Theory of the jamming transition at finite temperature

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I. INTRODUCTION

A wide range of amorphous materials including granular materials, foams, molecular glasses, and colloids exhibit a transition from liquid-like to solid-like behavior. In the solid phase, these materials display anomalous elastic properties. In particular, amorphous solids universally present an excess of vibrational modes over the Debye model (that treats vibrational modes as plane waves), a phenomenon referred to as the “boson peak.”\(^1\) The boson peak affects various properties of the solid, including heat transport\(^2–6\) as well as the spatial heterogeneity of the elastic response.\(^7–10\) Its presence indicates that glasses lie close to an elastic instability, suggesting a connection with the glass transition where rigidity emerges.\(^11,12\) For these reasons, this phenomenon is intensely studied.\(^13\)

It was proposed that in a variety of glasses,\(^14,15\) the boson peak is controlled by some aspects of the short-range microscopic structure, in particular, a measure of the particle connectedness\(^16–18\) as well as the characteristic force with which nearby particles interact,\(^19,20\) both well-known to affect the stability of engineering structures.\(^21\) Detailed predictions on transport and sound dispersion can be made in this framework,\(^15\) which have been recently supported by experiments.\(^22\) In this approach, particles interacting via a purely repulsive potential at zero temperature,\(^23–25\) are predicted to display singular vibrational properties: the spectrum has a characteristic frequency \(\omega_0\) satisfying \(\omega_0^2 \sim z \sim z_c\) near the jamming transition,\(^13\) as confirmed numerically.\(^13\) Here, \(z\) is coordination, measured by the average number of contacts per particle, and \(z_c = 2d\) is the minimal coordination for mechanical stability in dimension \(d\), the so-called Maxwell threshold. The boson peak frequency \(\omega_{BP}\), however, is essentially zero, with \(\omega_{BP} \ll \omega_0\) indicating that the system is marginally stable\(^20\) and implying that \(z - z_c \sim \sqrt{\phi - \phi_c}\), where \(\phi_c\) is the jamming packing fraction where pressure vanishes (that can depend on the configuration considered).

Since, in practice, interaction potentials are always anharmonic (AH), one may question if these results survive at finite temperature.\(^30,31\) Hard spheres (HS), arguably the simplest glass former, are a particularly challenging case for which the potential is discontinuous, implying that the Hessian of the energy (whose eigenvectors correspond to the normal modes) is not well-defined. However, it was argued that a coarse-grained free energy can be computed in that case\(^32–34\) if one can find times \(\tau\) such that \(\tau_c \ll \tau \ll \tau_r\), where \(\tau_c\) is a microscopic collision time and \(\tau_r\) is the relaxation time of the structure (this condition is always achieved in the glass phase). This free energy captures the volume of phase space around a given meta-stable state (or “vibrational entropy”) and can always be expressed in terms of the mean particle position within a meta-stable state. This approach leads to an effective interaction \(V_{\phi\phi}\) between particles, which is in general multi-body. Near the jamming point, however, this interaction is simply two-body (as recalled below) and only occurs between particles interacting (i.e., colliding) on the intermediary time \(\tau\), leading to the definition of a contact network and allowing to extend the notion of coordination to hard spheres. The Hessian of the coarse-grained free energy describes the linear response, in particular, how small external forces affect the mean particle positions. Its eigenvectors define normal modes whose thermal fluctuations are inversely proportional to their associated eigenvalue, as confirmed numerically.\(^35\)

Theoretical arguments using such an effective potential were used to predict scaling properties of the spectrum of the Hessian, as well as spatial properties of the eigenvectors.\(^33,34\) One finds that the normal modes slightly differ from the soft (S) sphere case: in both cases, modes are extended and heterogeneous, but for hard spheres, soft modes tend to distort a small amount of bonds (which are weak),...
whereas for soft spheres, modes tend to distort all the bonds in the system. We thus coin hard-sphere soft modes as sparse, whereas for soft spheres, we keep the previously used terminology of anomalous modes. This distinction leads to a small but detectable difference in vibrational properties. For the coordination, it was predicted that $z - z_c \sim (\phi_c - \phi)^{0.34.41}$. Other predictions, such as for the mean-squared displacement, were found to agree with recent replica calculations in infinite dimensions, supporting the validity of the two approaches.

The asymmetry between soft and hard spheres apparent in the scaling of coordination is surprising, since one can go continuously from one case to the other by considering soft spheres and by allowing to vary both $\phi$ and $T$.

II. EFFECTIVE POTENTIAL

A. Derivation

We consider a system of $N$ soft spheres at constant pressure $p$ that is fluctuating around a metastable state. Thermal averages taken around this state are written by $\langle \cdot \rangle$, while averages over the contacts will be denoted by $\langle \cdot \rangle$. We assume that the coordination of the network of interacting particles is $z_c = 2d$, i.e., the system is isostatic, as is the case at the jamming transition $p,T \to 0$. The computation of the vibrational free energy in such a meta-stable state is detailed in Appendix A, and here we sketch the argument. Isostaticity implies that the number of degrees of freedom in the particle displacements $\{ \delta r_i \}$, $dN$, is precisely equal to the number of contacts, $N_C = zN/2$. Thus, the partition function of the metastable state, originally an integral over the displacements $\{ \delta r_i \}$, can be written as an integral over the gaps $\{ h_u \}$ between contacting particles (with $h_u < 0$ for overlap). Assuming that all $|\delta r_i| \ll 1$, the map from $\{ \delta r_i \}$ to $\{ h_u \}$ is linear.

To compress or dilate the system from a volume $V_e$ (where all particles are just touching) to $V$ requires work $W = -p(V - V_e)$. Stability implies that the time-averaged forces $f_a$ between particles satisfy force balance; this can be written as $W = -\sum_a f_a h_a$, where the sum is over all contacts $a$ of the metastable state, and we have used the virtual work principle. Since $W$ and the elastic energy $U$ are sums from different contacts (we consider only pair potentials), this leads to a single-gap partition function:

$$Z(\beta,f) = e^{-\beta U(h)} e^{-\beta f h},$$

where the force $f$ fixes the time-averaged gap $\langle h \rangle$ through $\langle h \rangle = \partial G/\partial f$, and $\beta = 1/(k_B T)$. The effective potential $V_{\text{eff}}$ is obtained by a Legendre transform $V_{\text{eff}}(\langle h \rangle) = G(f - f(h))$, from which it follows that $f = -\partial V_{\text{eff}}(\langle h \rangle)/\partial \langle h \rangle$. We consider a finite-range harmonic potential $U(h) = \frac{1}{2} \epsilon |h|/\sigma^2$ when $-\frac{1}{2} \epsilon \tau < h < 0$ and 0 otherwise. We now take units in which $\epsilon = \sigma = k_B = 1$. As described in Appendix A, it is simple to analytically extract the limiting behavior: when $f \ll \sqrt{T}$, $\langle h \rangle \approx T/\tau$, whereas when $f \gg \sqrt{T}$, $\langle h \rangle \approx -f$. These correctly reduce to the effective hard-sphere potential from Refs. 32 and 33 in the small-force limit and the original harmonic potential in the large-force limit, respectively, and moreover they indicate the cross-over scales. In the intermediate regime, $|\langle h \rangle| \leq \sqrt{T}$, there is a smooth cross-over between these behaviors.

Since our goal is to obtain scaling behavior, it is convenient to have a simple form that incorporates the salient features of $V_{\text{eff}}$, without adding extra structure. The simplest is the one satisfying $\langle h \rangle = -f + T/f$, which leads to an effective force law

$$f(h) = -\frac{1}{2} \langle h \rangle + \frac{1}{2} \sqrt{\langle h \rangle^2 + 4T},$$

from which we can compute the effective potential $V_{\text{eff}}(\langle h \rangle) = -\frac{1}{2} \langle h \rangle f(\langle h \rangle) - T \log(\langle h \rangle + \sqrt{\langle h \rangle^2 + 4T})$ and stiffness

$$k(h) \equiv \frac{df}{dh} = \frac{1}{2} \frac{\langle h \rangle}{\sqrt{\langle h \rangle^2 + 4T}}.$$
TABLE I. Regimes of the soft-sphere glass. Shown is the scaling behavior of pressure $p$, typical time-averaged gap $(h)$, characteristic frequency $\omega^*$, mean-squared displacement $\langle \delta R^2 \rangle$, intra- and shear modulus $\mu$, and correlation length of the normal modes $h_s(\omega^*)$ versus temperature $T$ and volume fraction deviation $\delta \phi = \phi - \phi_c$. As discussed in the main text, the soft regime contains a transition at a nontrivial temperature scale $T^* \sim \delta \phi^{(2+2\theta_e)/(2+4\theta_e)} \sim \delta \phi^{-2}$, invisible in the effective potential and equation of state (and therefore $p$ and $(h)$), but strongly affecting vibrational properties. The exponents $\kappa = (4 + 2\theta_e)/(3 + \theta_e) \approx 1.41$ and $a = (1 - \theta_e)/(3 + \theta_e) \approx 0.17$, where $\theta_e = 0.42$ characterizes the force distribution of “extended” contacts at jamming.26–29

<table>
<thead>
<tr>
<th>Regime</th>
<th>$T$</th>
<th>$\delta \phi$</th>
<th>$p$ $\propto (\delta \phi)^{1/2}$</th>
<th>$h$ $\propto (\delta \phi)^{1/2}$</th>
<th>$\omega^*$ $\propto (\delta \phi)^{1/2}$</th>
<th>$\langle \delta R^2 \rangle$ $\sim (\delta \phi)^2$</th>
<th>$\mu$ $\sim (\delta \phi)^{-2}$</th>
<th>$h_s(\omega^*)$ $\sim (\delta \phi)^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hard-sphere (HS)</td>
<td>$T &lt; \delta \phi^2$</td>
<td>$\delta \phi &lt; 0$</td>
<td>$T/</td>
<td>\delta \phi</td>
<td>$</td>
<td>$</td>
<td>\delta \phi</td>
<td>$</td>
</tr>
<tr>
<td>Soft-zero-T (S0)</td>
<td>$T' &lt; T &lt; \delta \phi^2$</td>
<td>$\delta \phi &gt; 0$</td>
<td>$\delta \phi$</td>
<td>$-\delta \phi$</td>
<td>$\delta \phi^{1/2}$</td>
<td>$T</td>
<td>\delta \phi</td>
<td>^{1/2}$</td>
</tr>
<tr>
<td>Soft-entropic (SE)</td>
<td>$T &lt; T'$</td>
<td>$\delta \phi &gt; 0$</td>
<td>$\delta \phi$</td>
<td>$-\delta \phi$</td>
<td>$\delta \phi^{1/2}$</td>
<td>$T</td>
<td>\delta \phi</td>
<td>^{1/2}$</td>
</tr>
<tr>
<td>Anharmonic (AH)</td>
<td>$T \gg \delta \phi^2$</td>
<td>$\sqrt{T}$</td>
<td>$\sqrt{T}$</td>
<td>$T^{1/4}$</td>
<td>$T^{1/4}$</td>
<td>$T^{1/4}$</td>
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The effective stiffness is plotted in Fig. 2(a), showing an entropic smoothing as $T$ is increased from zero. In the Introduction, it was argued that the effective potential can be measured by displacement covariances using the usual harmonic formula.31 To test this claim explicitly, in Fig. 2(b), we reproduce the effective stiffness $k_{\text{eff}}$ extracted from displacement covariances in Ref. 31 from numerical simulations of a thermal soft-sphere system in $d = 2$. A very good qualitative agreement is obtained, with no fitting parameters. Moreover, in Ref. 31, it was observed that by varying $\delta \phi = \phi - \phi_c$ from $\approx -0.02$ to $+0.05$, the effective stiffness function $k_{\text{eff}}(\phi)$ remained constant, and the different systems merely sampled different ranges of $(h)$; this feature is reproduced by Eq. (3), which has no explicit dependence on $\phi$. This observation supports that corrections to the effective potential away from isostaticity are small in this range of $\delta \phi$, as was checked previously for hard spheres.32

B. Force distribution

The disordered geometry of the metastable state is characterized by the statistics of time-averaged particle positions, which determines in turn the distribution of forces between particles. In Ref. 47, the force distribution in packings of frictionless particles at jamming was found to be singular,

$$P(f) \propto f^{\theta_e} e^{-f/f_0}.$$  \hspace{1cm} (4)

as confirmed by several numerical studies.26,29,34,48 Note that the exponential tail was observed earlier in Ref. 49 but is not crucial; a Gaussian cut-off would not change our scaling predictions below. The singularity at small $f$ was shown to be necessary for the stability of packings toward rewiring of their contact network.26,60 More precisely, contacts need to be classified in two groups. Local contacts have very little mechanical coupling with their surroundings, and their density follows Eq. (4). Extended contacts are coupled to their surroundings, and their density follows

$$P_e(f) \sim f^{\theta_e} e^{-f/f_0}.$$  \hspace{1cm} (5)

The latter are less numerous at low force, i.e., $\theta_e > \theta_f$, but more important for our purpose.31 Marginal stability of packings implies

$$\theta_f = \frac{\theta_e}{2 + \theta_e}$$  \hspace{1cm} (6)

in agreement with numerics indicating $\theta_f \approx 0.17$ and $\theta_e \approx 0.44$. Replica calculations27,28,53,54 in $d = \infty$ do not predict $\theta_f$ but yield $\theta_e = 0.4231 \ldots 28$ consistent with the value extracted from numerical observations in finite dimensions.

In what follows, we assume that the distribution of Eq. (5) holds true in the vicinity of the jamming transition. Note that away from the Maxwell point, $P_e(f)$ develops a plateau at small force.28,48 For simplicity, we neglect this plateau in our arguments, since as shown previously in the hard sphere regime,34 it is not expected to affect our results.

Assuming Eq. (4) with $\theta_f = 0.175$ and the effective potential, Eq. (2) immediately yields a prediction for the time-averaged gap distribution, as a function of $f_0$ and $T$. Using the equation of state derived below, this can be written as a function of $\delta \phi$, plotted in Fig. 3(a) at $T = 10^{-6}$. As $\delta \phi$ is varied, the distribution has a complex evolution. Comparing this to numerical results from Ref. 31, plotted in Fig. 3(b), again a very good qualitative agreement is obtained, with no fitting parameters. Moreover, the scaling behavior of $P(h)$ can easily be extracted. One finds, in particular, that $P(h)$ has a maximum at $h^* \sim \langle h \rangle$, where $\langle h \rangle$ denotes the average value.
over contacts, i.e., with respect to Eq. (4). By averaging \( \langle h \rangle = -f + T/f \) over contacts, the mean gap is

\[
\langle h \rangle = -(1 + \theta T) f_0 + T/\langle f_0 \theta T \rangle.
\]

(7)

The height of the maximum of \( \langle h \rangle \) scales as \( \langle h^\dagger \rangle \sim (f_0 + T/f_0)^{-1} \).

From \( \langle h \rangle \), one can also extract the instantaneous coordination \( z_{\text{inst}} \) by \( z_{\text{inst}} / z = \int_0^1 dh \langle h \rangle \). The result is that in most of the phase diagram, \( z_{\text{inst}} < z_c \); the system is instantaneously hypostatic. However, the instantaneous coordination is not the correct variable to characterize stability and vibrational properties—this role is played by the coordination coarse-grained in time.

**C. Equation of state**

The effective potential and force distribution also imply the equation of state. The Irving-Kirkwood expression for the stress tensor\(^5\) gives its contact contribution as \( p V/\langle h \rangle = \langle 1 + h \rangle f \), whose thermal average is \( p V/\langle h \rangle = \langle 1 + h \rangle f \). Meanwhile, mechanical stability of the metastable state allows to write the work done in compression from \( V_c \) in terms of forces and gaps. The latter expression, the virtual work principle derived in Appendix A, equates \( p V/\langle h \rangle \) to its microscopic expression \( N_c \langle h \rangle \). The thermal average is \( p V/\langle h \rangle = \langle 1 + h \rangle f \). Subtracting these expressions, we find \( p V_c/\langle h \rangle = \langle 1 + h \rangle f_0 \), using Eq. (4). Similarly, we use the effective potential \( \langle h \rangle = -f + T/f \) and Eq. (4) to evaluate \( \langle h \rangle = \langle 1 + h \rangle f_0 + T \). Substituting this into the virtual work principle and simplifying with \( \langle V \rangle = V \) and \( V_c - V = \phi/\phi \), valid in the thermodynamic limit, we find eventually the equation of state

\[
P \left( \frac{V_c}{1 + \theta T} \right)_{N_c} = f_0 \frac{c_1 T \phi^2}{2 \phi^2 + c_1 (1 + \theta T)}.
\]

(8)

where \( c_1 = 4(2 + \theta T)(1 + \theta T) \). Note that \( \langle h \rangle = (1 + \theta T) f_0 \).

**III. VARIATIONAL ARGUMENTS**

**A. Density of states**

The effective potential defines a harmonic shadow system whose density of vibrational states, \( D(\omega) \), can be bound with a variational argument.\(^14\) We follow Ref. 34, sketching only the salient modifications from the \( T \to 0 \) arguments presented there.

The shadow system is equivalent to an elastic network with a fixed time-averaged coordination \( z \geq z_c \). Our goal is to construct normalized trial displacement fields with a small elastic energy \( E \) as measured by the stiffness matrix of the elastic network. It is customary to use the notation \( E = \omega^2 \), although our predictions, based on thermodynamics, apply both to over-damped Brownian particles and inertial ones.

If \( Q \) orthonormal modes per unit volume can be found with a characteristic frequency \( \omega \), a variational inequality implies that\(^17\) \( D(\omega) \geq Q/\omega \), where here and in the remainder of this section, we ignore unimportant constants. To construct trial modes, a useful Ansatz near the Maxwell point is to cut a fraction \( q \ll 1 \) of bonds, creating a density \( q - \delta z / z_c \) of floppy (i.e., zero-energy) modes in the cut system. These floppy modes have motion transverse to all bonds, but motion parallel to bonds \( \textit{only} \) at the cut bonds. In the original, uncut system, these modes compress or extend springs at the cut bonds, but a judicious choice of cut bonds can lead to small energy and an optimal bound on \( D(\omega) \). Two Ansätze have proven useful: one that creates “anomalous” modes,\(^17\) and another that creates “sparse” modes.\(^34\) First, we suppose that the springs are at their rest length.

**B. Anomalous modes**

As discussed in Ref. 14, trial modes can be created by cutting bonds along blocks of size \( L \sim 1/q \gg 1 \) (see Fig. 4(a)). The induced floppy modes have large motions at the cut bonds; by modulating these modes with plane waves with nodes at the cut bonds, the resulting trial modes have a small frequency \( \omega \sim q/\sqrt{k} \). It turns out that in the regimes where anomalous modes can dominate the low-frequency spectrum, \( k \sim 1 \) and \( \omega \sim q \). This leads to a bound,

\[
D(\omega) \geq \omega^0 \equiv D_a(\omega),
\]

(9)

valid above the characteristic frequency \( \omega_a \sim \delta z \). This is sketched in Fig. 5(a). Since this argument is purely geometrical, it applies without change in the case of an effective potential, as considered here.
C. Sparse modes

The second Ansatz, discussed in Ref. 34, creates trial modes that only extend and compress a fraction $q$ of the weakest bonds; we call these modes “sparse.” The trial modes created by cutting these contacts have a characteristic stiffness $k_c$ and characteristic force $f_c$, satisfying $q = f_c k_c$. This leads to $f_c \sim p q^{1/(1+\theta_e)}$. From Eqs. (2) and (3), we find $k_c \sim p^2 q^{2/(1+\theta_e)} / (T + p^2 q^{2/(1+\theta_e)})$, so that the elastic energy of the trial modes is $E \sim q k_c$. These two scales are the only ingredients needed from the effective potential of Sec. II; in particular, the equation of state does not directly affect the trial modes.

Although, in principle, both localized and extended contacts could be cut, it was checked in Ref. 34 that only the extended contacts give a useful bound for hard spheres. We therefore use only them here, taking $\bar{\mathcal{P}}(f)$ from Eq. (5).

To obtain a useful bound from this Ansatz, the characteristic stiffness must be small; in particular, we must have $T/p^2 \gg q^{2/(1+\theta_e)}$ (otherwise $k_c \sim 1$). This can be written as $q \ll q_T$ with $q_T \sim (T^{1/2} / p)^{1+\theta_e}$. In this case, the modes have a characteristic frequency $\omega(q) \sim \sqrt{E} \sim \sqrt{q k_c} \sim p q^{1/(4b)} T^{-1/2}$, and the variational inequality gives

$$D(\omega) \gtrsim (T/p^2)^{2b} \omega^{-a} \equiv D_{\omega}(\omega),$$

with $a = (1 - \theta_e) / (3 + \theta_e)$, $b = (1 + \theta_e) / (6 + 2\theta_e)$.

as obtained previously for hard spheres. This holds for any $q \gg \delta z$, implying that $\omega \geq \omega_s$ with

$$\omega_s \approx (p/\sqrt{T}) \delta z^{1/4b}.$$  

D. Optimal bound

At finite $T$, both “anomalous” and “sparse” bounds are useful, in different parts of the phase diagram and different frequency ranges. The optimal bound on $D(\omega)$ is simply whichever is larger of Eqs. (10) and (9),

$$D(\omega) = \max(D_{\omega}(\omega), D_{\omega_a}(\omega)).$$

Accordingly, the characteristic frequency of the lowest-frequency modes is $\omega^* = \min(\omega_a, \omega_s)$. The equality $\omega_a = \omega_s$ defines a characteristic temperature,

$$T^* \sim p^2 \delta z^{a/2b},$$

and therefore two cases:

Case $T < T^*$: the vibrational spectrum is dominated by anomalous modes and the density of states is flat, as occurs at zero temperature for soft particles.

Case $T > T^*$: the lowest soft modes are sparse-like. However since Eq. (10) is a decreasing function of $\omega$, eventually Eq. (10) yields $D(\omega) \gtrsim 1$, and the bounds coincide. This occurs at a frequency,

$$\omega_T = (T/p^2)^{2b/a}.$$  

So the vibrational spectrum contains both features: for $\omega_s \ll \omega \ll \omega_T$, $D(\omega)$ is hard-sphere like and decays as a power-law of frequency. However it becomes flat for $\omega_T \lesssim \omega \lesssim 1$. We include in the latter case, the possibility that $\omega_T \sim 1$, in which case the flat regime is not visible. These two behaviors of $D(\omega)$ are sketched in Fig. 5, and the phase diagram is shown in Fig. 6.
E. Coordination and marginal stability

The coordination $z$ is a natural variable to describe vibrational properties, but it is generally not experimentally accessible. Here, we relate it to $T$ and $p$ by considering that the system is marginally stable, as previously argued from dynamical considerations and as confirmed by replica calculations in infinite dimension. The elastic energy of a spring network under compression has two components: a positive (stabilizing) one, due to motion parallel to springs, and a negative (destabilizing) one, due to motion transverse to springs. Marginal stability implies that for the softest sparse or anomalous modes, the destabilizing transverse part of the elastic energy is of the order of the stabilizing part. The most unstable (anomalous or sparse) trial modes used to bound $D(\omega)$ are those at frequency $\omega^*$, with energy $\omega^*$.

We thus get $\omega^* \sim \sqrt{p}$. This sets $\delta z$ and $T^*$

\[ \delta z \sim \left( \frac{\omega^*}{p} \right)^{1/2} T > T^* \]

and

\[ T^* \sim p^{1-\alpha}. \]

F. Mean-squared displacement

These results yield a bound on the particles’ mean-squared displacement ($\langle \delta R^2 \rangle$),

\[ \frac{\langle \delta R^2 \rangle}{T} = \int \frac{D(\omega)}{\omega^2} d\omega > \int_{\omega > \omega^*} \frac{D(\omega)}{\omega^2} d\omega > \begin{cases} \left( \frac{T}{p} \right)^{1/2} \omega^* & T > T^* , \\ \omega^* & T < T^* . \end{cases} \]

The results (20) and (25) display a striking asymmetry: the nontrivial temperature scale $T^*$, although it can be defined both above and below jamming, plays no role in the latter case. Physically, this is because when $\delta \phi > 0$, there must be a temperature scale where the softest modes transition from “anomalous” to “sparse,” whereas when $\delta \phi < 0$, the softest modes are always “sparse.”

\[ \langle \delta R^2 \rangle \gtrsim \frac{T}{\omega^*} \]

The scaling predictions of Sec. III can be derived and extended with EMT, a mean-field approximation to self-consistently treat disorder. Although EMT is formulated at $T = 0$, an effective potential facilitates its use at any $T$. An arbitrary distribution of disorder is allowed: here, we assume that forces are distributed as Eq. (5), as in the variational bounds above. We follow the same procedure as our previous works, discussing all details in Appendix B.

In addition to reproducing the previous results, with values for prefactors, EMT also gives the behavior of the shear modulus and density of states at all $\omega \ll 1$. Here, we focus on the results for $d = 3$ at marginal stability, and only work to leading order in $\delta z$. By numerical solution of the EMT equations at marginal stability, we obtain $\delta z(T, \phi)$, plotted in Fig. 7. The asymmetry between $\delta \phi > 0$ and $\delta \phi < 0$ is clearly visible. A curious feature is that at fixed $T$, $\delta z$ has a minimum at a finite $\delta \phi$. The effective medium predictions of Sec. III can be derived and extended with EMT, a mean-field approximation to self-consistently treat disorder. Although EMT is formulated at $T = 0$, an effective potential facilitates its use at any $T$. An arbitrary distribution of disorder is allowed: here, we assume that forces are distributed as Eq. (5), as in the variational bounds above. We follow the same procedure as our previous works, discussing all details in Appendix B.

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The EMT prediction for $D(\omega)$ is plotted in Fig. 8(a). Above $\omega^*$, it behaves as described in the foregoing text. Below $\omega^*$, we find $D(\omega) \sim \omega^2$; we note that our previous work\textsuperscript{34} erroneously predicted $D(\omega) \sim \omega^{2+\alpha}$ in this regime: an incorrect approximation was used to obtain scaling behavior below $\omega^*$, affecting only this prediction.

EMT predicts that the zero-frequency shear modulus $\mu \propto -\delta z + \sqrt{\delta z^2 + Cp}$, for a constant $C$. It can be checked that in all cases $p \lesssim \delta z^2$, so that

$$\mu \sim p/\delta z,$$

consistent with arguments presented earlier in the $T \to 0$ limit,\textsuperscript{34,62-64} and with the replica theory.\textsuperscript{65} This implies

$$\mu \sim \begin{cases} \delta \phi^{1/2} & (S0) \\ \delta \phi T^{1-x} & (SE) \\ T\delta \phi^{1-x} & (HS) \\ T^{1-z} & (AH) \end{cases}$$

plotted in Fig. 8(b). In all cases, we find

$$\mu(\delta R^2) \sim T.$$

We note that this shear modulus only describes relaxation within a metastable state.

Finally, EMT predicts the spatial correlation of mode displacements, $\ell_s(\omega)$. For $\omega \gtrsim \omega^*$, we find $\ell_s(\omega) \sim 1/\sqrt{\omega D(\omega)}$, leading to

$$\ell_s(\omega^*) \sim \begin{cases} \delta \phi^{1/2} & (S0) \\ (T/\delta \phi)^{\nu+1} & (SE) \\ |\delta \phi|^{\nu+1} & (HS) \\ T^{\nu+1} & (AH) \end{cases}.$$

In principle, $\ell_s$ can be measured by static response, as shown previously for $T = 0$ soft solids.\textsuperscript{26}

VI. COMPARISON WITH SIMULATIONS AND EXPERIMENTS

Packings of soft harmonic spheres at finite temperature have been studied numerically by several groups.\textsuperscript{30,31,36-41} A major goal of these works, particularly Refs. 30, 31, and 39, was to show that vibrational properties become strongly anharmonic as packings are heated. As evidence, it was observed in Refs. 30, 31, and 39 that as a jammed solid at $\delta \phi > 0$ is heated, the plateau in $D(\omega)$ develops a negative slope at low frequency. We have shown that this phenomenon can be understood within a harmonic effective theory and simply reflects the increasing importance of weak contacts (and therefore “sparse” modes) as the effective potential develops a small-force thermal tail.

In Refs. 38, 39, and 41, the three simple regimes HS, S, and AH were observed, with the scaling $T \sim |\delta \phi|^2$ predicted here.\textsuperscript{66} However, neither of these works found the subtle distinction between S0 and SE regimes. Because the temperature scale $T \sim |\delta \phi|^{2.20}$ (using $\theta_e = 0.42$) is close to $\delta \phi^2$, precise measurements of $D(\omega)$, $\langle \delta \phi^2 \rangle$, or $\mu$ are needed to test our predictions. However, our non-trivial prediction on the shape of the density of states (which can present a plateau or a power-law decay depending on the control parameters and the frequency) appears to be confirmed numerically, see, e.g., Fig. 2 in Ref. 39 and Fig. 3 in Ref. 38.

Several colloidal experiments have aimed at measuring finite-temperature vibrational properties near jamming.\textsuperscript{34,45,67} although these observations may not be close enough to the critical point to obtain accurate exponents.\textsuperscript{39,68} However, recent experiments on granular media\textsuperscript{69,70} may probe this regime, albeit in the presence of friction. In Refs. 69 and 70, heterogeneity associated with dynamics of contacts was used to infer Widom lines emerging from a common point at $T = 0, \phi = \phi_0$, consistent with the results of this work. A more detailed comparison could be possible by computing dynamical susceptibility, along the lines of Ref. 39.
VII. CONCLUSION

We have proposed a description of the vibrational properties of thermal soft spheres near the jamming transition, based on a real-space description of soft vibrational modes. These modes are of two types—sparse and anomalous—depending on packing fraction, temperature, and the frequency considered. Our work shows that even when anharmonicities are extremely strong, they can be tamed by time-averaging, allowing one to define an effective potential from which static linear response and thermal fluctuations can be computed. Ultimately, all our scaling predictions can be expressed in terms of one exponent θ, characterizing forces in jammed packings, which can be extracted numerically.

θ is also very well estimated by replica calculations in infinite dimensions.26 In the hard sphere case (φ < φc, T → 0), such calculations lead to identical results for the mean-square displacement28 and the elastic modulus.65,71 However, this approach currently neither fixes the exponents for soft spheres,66 nor does it access the shape of the vibrational spectrum nor the length scale characterizing normal modes. It would be very interesting to extend the replica method to these questions, enabling a full comparison with the present results.

Although we have focused on the proximity of the jamming transition, we expect our description based on an effective potential to be qualitatively appropriate away from it. For example, if the packing fraction is decreased (or the temperature increased), an elastic instability is expected to occur10,15,33 near the glass transition where configurations become unstable. Denoting φ0 such a packing fraction, effective medium15 predicts that the elastic modulus jumps and displays a square-root singularity at that point μ ≈ μ0 + Cφ/φ0, also as found in mode coupling theory,72,73 replica theory,65,71 and the random-first-order-transition scenario.74 Furthermore, numerics support that an elastic length scale diverges in two dimensions as10 l_c ∼ 1/(φ - φ0)1/4 and therefore decreases as the system enters the glass phase. We expect these behaviors to be smoothed to some extent, since in the vicinity of the glass transition, the separation of time scales required to define an effective potential disappears. Direct extraction of elastic length scales as a function of packing fraction or temperature would be very informative to test this prediction.

Finally, one may wonder what happens to the soft sphere phase diagram when the system is driven by an imposed shear. For T = 0 and φ < φc, it has been shown that the dynamics of over-damped hard spheres is governed by an operator whose low-energy modes are of the anomalous type,47 so that velocity correlations decay primarily on a length scale ℓ_c ∼ 1/√ω_c ∼ μ independent of φc.55,76 It would be interesting to see if the notion of effective potential could be used to extend such considerations to finite temperature, a path recently proposed in Ref. 77.

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APPENDIX A: EFFECTIVE POTENTIAL

In these appendices, we (A) derive the effective potential, and (B) describe the effective medium theory.

Here, we derive, in more detail, the effective potential used in the main text. We consider a system of N soft spheres at constant pressure p that is fluctuating around an isostatic metastable state. The latter has a Gibbs partition function

\[ Z(p, β) = \int D\delta r e^{-βpV} e^{-βU}, \]  

(A1)

where U is elastic energy, V is volume, p is pressure, \( \int D\delta r \equiv \prod_i \int d\delta r_i, \) and \( β = 1/(k_B T) \). The displacements \( \delta r_i \) are with respect to a configuration in which all particles are just touching, at volume \( V_c \).

Metastability of the state is interpreted to mean that although the state may have a finite lifetime, the time-averaged positions of the particles are in force balance. Then, there exist contact forces \( \{ f_a \} \) balancing the external forces \( \{ F_i \} \),

\[ f_a = \sum_{a} f_a(\bar{n}_a), \]  

(A2)

for each \( i \), where \( \langle \bar{n}_a \rangle = (\bar{r}_j - \bar{r}_i)/(\{\bar{r}_j - \bar{r}_i\}) \) is the time-averaged contact vector. Summing over all particles and contracting with an arbitrary displacement field, we get an expression for the work done in the displacement field,

\[ W = \sum_{i} F_i \cdot \delta r_i = -\sum_{a} f_a(\bar{n}_a) \cdot (\delta r_j - \delta r_i) = -\sum_{a} f_a(h_a + O(h_a^2)), \]  

(A3)

the virtual work principle.46 Here, we have defined the gap \( h_a \) between particles, \( h_a = \bar{n}_a \cdot (\delta r_j - \delta r_i) \) (with \( h_a < 0 \) for overlap). The error in Eq. (A3) comes from the deviation of time-averaged contact vectors from instantaneous ones; this is small if particle displacements are also small, \( |\delta r_i| \ll 1 \). Because of isostaticity, each force \( f_a \) in this expression can be written as \( f_a = p f_a \), where \( f_a \) is fixed on the mesoscopic time \( \tau \) and depends on the time-averaged positions of the particles. The pressure simply sets the force scale.

Isostaticity implies that the number of degrees of freedom in the particle displacements \( \{ \delta r_i \} \), dN, is precisely equal to the number of contacts, \( N_c = z N/2 \). Thus, Eq. (A1), originally an integral over the displacements \( \{ \delta r_i \} \), can be written as an integral over the gaps \( \{ h_a \} \) between contacting particles, i.e.,

\[ Z(p, β) = \int D h J e^{-βpV} e^{-βU}, \]  

(A4)
We see that the behavior of Eq. (A9) depends on the scaling \( \beta \), strictly, each gap \( h_\alpha \) should be bounded from above by some nontrivial function of the positions of the rest of the particles. However, since we are only interested in small displacements, we ignore this fact and let the upper limit on each \( h_\alpha \to \infty \): large gaps are strongly suppressed by the Boltzmann factor. (A posteriori, one can check the smallness of temperature needed for gaps to remain \( \ll 1 \).) Finally, we are led to a single-gap partition function,

\[
Z(\beta, f) = e^{-\beta G} = \int df e^{-\beta U(h)} e^{-\beta f h},
\]

where the force \( f \) fixes the time-averaged gap \( \langle h \rangle \) through \( \langle h \rangle = \partial G / \partial f \). The effective potential \( V_{\text{eff}} \) should be a function of the time-averaged gap \( \langle h \rangle \); we define it by Legendre transform \( V_{\text{eff}}(\langle h \rangle) = G(f) - f \langle h \rangle \), from which it follows that \( f = -\partial V_{\text{eff}}(\langle h \rangle) / \partial \langle h \rangle \), as desired. We consider a finite-range harmonic potential \( U(h) = \frac{1}{2} e |h| \sigma^2 \) when \( -\frac{1}{\sqrt{\beta}} \sigma < h < 0 \) and 0 otherwise. We now take units in which \( e = \sigma = k_B = 1 \).

Equation (A6) and \( f = -\partial V_{\text{eff}}(\langle h \rangle) / \partial \langle h \rangle \) define implicitly the effective potential. For our choice of \( U(h) \), we obtain an error function,

\[
Z = \int_0^\infty dh e^{-\beta f h} + \int_{-1/\sqrt{\beta}}^0 dh e^{-\beta f h} e^{-1/2|h|^2} = \frac{1}{\beta f} + \frac{1}{\sqrt{\beta}} e^{1/2 \beta f^2} \int_{\sqrt{\beta} f}^{1/2} dz e^{-z^2}. \tag{A7}
\]

We are interested in \( \beta \to \infty \) so \( \sqrt{\beta} (f - 1/\sqrt{2}) \approx -\infty \). Then, the equation defining the effective potential is

\[
\beta(h) = -\frac{\partial \ln Z}{\partial f} = -\frac{1}{Z} \left[ -\frac{1}{\beta f^2} + 1 + \beta^{1/2} f e^{1/2 \beta f^2} \int_{-\infty}^{\sqrt{\beta} f} dz e^{-z^2} \right] \tag{A9}
\]

We see that the behavior of Eq. (A9) depends on the scaling variable \( \sqrt{\beta} f \). When \( \beta f^2 \gg 1 \), the contact term dominates, while when \( \beta f^2 \ll 1 \), the entropic term dominates. The integral is always \( O(1) \), so we approximate it by \( \sqrt{\beta} f / 2 \).

**Entropic regime:** Let \( \beta f^2 \ll 1 \). Then, \( Z \approx 1 / (\beta f) \) and

\[
\langle h \rangle \approx \frac{1}{\beta f}. \tag{A10}
\]

This recovers the hard-sphere effective potential derived in Ref. 33. It holds when \( f \ll 1 / \sqrt{\beta} \) or \( \langle h \rangle \gg 1 / \sqrt{\beta} \).

**Contact regime:** Let \( \beta f^2 \gg 1 \). Then, \( Z \approx \sqrt{\pi \beta} / 2 e^{1/2 \beta f^2} \) and

\[
\langle h \rangle \approx -f. \tag{A11}
\]

This recovers the original harmonic potential. It holds when \( f \gg 1 / \sqrt{\beta} \) or \( \langle h \rangle \ll -1 / \sqrt{\beta} \).

Therefore, there is a characteristic scale \( 1 / \sqrt{\beta} = \sqrt{T} \) both for gaps and overlaps. We cannot analytically solve the equations in the nontrivial regime \( -\sqrt{T} < \langle h \rangle < \sqrt{T} \) but there is a smooth cross-over (for example, there is no \( f \) with \( d\langle h \rangle / df = 0 \), since \( d\langle h \rangle / df \approx -((\langle h \rangle - \langle h \rangle)^2) < 0 \)).

In the main text, we want to use \( V_{\text{eff}} \) to obtain scaling behavior of vibrational properties; we can do so by replacing the cumbersome implicit expression with a simple form that incorporates the correct limiting behavior. The simplest is the one satisfying \( \langle h \rangle = -f + T / f \), which leads to an effective force law

\[
f(h) = -\frac{1}{2} (h) + \frac{1}{2} \sqrt{(h)^2 + 4T}, \tag{A12}
\]

from which we can compute the effective potential \( V_{\text{eff}}(\langle h \rangle) = -\frac{1}{2} (h) f(h) - T \log(\langle h \rangle) + \sqrt{(h)^2 + 4T} \) and stiffness

\[
k(h) = \frac{d f}{d (h)} = \frac{1}{2} \frac{(h)}{2 \sqrt{(h)^2 + 4T}}. \tag{A13}
\]

These relations are valid for \( T \ll f^2 \) and \( T \gg f^2 \), but perhaps not close enough to \( T \sim f^2 \).

**APPENDIX B: EFFECTIVE MEDIUM THEORY**

EMT is a self-consistent approximation scheme to treat disorder. Here, we follow our previous works,15,34 the only difference with respect to Ref. 34 being the effect of softness on the effective potential Eq. (A12) (in that work we had \( f(\langle h \rangle) = T / (\langle h \rangle) \)). Accordingly, we only sketch the derivation of our results.

**Equations:** We assume that contact forces have a distribution

\[
\mathbb{P}(f) = C f^\theta e^{-f/\beta h}, \tag{B1}
\]

and that forces and bond stiffnesses follow the effective potential Eqs. (A12) and (A13). We fix the bond length to one, since incorporating the dependence of bond length with force leads to subdominant corrections near jamming. A random elastic network of coordination \( z \) is constructed by random dilution of a regular lattice of coordination \( z_0 \) down to \( z \). The stiffness in contact \( \alpha, k_\alpha \), and the force in the contact, \( f_\alpha \) are random variables distributed according to

\[
\mathbb{P}_{\text{EMT}}(k_\alpha) = (1 - P) \delta(k_\alpha) + P \mathbb{P}(k_\alpha), \tag{B2}
\]

\[
\mathbb{P}_{\text{EMT}}(f_\alpha) = (1 - P) \delta(f_\alpha) + P \mathbb{P}(f_\alpha), \tag{B3}
\]

where \( P = z / z_0 \). The bond stiffness distribution is \( \mathbb{P}(k) = df / dk \mathbb{P}(f) \). In EMT, the elastic behavior of a random material is modelled by a regular lattice with effective frequency-dependent stiffnesses; here, we will have a longitudinal stiffness, \( k^L \), and a transverse stiffness \( -k^T \). Writing \( \tau \) for disorder average, the EMT equations are

\[
0 = \frac{k^L - k_\alpha}{1 - (k^L - k_\alpha) G^L} = \frac{k^T - f_\alpha}{1 + (k^T - f_\alpha) G^T}, \tag{B4}
\]

where \( G^L \) and \( G^T \) are related to the Green’s function \( \tilde{G}(\omega) = (M - m \omega^2)^{-1} \) by

\[
G^L = \tilde{n}_\alpha \cdot \langle \tilde{G} \rangle | \tilde{n}_\alpha, \tag{B5}
\]

\[
G^T = \frac{1}{d - 1} [\text{tr} (\langle \tilde{G} \rangle | \tilde{n}_\alpha) - G^L], \tag{B6}
\]
with $\langle a \rangle \equiv \langle i \rangle - \langle j \rangle$. Using Eq. (A12), one obtains the EMT equations

\[ 0 = \frac{(1-P)k^l}{1-k^lG^l} + P \left[ -\frac{1}{G^l} + \frac{1}{G^l(1+c)} \right] \times \left[ 1 + C_T f_0^{1-\theta} \left[ (1-k^lG^l)^{\alpha} \right] + \cdots \right], \]

\[ 0 = \frac{(1-P)k^l}{1-k^lG^l} + P \left[ \frac{1}{G^l} - \frac{C_T f_0^{1-\theta}}{G^l(1+c)} \right] \times \left[ 1 + \frac{1}{G^l} - \frac{f_0^{1-\theta}}{c_2-f_2} \right], \]

where $c = (1-k^lG^l)/G^l$, $\bar{c} = c/(1+c)$, and $c_2 = (1+k^lG^l)/f_0G^l$. Near the Maxwell point, we expect $|c| \ll 1$ and $c_2 \gg 1$ (which can be checked a posteriori), leading to

\[ 0 = k^lG^l - P \left[ \frac{1}{G^l} - \frac{f_0^{1-\theta}}{c_2-f_2} \right] \times \left[ 1 + C_T f_0^{1-\theta} \left[ (1-k^lG^l)^{\alpha} \right] + \cdots \right], \]

\[ 0 = k^lG^l - P \left[ \frac{1}{G^l} - \frac{f_0^{1-\theta}}{c_2-f_2} \right] \times \left[ 1 + C_T f_0^{1-\theta} \left[ (1-k^lG^l)^{\alpha} \right] + \cdots \right], \]

with $\alpha = (\theta-1)/2$, $C_1 = \pi/(2\Gamma_{1+\theta}\sin|\pi\alpha|)$, $\Gamma_{r} = \frac{\pi}{\sin(\pi r)}$, and $\delta z_k \sim 1/\Lambda$. Isotropy of $G$ implies an identity

\[ G^l = G^l = \frac{2d}{\lambda_0 k^l - k^l} \left[ 1 + \frac{\lambda_0}{d} \text{tr}(G(0,0)) \right] \]

Assuming $\omega \ll \sqrt{k^l/m}$ and $d \geq 3$, it can be checked that

\[ \frac{1}{d} \text{tr}(G(0,0)) = \frac{A_1}{k^l - k^l} + \cdots, \]

with

\[ A_1 = \frac{2\pi^{d/2}}{\rho^2d/(2\pi)^d} \Lambda^{-2} \frac{A^{d-2}}{d-2}. \]

Equations (B7), (B8), (B10), and (B11) are solved for $\delta z \ll 1$ by supposing

\[ k^l \sim \delta z^2, \quad k^l \sim \delta z^2, \quad \omega \sim \delta z^2, \quad T \sim \delta z^2, \quad f_0 \sim \delta z^2, \]

and balancing terms in the above equations. This necessarily leads to a description of the behavior near $T^*$, where both hard-sphere physics and soft-sphere physics are present at a small frequency. We find

\[ \eta = \gamma = 2\varepsilon = 2\zeta = 2, \quad \nu = \frac{5 + 3\theta}{1 + \theta}, \]

recovering the scalings described in the main text.

Results: The leading order equations for $k^l$, $k^l$ are

\[ k^l = Pf_0(1+\theta) \sim p \]

and

\[ 0 = z_0A_2\omega^2 - k^l\delta z + \tilde{k}^l \zeta + ak^l_{\omega} + c_3k^l \left( \frac{Tk^l}{f_0^2} \right)^{\alpha+1}, \]

with $a = z_0 - \zeta_c$ and $c_3 = C_1z_0(1 - \zeta_c/z_0)^{\alpha+1}(z_0/\zeta_c)^{\alpha}$. This equation contains the leading-order terms (in $\delta z$) for both the harmonic $T = 0$ theory from Ref. 15 and the hard-sphere theory from Ref. 24. When all terms are important, it describes behavior near $T^*$. Other regimes are obtained when one or several terms become small. We cannot analytically solve Eq. (B17), but we can determine some of its key properties.

For example, we expect $k^l(\omega)$ to have an onset frequency $\omega_0$ where the density of states rises from zero. At this point, we must have $|dk^l/d\omega| = \infty$, implying

\[ 0 = \delta z - 2ak^l_0 - (\alpha + 2)c_0 \left( \frac{Tk^l}{f_0^2} \right)^{\alpha+1} \]

and

\[ 0 = \gamma_2k^l_0 + \gamma_1\delta z_k - \zeta_c(A_1\omega_0^2 + \tilde{k}^l), \]

where $k_0 = k^l(\omega_0)$, with $\gamma_1 = (1+\theta)/(3+\theta)$, $\gamma_2 = \alpha/(3+\theta)$. $k_0$ and $\omega_0$ can be found by numerical solution of Eqs. (B18) and (B19) for a prescribed value of $\delta z$.

Marginal stability: The condition of marginal stability corresponds to $\partial^2/\partial \omega^2 = 0$. Therefore, $\delta z(p,T)$ at marginal stability can be found by solving Eqs. (B18) and (B19) in this case, leading to Figs. 6 and 7 in the main text. Since $k_0 = k^l(\omega_0)$, at marginal stability, $k_0 - \tilde{k}^l = k_0(1 + O(\delta z))$ is precisely the shear modulus $\mu$. Hence,

\[ \mu = \frac{\gamma_1}{2\gamma_2} \left[ -\delta z + \sqrt{\delta z^2 + \gamma_3f_0} \right], \]

as discussed in the main text and plotted in Fig. 8(b).

Density of states: The density of states

\[ D(\omega) = \frac{2\omega^2}{\pi} \text{Im} \left[ \text{tr} \left( \hat{G}(0,\omega) \right) \right] \]

\[ = \frac{2\rho k^l}{\pi} \text{Im} \left[ \frac{A^{d-2}}{d-2} \frac{d}{\lambda_0} \text{tr}(G(0,\omega)) \right] \]

with $A_k = k^l - \tilde{k}^l$. We determine it by numerically solving Eq. (B17) at each $\omega$. It is plotted in Fig. 8(a).

Scattering length: Finally, we can extract the asymptotic behavior of the Green’s function for large $r$. To leading order, log($\hat{G}(r,\omega)$) $\sim -r/\ell_s(\omega) + i\omega r/\nu(\omega)$, where $\ell_s(\omega) = -\omega^{-1}A_k/\text{Im}[\hat{G}(0,\omega)]$ and $\nu(\omega) = |\Delta k|/\text{Re}[\hat{G}(0,\omega)]$ are, respectively, the scattering length and sound velocity at frequency $\omega$.

To extract $\ell_s$, at the characteristic frequency $\omega_s$, we use our knowledge of the shape of $|\Delta k| \sim k^l$ known from our previous works,\textsuperscript{15,34} which is confirmed by numerical solutions to Eq. (B17): near $\omega_s$, we have $\text{Re}[k^l] \sim \text{constant} \sim \mu$, while $\text{Im}[k^l] \gg \text{Re}[k^l]$. This implies that $|\Delta k| \sim \text{Im}[k^l]$. Using $2\rho k^l \sqrt{\Delta k} = |\Delta k| \sim |\Delta k| \approx |\Delta k|$ along with the definitions of $\ell_s$ and Eq. (B21), we find

\[ \ell_s(\omega) = -\frac{|\Delta k|}{\omega \text{Im}[\sqrt{\Delta k}]} \sim -\frac{|\Delta k|^{1/2}}{\omega^s} \sim |D(\omega)\omega^s|^{-1/2}, \]

from which we can determine the scaling properties of $\ell_s(\omega)$.


J. Maxwell, Philos. Mag. 27, 294 (1864).


