{1}{N} \sum_{m=0}^{n+1} \binom{n+1}{m} (-1)^m \psi\left(\frac{m}{N}+1\right) \\
&= \frac{1}{N}\left(\gamma - \sum_{m=1}^{n+1} \binom{n+1}{m} (-1)^m \psi\left(\frac{m}{N}\right)\right) + \sum_{m=1}^{n+1} \binom{n+1}{m} (-1)^{m+1} \frac{1}{m},
\end{aligned}
$$

where the second sum is $\sum_{m=1}^{n+1} \frac{1}{m}$, as stated in [27, 0.155 (4)].

Finally from (26) we get (5)

$$
\begin{aligned}
\mathbb{E}[E_{-2n}] = 2^{2n} N^2 \Bigg[& \frac{1}{n+1} - n(1-n) \left(-\frac{1}{N} \sum_{m=0}^{n} \binom{n}{m} (-1)^m \psi\left(\frac{m+1}{N}\right) - \frac{1}{n+1}\right) \\
& - n \left(\frac{1}{N} \left(\gamma - \sum_{m=1}^{n+1} \binom{n+1}{m} (-1)^m \psi\left(\frac{m}{N}\right)\right) + \sum_{m=1}^{n+1} \frac{1}{m}\right) \Bigg] \\
= 2^{2n} N^2 & \left(\frac{1}{n+1} - \frac{n(n-1)}{n+1} - n \sum_{m=1}^{n+1} \frac{1}{m}\right) \\
& + 2^{2n} n N \left(-\gamma + \sum_{m=1}^{n+1} \binom{n+1}{m} (-1)^m \psi\left(\frac{m}{N}\right) \left(\frac{n-1}{n+1} m + 1\right)\right).
\end{aligned}
$$

In order to compute $\mathbb{E}[E_0]$, i.e. formula (3) from [3], we take the derivative of $\mathbb{E}[E_s]$ at $s = 0$. Consider the continuous function

$$g(r) = \begin{cases} \mathbb{E}[E_{2r}], & \text{for } r \neq 0, \\ N^2 - N, & \text{for } r = 0, \end{cases}$$

where $r = 0$ matches the Riesz 0-energy, which trivially is $N^2 - N$ for any configuration of points. Then

$$\mathbb{E}[E_0] = \frac{1}{2} g'(0).$$

Since $g'(0)$ exists, we can derive it by restricting to $r < 0$

$$g'(0) = \lim_{r \to 0^-} \frac{g(r) - g(0)}{r},$$

where

$$g(r) = 2^{-2r} N^2 \left(\frac{1}{1-r} + r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt \right. \\ \left. + r \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt \right),$$

according to (25).

Then

$$\begin{aligned} \lim_{r \to 0^-} g(r) &= N^2 + N^2 \lim_{r \to 0^-} r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt \\ &\quad + N^2 \lim_{r \to 0^-} r \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt \\ &= N^2 + N^2 \lim_{r \to 0^-} r(1+r) \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt, \end{aligned}$$

because $(1-t)^{1-r} \uparrow (1-t)$ when $r \to 0^-$ and $\int_0^1 (1-t) \frac{t^{N-1}}{1-t^N}\, dt < \infty$. By continuity, we also have $\lim_{r \to 0^-} g(r) = g(0) = N^2 - N$, so we deduce that

$$\lim_{r \to 0^-} r \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt = -\frac{1}{N}. \tag{28}$$

Therefore,

$$\frac{g'(0)}{N^2} = (1 - \log 4) + \lim_{r \to 0^-} \frac{\frac{r(1+r)}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r}$$

$$
\begin{aligned}
&+ \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{1-r} \frac{t^{N-1}}{1-t^N}\, dt}{r} \\
&= (1-\log 4) + \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r} \\
&+ \underbrace{\lim_{r\to 0^-} r \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt}_{=-1/N \text{ by } (28)} \\
&+ \int_0^1 (1-t) \frac{t^{N-1}}{1-t^N}\, dt = (1-\log 4) + \underbrace{\lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{t^N}{1-t^N}\, dt + \frac{1}{N}}{r}}_{I_3} \\
&- \frac{1}{N} - \frac{1}{N}\left(\psi(1) - \psi\left(1+\frac{1}{N}\right)\right),
\end{aligned} \tag{29}
$$

where we have applied (27).

It remains to compute the limit I_3

$$
\begin{aligned}
I_3 &= \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)}\right) dt}{r} \\
&\quad + \frac{1}{N} \lim_{r\to 0^-} \frac{\frac{r}{2^{2r}} \int_0^1 (1-t)^{-r} \frac{1}{1-t}\, dt + 1}{r} \\
&= \lim_{r\to 0^-} \int_0^1 (1-t)^{-r} \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)}\right) dt + \frac{1}{N} \lim_{r\to 0^-} \frac{-2^{-2r}+1}{r} \\
&= \underbrace{\int_0^1 \left(\frac{t^N}{1-t^N} - \frac{1}{N(1-t)}\right) dt}_{I_4} + \frac{2}{N}\log 2,
\end{aligned}
$$

where the limit of the last integral is justified by monotone convergence theorem. Using (27), we obtain

$$
\begin{aligned}
I_4 &= \frac{1}{N} \int_0^1 \frac{N t^N - \sum_{j=0}^{N-1} t^j}{1-t^N}\, dt = \frac{1}{N} \sum_{j=0}^{N-1} \int_0^1 \frac{t^N - t^j}{1-t^N}\, dt \\
&= -\frac{1}{N^2} \sum_{j=0}^{N-1} \left(\psi\left(1+\frac{1}{N}\right) - \psi\left(\frac{j+1}{N}\right)\right) \\
&= -\frac{1}{N}\psi\left(1+\frac{1}{N}\right) + \frac{1}{N^2} \sum_{j=0}^{N-1} \psi\left(\frac{j+1}{N}\right) \\
&= -\frac{1}{N}\psi\left(1+\frac{1}{N}\right) - \frac{1}{N}(\log N + \gamma),
\end{aligned}
$$

where we have used that $\sum_{j=0}^{N-1}\psi\left(\frac{j+1}{N}\right)=-N\log N-\gamma N$.

From (29) we finally get

$$\begin{aligned}
&2\mathbb{E}[E_0]\\
&\quad = g'(0) = (1-\log 4)\,N^2+N^2\left(-\frac{1}{N}\psi\left(1+\frac{1}{N}\right)-\frac{1}{N}\left(\log N+\gamma\right)+\frac{2}{N}\log 2\right)\\
&\qquad -N-N\left(\psi\left(1\right)-\psi\left(1+\frac{1}{N}\right)\right)=(1-\log 4)\,N^2-N\log N-(1-\log 4)\,N.
\end{aligned}$$

□

Proposition 3.1 *Let $r<2$ and $m\geq 1$. Then*

$$\begin{aligned}
&\lim_{M\to\infty}\Bigg[2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}+2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}\\
&\quad -2(1+r)N^{r-1}M^r-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg]\\
&\quad = 2r(1+r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}N^{r-1-2j}\zeta\left(1-r+2j,1+\frac{2-r}{2N}\right)\\
&\qquad +2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}N^{r-2-2j}\zeta\left(2-r+2j,1+\frac{1-r}{2N}\right)\\
&\qquad +O\left(N^{r-1-2m}\right)
\end{aligned}\tag{30}$$

as $N\to+\infty$.

Proof We will use the following Fields' approximation for the quotient of gamma functions, see [36, Eq. 5.11.14] or [26]

$$\frac{\Gamma(z+a)}{\Gamma(z+b)}=\sum_{j=0}^{m-1}\frac{B_{2j}^{(2\rho)}(\rho)(b-a)_{2j}w^{a-b-2j}}{(2j)!}+O\left(w^{a-b-2m}\right),$$

as $w\to\infty$ with $|\arg(w+\rho)|<\pi$ where a and b are fixed complex numbers, $w=z+\rho$ and $2\rho=1+a-b$. Then,

$$\begin{aligned}
&\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}\\
&\quad =\sum_{k=1}^{M}\left(Nk+\frac{2-r}{2}\right)^{r-1}+\sum_{j=1}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}\sum_{k=1}^{M}\left(Nk+\frac{2-r}{2}\right)^{r-1-2j}
\end{aligned}$$

$$+\sum_{k=1}^{M} O\left(\left(Nk+\frac{2-r}{2}\right)^{r-1-2m}\right) = N^{r-1} \underbrace{\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}}_{D}$$

$$+\sum_{j=1}^{m-1} \frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!} N^{r-1-2j} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{2-r}{2N}\right)^{1-r+2j}}}_{E_j}$$

$$+ O\left(N^{r-1-2m}\right) \underbrace{\sum_{k=1}^{M} \frac{1}{k^{1-r+2m}}}_{F}, \tag{31}$$

and

$$\sum_{k=1}^{M} \frac{\Gamma(Nk)}{\Gamma(Nk+2-r)} = \sum_{k=1}^{M}\left(Nk+\frac{1-r}{2}\right)^{r-2}$$

$$+\sum_{j=1}^{m-1} \frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!} \sum_{k=1}^{M}\left(Nk+\frac{1-r}{2}\right)^{r-2-2j}$$

$$+\sum_{k=1}^{M} O\left(\left(Nk+\frac{1-r}{2}\right)^{r-2-2m}\right) = N^{r-2} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{1-r}{2N}\right)^{2-r}}}_{G}$$

$$+\sum_{j=1}^{m-1} \frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!} N^{r-2-2j} \underbrace{\sum_{k=0}^{M-1} \frac{1}{\left(k+1+\frac{1-r}{2N}\right)^{2-r+2j}}}_{H_j}$$

$$+ O\left(N^{r-2-2m}\right) \underbrace{\sum_{k=1}^{M} \frac{1}{k^{2-r+2m}}}_{I}. \tag{32}$$

To compute the limit as $M \to \infty$, observe that $E_j \to \zeta\left(1-r+2j, 1+\frac{2-r}{2N}\right)$ and $H_j \to \zeta\left(2-r+2j, 1+\frac{1-r}{2N}\right)$ for $j \geq 1$, since $1-r+2j, 2-r+2j > 1$. The sums F and I are convergent and G can be written as (see [36, Eq. 25.11.5])

$$\sum_{k=1}^{M} \frac{1}{\left(k+\frac{1-r}{2N}\right)^{2-r}} = \zeta\left(2-r, 1+\frac{1-r}{2N}\right) - \frac{\left(M+\frac{1-r}{2N}\right)^{r-1}}{1-r}$$
$$-(2-r)\int_{M-1}^{\infty} \frac{x-\lfloor x\rfloor}{\left(x+1+\frac{1-r}{2N}\right)^{3-r}}\, dx.$$

The same formula holds to approximate D for $r < 1$

$$\sum_{k=1}^{M} \frac{1}{\left(k+\frac{2-r}{2N}\right)^{1-r}} = \zeta\left(1-r, 1+\frac{2-r}{2N}\right) + \frac{\left(M+\frac{2-r}{2N}\right)^r}{r} \\ -(1-r)\int_{M-1}^{\infty} \frac{x-\lfloor x \rfloor}{\left(x+1+\frac{2-r}{2N}\right)^{2-r}}\, dx, \tag{33}$$

while if $r > 1$, by the Euler–Maclaurin formula,

$$\begin{aligned}
&\sum_{k=1}^{M} \left(k+\frac{2-r}{2N}\right)^{r-1} \\
&= \int_1^M \left(x+\frac{2-r}{2N}\right)^{r-1} dx + \frac{1}{2}\left[\left(M+\frac{2-r}{2N}\right)^{r-1} + \left(1+\frac{2-r}{2N}\right)^{r-1}\right] \\
&\quad + (r-1)\int_1^M \frac{x-\lfloor x \rfloor - 1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\, dx \\
&= \frac{\left(M+\frac{2-r}{2N}\right)^r}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} - \frac{\left(1+\frac{2-r}{2N}\right)^r}{r} \\
&\quad + \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} + (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{M} \frac{x-\lfloor x \rfloor - 1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\, dx - (r-1) \\
&\quad \times \int_{-\left(\frac{2-r}{2N}\right)}^{1} \frac{x-\lfloor x \rfloor - 1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\, dx \\
&= \frac{\left(M+\frac{2-r}{2N}\right)^r}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} - \frac{\left(1+\frac{2-r}{2N}\right)^r}{r} + \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} \\
&\quad + (r-1)\int_{-\left(\frac{2-r}{2N}\right)}^{M} \frac{x-\lfloor x \rfloor - 1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\, dx - \left(\frac{2-r}{2N}\right)^{r-1} \\
&\quad + \frac{\left(1+\frac{2-r}{2N}\right)^r}{r} - \frac{\left(1+\frac{2-r}{2N}\right)^{r-1}}{2} \\
&= \frac{\left(M+\frac{2-r}{2N}\right)^r}{r} + \frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2} + (r-1) \\
&\quad \times \int_{-\left(\frac{2-r}{2N}\right)}^{M} \frac{x-\lfloor x \rfloor - 1/2}{\left(x+\frac{2-r}{2N}\right)^{2-r}} dx - \left(\frac{2-r}{2N}\right)^{r-1},
\end{aligned} \tag{34}$$

where the last integral converges for $1 < r < 2$ when $M \to +\infty$ to $\zeta\left(1-r, \frac{2-r}{2N}\right)$, see [36, Eq. 25.11.26].

Using all the previous computations, we get

$$\lim_{M\to\infty}\Bigg[2r(1+r)\sum_{k=1}^{M}\frac{\Gamma(Nk+1)}{\Gamma(Nk+2-r)}+2r(1-r)\sum_{k=1}^{M}\frac{\Gamma(Nk)}{\Gamma(Nk+2-r)}-2(1+r)N^{r-1}M^{r}$$
$$-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg]=\lim_{M\to\infty}\Bigg[2r(1+r)\left(N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}\right.$$
$$\left.+\sum_{j=1}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}\sum_{k=0}^{M-1}\frac{N^{r-1-2j}}{\left(k+1+\frac{2-r}{2N}\right)^{1-r+2j}}+O\left(N^{r-1-2m}\right)\sum_{k=1}^{M}\frac{1}{k^{1-r+2m}}\right)$$
$$+2r(1-r)\left(N^{r-2}\left(\zeta\left(2-r,1+\frac{1-r}{2N}\right)-\frac{\left(M+\frac{1-r}{2N}\right)^{r-1}}{1-r}\right.\right.$$
$$\left.-\int_{M-1}^{\infty}\frac{(2-r)(x-\lfloor x\rfloor)}{\left(x+1+\frac{1-r}{2N}\right)^{3-r}}\,dx\right)+\sum_{j=1}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}\sum_{k=0}^{M-1}\frac{N^{r-2-2j}}{\left(k+1+\frac{1-r}{2N}\right)^{2-r+2j}}$$
$$\left.+O\left(N^{r-2-2m}\right)\sum_{k=1}^{M}\frac{1}{k^{2-r+2m}}\right)-2(1+r)N^{r-1}M^{r}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg]$$
$$=\lim_{M\to\infty}\Bigg[2r(1+r)N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}-2(1+r)N^{r-1}M^{r}$$
$$-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg]$$
$$+2r(1-r)\sum_{j=0}^{m-1}\frac{B_{2j}^{(r-1)}(\frac{r-1}{2})(2-r)_{2j}}{(2j)!}N^{r-2-2j}\zeta\left(2-r+2j,1+\frac{1-r}{2N}\right)$$
$$+2r(1+r)\sum_{j=1}^{m-1}\frac{B_{2j}^{(r)}(\frac{r}{2})(1-r)_{2j}}{(2j)!}N^{r-1-2j}\zeta\left(1-r+2j,1+\frac{2-r}{2N}\right)+O\left(N^{r-1-2m}\right). \tag{35}$$

Everything reduces to compute the limit appearing in (35). If $r<1$, using (33),

$$\lim_{M\to\infty}\Bigg[2r(1+r)N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}-2(1+r)N^{r-1}M^{r}$$
$$-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^2)N^{r-2}M^{r-1}\Bigg]$$
$$=\lim_{M\to\infty}\Bigg[2r(1+r)N^{r-1}\left(\zeta\left(1-r,1+\frac{2-r}{2N}\right)\right.$$
$$\left.+\frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r}-(1-r)\int_{M-1}^{\infty}\frac{x-\lfloor x\rfloor}{\left(x+1+\frac{2-r}{2N}\right)^{2-r}}\,dx\right)-2(1+r)N^{r-1}M^{r}\Bigg]$$
$$=2r(1+r)N^{r-1}\zeta\left(1-r,1+\frac{2-r}{2N}\right)$$

$$
\begin{aligned}
&+2(1+r)N^{r-1}\lim_{M\to\infty}\\
&\quad\times\left(\left(M+\frac{2-r}{2N}\right)^{r}-M^{r}\right)\\
&=2r(1+r)N^{r-1}\zeta\left(1-r,1+\frac{2-r}{2N}\right).
\end{aligned}
$$

If $r>1$, using (34),

$$
\begin{aligned}
&\lim_{M\to\infty}\Bigg[2r(1+r)N^{r-1}\sum_{k=1}^{M}\left(k+\frac{2-r}{2N}\right)^{r-1}-2(1+r)N^{r-1}M^{r}\\
&\quad-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^{2})N^{r-2}M^{r-1}\Bigg]\\
&=\lim_{M\to\infty}\Bigg\{2r(1+r)N^{r-1}\Bigg(\frac{\left(M+\frac{2-r}{2N}\right)^{r}}{r}+\frac{\left(M+\frac{2-r}{2N}\right)^{r-1}}{2}\\
&\quad+\int_{-\left(\frac{2-r}{2N}\right)}^{M}\frac{(r-1)(x-\lfloor x\rfloor-\frac{1}{2})}{\left(x+\frac{2-r}{2N}\right)^{2-r}}\,dx-\left(\frac{2-r}{2N}\right)^{r-1}\Bigg)-2(1+r)N^{r-1}M^{r}\\
&\quad-2rN^{r-2}\left(M+\frac{1-r}{2N}\right)^{r-1}-r(N+r+Nr-r^{2})N^{r-2}M^{r-1}\Bigg\}\\
&=\lim_{M\to\infty}\Bigg[2(1+r)N^{r-1}M^{r}\left(\left(1+\frac{2-r}{2NM}\right)^{r}-1\right)\\
&\quad+rN^{r-2}M^{r-1}\Bigg((1+r)\left(1+\frac{2-r}{2NM}\right)^{r-1}N-2\left(1+\frac{1-r}{2NM}\right)^{r-1}\\
&\quad-\left(N+r+Nr-r^{2}\right)\Bigg)\Bigg]\\
&\quad+2r(1+r)N^{r-1}\left(\zeta\left(1-r,\frac{2-r}{2N}\right)-\left(\frac{2-r}{2N}\right)^{r-1}\right)\\
&=\lim_{M\to\infty}\Bigg[rN^{r-2}M^{r-1}\underbrace{[(1+r)(2-r)+(1+r)N-2-(N+r+Nr-r^{2})]}_{=0}\\
&\quad+O\left(M^{r-2}\right)\Bigg]\\
&\quad+2r(1+r)N^{r-1}\zeta\left(1-r,1+\frac{2-r}{2N}\right)=2r(1+r)N^{r-1}\zeta\left(1-r,1+\frac{2-r}{2N}\right),
\end{aligned}
$$

where we have used that $\zeta(s,a)-a^{-s}=\zeta(s,1+a)$.

Applying this limit on (35) we get the desired result. □

4 Bounds for the Minimal Energy Asymptotic Expansion

We will start this section by recalling some known results, and some conjectures, about the asymptotic expansion of the extremal energy $\mathcal{E}_s(N)$ attained by a set of N points on the sphere $\mathbb{S}^2$. For a more complete picture see [19].

The current knowledge about the asymptotic expansion of the minimal energy is far from complete even in the case of $\mathbb{S}^2$, but for $s \leq -2$ the situation is well known. Indeed, the minimizers of the Riesz energy for $s < -2$ are points placed at each of the two endpoints of some diameter (for even N), [15], and for $s = -2$, formula (8) shows that any configuration with center of mass at the origin attains the maximum $2N^2$.

For $0 < |s| < 2$, it is known that there exist $c, C > 0$ (depending on s) such that

$$-cN^{1+s/2} \leq \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \leq -CN^{1+s/2}, \tag{36}$$

see [37, 41, 42] and [1, 21] for improvements in the value of the constants leading to the bounds

$$\begin{aligned} \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\leq -\frac{\Gamma(1-s/2)}{2^s}N^{1+s/2}, \quad \text{if } 0 < s < 2, \\ \mathcal{E}_s(N) - \frac{2^{1-s}}{2-s} &\geq -\frac{\Gamma(1-s/2)}{2^s}N^{1+s/2}, \quad \text{if } -2 < s < 0, \end{aligned} \tag{37}$$

which were obtained with the bound given by the expected energy of random points from the spherical ensemble [1].

In the boundary case $s = 2$, it was shown in [22, Proposition 3] that

$$-\frac{1}{4}N^2 + O(N\log N) \leq \mathcal{E}_2(N) - \frac{1}{4}N^2\log N \leq \frac{1}{4}N^2\log\log N + O(N^2),$$

and the upper bound was improved in [1] to

$$\mathcal{E}_2(N) - \frac{1}{4}N^2\log N \leq \frac{\gamma}{4}N^2, \tag{38}$$

where γ is the Euler–Mascheroni constant.

For the logarithmic potential, it is known that there exists a constant, $C_{\log}$, such that

$$-0.0569\ldots \leq C_{\log} \leq 2\log 2 + \frac{1}{2}\log\frac{2}{3} + 3\log\frac{\sqrt{\pi}}{\Gamma(1/3)} = -0.0556\ldots,$$

for which

$$\mathcal{E}_0(N) = \left(\frac{1}{2} - \log 2\right)N^2 - \frac{1}{2}N\log N + C_{\log}N + o(N) \text{ as } N \to +\infty, \tag{39}$$

see [13, 33] and [10] for a recent direct computation of the lower bound. The upper bound for $C_{\log}$ has been conjectured to be an equality by two different approaches [13, 22].

For $-2 < s < 4$, $s \neq 0$, the asymptotic expansion of the optimal Riesz s-energy has been conjectured in [22] to be, for $s \neq 2$,

$$\mathcal{E}_s(N) = \frac{2^{1-s}}{2-s}N^2 + \frac{(\sqrt{3}/2)^{s/2}\zeta_{\Lambda_2}(s)}{(4\pi)^{s/2}}N^{1+\frac{s}{2}} + o(N^{1+\frac{s}{2}}) \text{ as } N \to +\infty, \tag{40}$$

where $\zeta_{\Lambda_2}(s)$ is the zeta function of the hexagonal lattice, while for $s = 2$ the conjectured expansion is

$$\mathcal{E}_2(N) = \frac{1}{4}N^2 \log N + CN^2 + O(1) \text{ as } N \to +\infty, \tag{41}$$

where $C = \frac{1}{4}\left[\gamma - \log(2\sqrt{3}\pi)\right] + \frac{\sqrt{3}}{4\pi}[\gamma_1(2/3) - \gamma_1(1/3)] \approx -0.08577$. Here, $\gamma_n(a)$ is the generalized Stieltjes constant in the Laurent expansion of the Hurwitz zeta function $\zeta(s, a)$ around $s = 1$.

It is clear that the minimal energy is always bounded by the expected energy with respect to a given random configuration. Therefore, one can bound the asymptotic expansion of the minimal energy by the asymptotic expansion of the expected energy. This idea was used in [3] to get bounds for the minimal logarithmic energy using (1) and in [1] to get (37) and (38). For other computations of expected energies in different settings, see [2, 4–6, 8, 11, 20, 34]. From our main result, Theorem 1.1, we obtain the asymptotic expansion (6) which is close to the conjectured expansion for the minimal energy, see Fig. 4, and we can prove the following bounds.

Corollary 4.1 *Let $C(s)$ be the constant in (7). Then*

(i) *For $0 < s < 2$, there exists an $N_0 = N_0(s)$ such that, for any $N \geq N_0$,*

$$\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \leq C(s)N^{1+s/2}.$$

(ii) *For $-2 < s < 0$ and a given $\epsilon > 0$, there exists an $N_1 = N_1(\epsilon, s)$ such that, for any $N \geq N_1$,*

$$\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2 \geq C(s)(1+\epsilon)N^{1+s/2}.$$

(iii) *For any $N \geq 2$,*

$$\mathcal{E}_2(N) - \frac{N^2 \log N}{4} \leq \frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right)N^2. \tag{42}$$

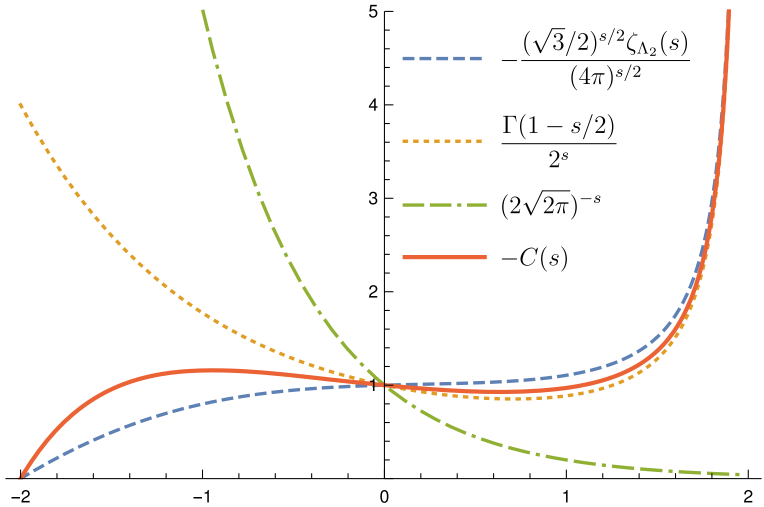

Fig. 4 All curves are related to $\left(\frac{2^{1-s}}{2-s}N^2 - \mathcal{E}_s(N)\right)/N^{1+s/2}$. The dashed blue curve is given by the conjectured valued for the second order constant, (40). The dotted yellow and the dash-dotted green curves corresponds to [1] and [37], respectively, and the thick red is our constant (7)

Remark 2 These bounds improve (37) and (38) from [1]. In the proof we show also that

$$\mathbb{E}[E_2] = \frac{N^2 \log N}{4} + \frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right) N^2 - \frac{N}{8} + O(1) \text{ as } N \to +\infty,$$

see (46). In fact, it is possible to write complete asymptotic expansions of the energy with the known asymptotic expansions of the cotangent sum (4), the so called Vasyunin sum, see [14].

Proof For $0 < s < 2$, from (6),

$$\begin{aligned}\frac{\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} &\le \frac{\mathbb{E}[E_s] - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \\ &= C(s) + \frac{s}{16}C(s-2)N^{-1} + O(N^{-2}) \text{ as } N \to +\infty.\end{aligned}$$

Since $C(s-2)$ is negative, the last expression is bounded above by $C(s)$ for N big enough.

For $-2 < s < 0$, using (6) again,

$$\frac{\mathcal{E}_s(N) - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \ge \frac{\mathbb{E}[E_s] - \frac{2^{1-s}}{2-s}N^2}{N^{1+s/2}} \xrightarrow[N\to\infty]{} C(s).$$

Therefore, given $\delta > 0$, for N large enough the right-hand side is bounded from below by $C(s) - \delta$. Since the constant $C(s)$ is negative, we can choose $\delta = -\epsilon C(s)$ to obtain the result.

For $s = 2$, the energy is (4):

$$\mathbb{E}[E_2] = -\frac{N\pi}{4}\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) + \frac{3N^2}{8} - \frac{3N}{8}.$$

We can rewrite the sum as

$$-\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) = \underbrace{\sum_{j=1}^{N-1}\left[-\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) - \frac{1}{\pi(1-j/N)}\right]}_{A} + \underbrace{\sum_{j=1}^{N-1}\frac{1}{\pi(1-j/N)}}_{B}, \tag{43}$$

in such a way that the term corresponding to $j = N$ in the first sum is well-defined. Let us apply the Euler–Maclaurin formula to $f(x) = g(x/N)$, with $g(x) = -x\cot(\pi x) - \frac{1}{\pi(1-x)}$:

$$\begin{aligned}
A &= \sum_{j=0}^{N} f(j) - f(0) - f(N)\\
&= \int_0^N f(x)\,dx - \frac{f(0)+f(N)}{2} + \frac{B_2}{2!}[f'(N) - f'(0)]\\
&\quad + \frac{B_4}{4!}[f^{(3)}(N) - f^{(3)}(0)] + R_N^A\\
&= N\int_0^1 g(x)\,dx - \frac{g(0)+g(1)}{2} + \frac{1}{12N}[g'(1) - g'(0)]\\
&\quad - \frac{1}{720N^3}[g^{(3)}(1) - g^{(3)}(0)] + R_N^A,
\end{aligned}$$

where B_j are the Bernoulli numbers and R_N^A is the remainder term, that satisfies

$$|R_N^A| \le \frac{2\zeta(5)}{(2\pi)^5}\int_0^N |f^{(5)}(x)|\,dx = \frac{2\zeta(5)}{(2\pi)^5 N^4}\int_0^1 |g^{(5)}(x)|\,dx. \tag{44}$$

We get

$$A = -\frac{\log(2\pi)}{\pi}N + \frac{3}{2\pi} + \frac{\pi^2+3}{36\pi N} - \frac{\pi^4+45}{5400\pi N^3} + R_N^A.$$

The second sum in (43) is

$$B = \frac{N}{\pi}\sum_{j=1}^{N-1}\frac{1}{N-j} = \frac{N}{\pi}\sum_{j=1}^{N-1}\frac{1}{j} = \frac{N}{\pi}\left(H_N - \frac{1}{N}\right),$$

where H_N is the N-th harmonic number. Its expansion as $N \to \infty$, see [23], is

$$H_N = \log N + \gamma + \frac{1}{2N} - \frac{1}{12N^2} + R_N^H,$$

where

$$0 < R_N^H < \frac{1}{120N^4}. \tag{45}$$

With these expansions, formula (43) reads

$$\begin{aligned}
-\sum_{j=1}^{N-1}\frac{j}{N}\cot\left(\frac{\pi j}{N}\right) &= -\frac{\log(2\pi)}{\pi}N + \frac{3}{2\pi} + \frac{\pi^2+3}{36\pi N} - \frac{\pi^4+45}{5400\pi N^3} + R_N^A \\
&\quad + \frac{N}{\pi}\left(\log N + \gamma - \frac{1}{2N} - \frac{1}{12N^2} + R_N^H\right) \\
&= \frac{1}{\pi}\left[N\log N + (-\log(2\pi)+\gamma)N + 1 + \frac{\pi^2}{36N} + NR_N^H - \frac{\pi^4+45}{5400N^3} + \pi R_N^A\right].
\end{aligned}$$

Plugging this into the formula (4), we obtain

$$\begin{aligned}
\mathbb{E}[E_2(x_1,\ldots,x_N)] &= \frac{N}{4}\left[N\log N + \left(\frac{3}{2} - \log(2\pi) + \gamma\right)N - \frac{1}{2}\right. \\
&\quad \left. + \frac{\pi^2}{36N} + NR_N^H - \frac{\pi^4+45}{5400}\frac{1}{N^3} + \pi R_N^A\right] \\
&= \frac{N^2\log N}{4} + \frac{1}{4}\left(\frac{3}{2} - \log(2\pi) + \gamma\right)N^2 - \frac{1}{8}N \\
&\quad + \underbrace{\frac{\pi^2}{144} + \frac{N^2R_N^H}{4}}_{C} + \frac{1}{4}\Bigg(\underbrace{-\frac{\pi^4+45}{5400}\frac{1}{N^2} + \pi NR_N^A}_{D}\Bigg).
\end{aligned} \tag{46}$$

Finally, from (45), we have

$$C \leq \frac{\pi^2}{144} + \frac{1}{480N^2} \leq \frac{\pi^2}{144} + \frac{1}{480} < 0.25 \leq \frac{N}{8}$$

for any $N \geq 2$, and $D \leq 0$ because

$$\pi N|R_N^A| \leq \frac{2\pi\zeta(5)}{(2\pi)^5 N^3}\int_0^1 |g^{(5)}(x)|\,dx \leq \frac{2\pi\zeta(5)}{(2\pi)^5 N^3}|g^{(5)}(1)| \leq \frac{\pi^4+45}{5400}\frac{1}{N^2},$$

if $N \geq 2$. This proves (42). ◻

5 Proof of Theorem 1.2

Proof Since the function $F(p,q) = \mathbf{1}_{\{|p-q|\leq t\}}$ is rotational invariant, we can apply the formula (15)

$$\begin{aligned}
&2\mathbb{E}[G(t,X_N)] \\
&= \mathbb{E}\left[\sum_{i\neq j}\mathbf{1}_{\{|p_i-p_j|\leq t\}}\right] = \pi\int_{z\in\mathbb{C},\ \frac{2|z|}{\sqrt{1+|z|^2}}\leq t}\rho_2(z,0)dz \\
&= N^2\int_0^{\frac{t^2}{4-t^2}} \frac{\left((1+x)^N-1-Nx\right)^2(1+x)^{N-2}+\left((1+x)^N-1-Nx(1+x)^{N-1}\right)^2}{((1+x)^N-1)^3}dx,
\end{aligned}$$

where we have applied the change of variables $r=\sqrt{x}$. After a lengthy computation one can compute a primitive of above integral to get

$$\begin{aligned}
&2\mathbb{E}[G(t,X_N)] \\
&= N^2\left(\frac{s}{1+s}-\frac{1}{N}+\frac{s(2+s)}{(1+s)\left((1+s)^N-1\right)}-\frac{Ns^2(1+s)^N}{(1+s)\left((1+s)^N-1\right)^2}\right)
\end{aligned}$$

with $s=t^2/(4-t^2)$ and then (10) follows.

Now we prove inequality (12). In terms of s, since $t^2=4s/(1+s)$, it reads

$$\begin{aligned}
&\frac{N^2}{4}\left(-\frac{2}{N}+\frac{2s}{1+s}+\frac{2s(2+s)}{(1+s)\left((1+s)^N-1\right)}-\frac{2Ns^2(1+s)^N}{(1+s)\left((1+s)^N-1\right)^2}\right) \\
&\leq \frac{N^3s^2}{8(1+s)^2}.
\end{aligned}$$

Then, with the substitution $X=(1+s)^N-1$, we have to show that

$$s-\frac{1+s}{N}+\frac{s(2+s)}{X}-\frac{Ns^2(1+X)}{X^2}\leq\frac{Ns^2}{4(1+s)}$$

and since $s>0$,

$$\frac{s-\frac{1+s}{N}}{Ns^2}+\frac{\frac{2+s}{Ns}-1}{X}-\frac{1}{X^2}\leq\frac{1}{4(1+s)}.$$

Rearranging terms and completing a square we arrive to

$$\left(\frac{1}{X}-\frac{\frac{2+s}{Ns}-1}{2}\right)^2+\frac{1}{4}\left(-\frac{(N-1)^2)}{N^2}+\frac{1}{1+s}\right)\geq 0.$$

If $N\geq 2$ and $s>0$ are such that $-\frac{(N-1)^2)}{N^2}+\frac{1}{1+s}\geq 0$, then the above inequality is trivially satisfied. Let now $-\frac{(N-1)^2)}{N^2}+\frac{1}{1+s}<0$, which is equivalent to $s>\frac{N^2}{(N-1)^2}-1$. We have to show that

$$\left(\frac{1}{X}-\frac{\frac{2+s}{Ns}-1}{2}-\frac{1}{2}\sqrt{\frac{(N-1)^2)}{N^2}-\frac{1}{1+s}}\right)\left(\frac{1}{X}-\frac{\frac{2+s}{Ns}-1}{2}+\frac{1}{2}\sqrt{\frac{(N-1)^2)}{N^2}-\frac{1}{1+s}}\right)\geq 0$$

or, equivalently,

$$\left(\frac{2}{X}+\left(1-\frac{1+\frac{2}{s}}{N}-\sqrt{\frac{(N-1)^2}{N^2}-\frac{1}{1+s}}\right)\right)\left(\frac{2}{X}+\left(1-\frac{1+\frac{2}{s}}{N}+\sqrt{\frac{(N-1)^2}{N^2}-\frac{1}{1+s}}\right)\right)\geq 0.$$

Under the given assumption

$$1-\frac{1+\frac{2}{s}}{N}\geq\sqrt{\frac{(N-1)^2}{N^2}-\frac{1}{1+s}}>0$$

and both factors in the factorization above are non-negative for $X>0$. □

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