Universal non-mean-field scaling in the density of state of amorphous solids

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Amorphous solids have excess soft modes in addition to the phonon modes described by the Debye theory. Recent numerical results show that if the phonon modes are carefully removed, the density of state of the excess soft modes exhibit universal quartic scaling, independent of the interaction potential, preparation protocol, and spatial dimensions. We hereby provide a theoretical framework to describe this universal scaling behavior. For this purpose, we extend the mean-field theory to include the effects of finite dimensional fluctuation. Based on a semi-phenomenological argument, we show that mean-field quadratic scaling is replaced by the quartic scaling in finite dimensions. Furthermore, we apply our formalism to explain the pressure and protocol dependence of the excess soft modes.

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Introduction. – The vibrational density of state $D(\omega)$ of amorphous solid differs dramatically from that of crystals. The low-frequency modes of crystals are phonons that follow the Debye law $D(\omega) \sim \omega^{d-1}$, where $d$ denotes the spatial dimensions $[1]$. On the contrary, $D(\omega)/\omega^{d-1}$ of amorphous solids exhibit a sharp peak at the characteristic frequency $\omega = \omega_{BP}$, which is referred to as the Boson peak (BP). This behavior suggests the existence of excess soft modes (ESMs) beyond that predicted by the Debye law $[2, 3]$. For $\omega < \omega_{BP}$, the ESMs are spatially localized $[5, 6]$. These localized modes play a central role in controlling the various low-temperature properties of amorphous solids, such as the specific heat, thermal conduction, and sound attenuation $[2, 6-12]$. Furthermore, recent numerical studies have established that the ESMs facilitate the structural relaxation of supercooled liquids at finite temperatures $[13, 14]$, and the local rearrangement of sheared amorphous solids at low temperature $[15-20]$.

The detailed statistical properties of ESMs have been only recently investigated via numerical simulations. The ESMs can be separated from the background phonon modes by using a small size system $[21]$, observing the participation ratio $[22]$, or introducing impurities $[23, 24]$. Remarkably, after successfully removal of the phonons, the mean-field replica calculation predicts another universal quartic scaling, independent of the interaction potentials, preparation protocols and dimensions $[21, 25, 26]$. Considering the relationship with other physical quantities, it is important to gain an understanding the mechanism that yields the $D(\omega) = A_4 \omega^4$ law and controls the prefactor $A_4$.

The $d$ independence of the quartic law motivates us to apply mean-field theory to understand this scaling behavior. The replica theory is now one of the most mature mean-field theories of amorphous solids $[27, 30]$. In particular, near the (un) jamming transition point at which the system loses rigidity $[3, 31]$, the theory predicts the exact critical exponents of the contact number and shear modulus $[30, 32]$. Furthermore, the theoretical result of $D(\omega)$ agrees very well with the numerical results for $\omega > \omega_{BP}$ in $d = 2$ and $3$ $[32, 33]$. The replica theory predicts that amorphous solids near the jamming transition point are in the Gardner phase $[30, 34]$, which has been originally investigated in a class of mean-field spin glasses $[35, 36]$. In the Gardner phase, the density of state has the gapless excitation $D(\omega) \sim \omega^2$ for $\omega < \omega_{BP}$ $[32]$. However, the numerical results indicate that $D(\omega) \sim \omega^2$ scaling is observed only near $\omega \sim \omega_{BP}$, and it is replaced by $D(\omega) \sim A_4 \omega^4$ for $\omega \ll \omega_{BP}$ $[22]$. The mean-field replica calculation predicts another source of the singularity that creates the ESMs, in addition to the trivial phonon modes. This singularity is related to the quenching rate, or from a theoretical perspective, the initial temperature $T_{ini}$ of the equilibrium supercooled liquid before quenching to produce glass. When $T_{ini}$ is sufficiently low, the supercooled liquid becomes highly viscous because of the complex structure of the free-energy landscape containing multiple minima $[37]$.

After quenching, the system falls to one of the minima. The minima become gradually unstable with an increase in temperature and eventually disappear above the so-called mode coupling transition point $T_{mct}$ $[27, 28]$. This instability affects the vibrational properties of the zero-temperature amorphous solids and creates ESMs $[38]$. This view seems to be consistent with the numerical result that the excess soft modes close to $\omega \sim \omega_{BP}$ are indeed enhanced for samples quenched from higher temperatures $[39]$. However, the mean-field prediction, $D(\omega) \sim \omega^2$ for $\omega < \omega_{BP}$, is again inconsistent with the numerical result where $D(\omega) \sim A_4 \omega^4$ scaling is robustly observed irrespective of $T_{ini}$ $[22]$. In this Letter, we reconcile the aforementioned discrepancies between the mean-field replica theory and the numerical results in finite $d$ for small $\omega$ by introducing the effect of the finite $d$ fluctuation to the mean-field density of state in a semi-phenomenological way. We initially construct a theory to describe the asymptotic behavior...
of $D(\omega)$ in high $d$ and show that the quartic law naturally arises as a consequence of finite $d$ fluctuation. Next, motivated by the $d$ independence of the $D(\omega) \sim A_4 \omega^4$ scaling [24], we apply our formalism to explain the numerical results in $d = 3$. We show that our theory well reproduces the correct scaling behavior of the prefactor $A_4$ near jamming and the $T_{\text{ini}}$ dependence of $A_4$ for $T_{\text{ini}} \sim T_{\text{met}}$.

**Effect of the finite dimensional fluctuation.** Recent numerical results confirm that the small $\omega$ behavior of the ESMs, $D(\omega) \sim A_4 \omega^4$, does not depend on the spatial dimensions $d$ [26]. Despite this seemingly mean-field like behavior, mean-field theory fails to reproduce this quartic law. We first review the discrepancy between the mean-field and numerical results in high but finite $d$ and then discuss an approach for solving this problem.

In the mean-field replica theory, amorphous solids are modeled by fully connected models, which are considered to correspond to the $d \to \infty$ limit of the system. The fully connected models have the universal form of the eigenvalue distribution function for small $\lambda$, $\rho(\lambda) \sim \sqrt{\lambda - \varepsilon}$ [40], where $\varepsilon$ is proportional to the distance to the instability point. The mean-field theory predicts that if an amorphous solid is quenched from high temperature or located near the jamming transition point, the system becomes marginally stable $\varepsilon = 0$ [41, 42], thus we have

$$
\rho_{\text{MF}}(\lambda) \sim \sqrt{\lambda - \theta(x)},
$$

where $\theta(x)$ denotes the Heaviside step function. The density of state $D(\omega)$ is obtained by changing the variable as $\omega = \sqrt{\lambda}$, which leads to $D(\omega) = 2\omega \rho_{\text{MF}}(\lambda = \omega^2) \sim \omega^2$ for small $\omega$. In Fig. 1 we compare the mean-field prediction with the numerical result in $d = 4$ to 7. For $\omega > \omega_0 \approx 0.12$, the numerical result converges to the mean-field prediction $D(\omega) \sim \omega^2$ for an increase of $d$. On the contrary, for $\omega < \omega_0$, the data systematically deviate from the mean-field prediction and are well fitted by $D(\omega) \sim \omega^4$, as already confirmed by previous numerical simulations in $d = 3$ and 4 [21, 20]. For very small $\omega$, the numerical results are scattered around $10^{-2}$, presumably owing to the finite size effect or the lack of statistics (not shown). We are aware that the size of the current system $N = 8192$ is not large enough to observe the effects of phonons [26]. Nevertheless, we believe that these effects can be negligible in $d > 5$ because the contribution of the ESMs, $D(\omega) \sim \omega^4$, overwhelms the phonon contribution, $D(\omega) \sim \omega^{d-1}$.

To clarify the reason for the above discrepancy between the mean-field and numerical result for finite $d$, we decompose the $i$-th eigenvalue $\lambda_i$ into the following two parts:

$$
\lambda_i = \lambda_i^{\text{MF}} + \varepsilon_i,
$$

where $\lambda_i^{\text{MF}}$ follows the mean-field result Eq. (1) and $\varepsilon_i$ represents the finite $d$ fluctuation. Then, the distribution function of $\lambda_i$ is

$$
\rho(\lambda) = \langle \delta(\lambda - \lambda_i) \rangle = \int_0^\infty d\varepsilon P_\lambda(\varepsilon) \rho_{\text{MF}}(\lambda - \varepsilon),
$$

(3)

where the lower bound of the integral arises from the stability condition, $\rho(\lambda) = 0$ for $\lambda < 0$, and we introduced the conditional probability distribution:

$$
P_\lambda(\varepsilon) = \frac{\langle \delta(\varepsilon - \varepsilon_i) \delta(\lambda - \varepsilon - \lambda_i^{\text{MF}}) \rangle}{\langle \delta(\lambda - \varepsilon - \lambda_i^{\text{MF}}) \rangle}. \quad (4)
$$

In the $d \to \infty$ limit, the system can be identified with the fully connected model and thus $P_\lambda(\varepsilon) = \delta(\varepsilon)$ to recover the mean-field result. For high but finite $d$, $P_\lambda(\varepsilon)$ is expected to have a narrow distribution close to $\varepsilon = 0$. Thus, we set a small cutoff $\Delta$ and assume that $P_\lambda(\varepsilon) = O(1)$ for $\varepsilon \ll \Delta$ and $P_\lambda(\varepsilon) \sim 0$ for $\varepsilon \gg \Delta$. Using Eqs. (1) and (3), we obtain the following for $\lambda \ll \Delta$:

$$
\rho(\lambda) \sim P_0(0) \int_0^\lambda d\varepsilon \sqrt{\lambda - \varepsilon} \sim P_0(0) \lambda^{3/2}, \quad (5)
$$

leading to $D(\omega) \sim \omega^4$. Thus, the mean-field result is replaced by the quartic scaling unless the finite dimensional fluctuation is negligible, i.e., $P_\lambda(\varepsilon) = \delta(\varepsilon)$. A similar calculation leads to $\rho(\lambda) \sim \rho_{\text{MF}}(\lambda)$ for $\lambda \gg \Delta$, meaning that $D(\omega) \sim \omega^2$ for $\omega \gg \omega_0 \equiv \sqrt{\Delta}$. Hereafter we recover the numerical results for high $d$ in Fig. 1.

The $D(\omega) \sim \omega^4$ law is also obtained by a seemingly different approach: the so-called soft-potential model where the localized modes are modeled by the collection of anharmonic oscillators of different stiffnesses [44–46]. The advantage of our approach over that of the soft-potential model is that we can consider how the control parameters and preparation protocols affect the prefactor $A_4$ by relying on the mature replica theory, as shown in the following sections.
In general, it is impossible to calculate $\mathcal{P}_\lambda(\varepsilon)$ exactly for finite $d$. To simplify the treatment, we neglect the $\lambda$ dependence $\mathcal{P}_\lambda(\varepsilon) \approx \mathcal{P}(\varepsilon)$, which is tantamount to neglecting the higher order terms of $\lambda$ and can be justified for small $\lambda$. Then, Eq. (4) reduces to

$$\rho(\lambda) = \int_0^\infty d\varepsilon \mathcal{P}(\varepsilon) \rho_{\text{MF}}(\lambda - \varepsilon). \quad (6)$$

From the normalization conditions of $\rho(\lambda)$ and $\rho_{\text{MF}}(\lambda)$, it can be shown that $\int_0^\infty d\varepsilon \mathcal{P}(\varepsilon) = 1$, suggesting that $\mathcal{P}(\varepsilon)$ can be considered as the distribution function of the distance to the instability point $\varepsilon$. The fluctuation of $\varepsilon$ is a consequence of the spatial heterogeneity of amorphous solids, which are not considered in the fully connected mean-field models [34,49]. The width $\Delta$ of the distribution $\mathcal{P}(\varepsilon)$ decreases with an increase of $d$ as the system approaches the fully connected model. From the central limit theorem, we expect $\Delta \sim d^{-1/2}$ and the crossover frequency decreases as $\omega_0 \sim d^{-1/4}$. However, it is difficult to detect such weak $d$ dependence from the current numerical result in Fig. 1. Further numerical investigations are necessary to confirm the $d$ dependence of $\Delta$.

Hereafter, we use a similar argument as that used to derive Eq. (6) to analyze the numerical results in $d = 3$. Given that the proposed theory does not taken into account the phonon mode, the phonon contribution should be removed from the numerical results as in Refs. [21,22,23], before comparing with the theoretical prediction.

**Pressure dependence near jamming.** Here we investigate the pressure $p$ dependence of $D(\omega)$ near jamming. For this purpose, we investigate the negative perceptron model, a mean-field model of the jamming transition that belongs to the same universality class of hard/harmonic spheres in the $d \to \infty$ limit [33,50]. The simplicity of the model allows for analytical calculation of the eigenvalue distribution function [11]. Near jamming, the model predicts for $\lambda \ll 1$ [41]

$$\rho_{\text{MF}}(\lambda) \sim \frac{\sqrt{\lambda}}{\lambda + \omega_*^2} \rho(\lambda), \quad (7)$$

where $\omega_* = c\sqrt{p}$, and $c$ is a constant. Essentially the same result as Eq. (7) is obtained by the effective medium theory, except for the trivial Debye modes [32]. The gapless form of Eq. (7) is a consequence of the Gardner transition [32], which is the continuous replica symmetric breaking transition originally discovered in the mean-field spin glasses [33,60]. From Eq. (7), the scaling behavior of $D(\omega)$ near jamming ($p \ll 1$) is given as:

$$D(\omega) \sim \begin{cases} \text{constant} & (\omega \gtrsim \omega_*), \\ \left(\omega/\omega_*\right)^2 & (\omega \ll \omega_*). \end{cases} \quad (8)$$

However, this is inconsistent with the numerical result in $d = 3$. The numerical results shows that if one carefully removes the phonon modes by using the participation ratio, one obtains 22

$$D(\omega) \sim \begin{cases} \text{constant} & (\omega \gtrsim \omega_*), \\ \left(\omega/\omega_*\right)^2 & (\omega_0 \ll \omega \ll \omega_*), \\ \left(\omega/\omega_*\right)^4 & (\omega \ll \omega_0), \end{cases} \quad (9)$$

where $\omega_0 \propto \sqrt{p}$ but the proportionality constant is much smaller than that of $\omega_*$. One of the reasons for the discrepancy between the mean-field theory and the numerical results is the absence of the marginal stability for finite $d$. The numerical results show that the mean distance to the instability point has a finite value $[32,51]$,

$$\langle \varepsilon \rangle = p\Delta_G, \quad (10)$$

where $\Delta_G$ is a small positive constant. As in Eq. (10), we introduce the fluctuation of $\varepsilon$ and assume that the mean value of the eigenvalue distribution function can be written as follows:

$$\rho(\lambda) = \int_0^\infty d\varepsilon \mathcal{P}(\varepsilon) \rho_{\text{MF}}(\lambda - \varepsilon). \quad (11)$$

From Eq. (10), $\mathcal{P}(\varepsilon)$ should be $\mathcal{P}(\varepsilon) = O(p^{-1}\Delta_G^{-1})$ for $\varepsilon < p\Delta_G$ and quickly decreases for $\varepsilon > p\Delta_G$. Repeating a similar argument in Eq. (5), we obtain for $\lambda \ll p\Delta_G$

$$\rho(\lambda) \sim c^2\Delta_G^{-1}\omega_*^4\lambda^{3/2}, \quad (12)$$

which leads to $D(\omega) \sim c^2\Delta_G^{-1}(\omega/\omega_*)^4$. This scaling smoothly connects to the mean-field scaling Eq. (3) at $\omega \sim \omega_0 \equiv \sqrt{p}\Delta_G$. Thus, we reproduced the numerical result, Eq. (9). Finally, for concreteness, in Fig. 2 we show $D(\omega)$ calculated by Eq. (11) assuming $\mathcal{P}(\varepsilon) = (p\Delta_G)^{-1}e^{-(p\Delta_G)^{-1}\varepsilon}$; $\Delta_G = 10^{-4}$, and $c = 1$. If one rescales $\omega$ by $\omega_*$, the data for different $p$ are collapsed on a single curve as expected from Eq. (9).

**Initial temperature dependence.** Here, we discuss the influence of $T_{\text{ini}}$ on the vibrational properties of amorphous solids at zero temperature. For this purpose, we
start from the $p$-spin spherical model (PSM), which is a prototypical mean-field model for glass transition to discuss the connection between the glassy slow dynamics and complex free energy landscape [23, 24]. The replica calculation of the PSM shows that there are many metastable states on the free energy landscape below $T_{\text{mct}}$. After quenching, the system falls to one of the minima. On the minima, the eigenvalue distribution function of the PSM follows the Wigner semicircle law [29, 52]. For $\lambda \ll 1$ and $T_{\text{ini}} \approx T_{\text{mct}}$, this can be written as

$$\rho_{\text{MF}}(\lambda) \sim \sqrt{\lambda - \lambda_{\min}} \theta(\lambda - \lambda_{\min}),$$  \hspace{1cm} (13)

where $\lambda_{\min} = c(T_{\text{mct}} - T_{\text{ini}})$ for $T_{\text{ini}} < T_{\text{mct}}$, and $\lambda_{\min} = 0$ for $T_{\text{ini}} \geq T_{\text{mct}}$ [42]. $c$ is a positive constant. Repeating a similar argument that used to derive Eq. (3), we obtain

$$\rho(\lambda) = \int_{-\lambda_{\min}}^{\infty} d\varepsilon P(\varepsilon) \rho_{\text{MF}}(\lambda - \varepsilon),$$  \hspace{1cm} (14)

where the lower bound of the integral is followed by the stability condition, $\rho(\lambda) = 0$ for $\lambda < 0$. As mentioned, $P(\varepsilon)$ is expected to have a narrow distribution close to $\varepsilon = 0$. To express this distribution, we assume

$$P(\varepsilon) \sim \Delta_{\text{mct}}^{-1} \exp \left[-\left|\varepsilon \over \Delta_{\text{mct}}\right|^\alpha \right],$$  \hspace{1cm} (15)

where $\Delta_{\text{mct}}$ and $\alpha$ are constants. Then, the eigenvalue distribution for small $\lambda$ is calculated as

$$\rho(\lambda) \sim \rho(-\lambda_{\min}) \int_{-\lambda_{\min}}^{\lambda - \lambda_{\min}} d\varepsilon \sqrt{\lambda - \lambda_{\min} - \varepsilon} \sim \rho(-\lambda_{\min}) \lambda^{3/2},$$  \hspace{1cm} (16)

leading to

$$D(\omega) = A_4 \omega^4,$$  \hspace{1cm} (17)

where the prefactor is given as:

$$A_4 = \begin{cases} A & (T_{\text{ini}} \geq T_{\text{mct}}) \\ A \exp \left[-\left(T_{\text{mct}} - T_{\text{ini}} \over \Delta_{\text{mct}}\right)^\alpha \right] & (T_{\text{ini}} < T_{\text{mct}}) \end{cases}.$$  \hspace{1cm} (18)

$A$ is a constant and $\Delta_{\text{mct}} = \Delta_{\text{mct}}/c$. The preceding equation shows that $A_4$ rapidly decreases for $T_{\text{mct}} - T_{\text{ini}} > \Delta_{\text{mct}}$. In Fig. 3 we compare our prediction with the numerical results of an amorphous solid in $d = 3$. An excellent agreement is realized which proves the validity of our theory.

**Conclusions and discussions.** In summary, we discussed the process by which finite dimensional fluctuation alters the mean-field scaling $D(\omega) \sim \omega^2$ of amorphous solids. Our theory successfully captures quartic scaling, $D(\omega) \sim A_4 \omega^4$, reported in previous numerical simulations. We applied the theory to describe the pressure $p$ and initial temperature $T_{\text{ini}}$ dependence of the prefactor $A_4$. In both cases, the theoretical results are in good agreement with the previous numerical results. It should be noted that the argument in Eq. (5) does not depend on the precise form of $P_\lambda(\varepsilon)$. If $P_\lambda(\varepsilon)$ is finite and continuous at $\varepsilon = 0$ and $\rho(\lambda)$, one always obtains the quartic scaling for small $\omega$. This may explain the robustness of the quartic scaling against the different interaction potentials, preparation protocol, and dimensions [21, 22, 25, 26, 53].

In this Letter, we proposed two singularities to yield the quartic scaling: singularities related to the Gardner and MCT transitions. Near the jamming transition point ($p \ll 1$), one can conclude that the Gardner transition plays the dominant role in generating quartic scaling considering the numerical and experimental evidence for the Gardner transition [54, 55], and the consistency between the mean-field and numerical results [30, 57]. However, this scenario may not hold apart from jamming where amorphous solids do not show the strong signature of the Gardner transition [55, 59]. In this region, the MCT transition would be the main cause of the quartic scaling. For the intermediate value of $p$, the situation is more complex and further investigations are needed to determine which singularity plays the dominant role.

If $P_\lambda(\varepsilon)$ is not finite at $\varepsilon = 0$ and $\lambda = 0$, the $D(\omega) \sim \omega^4$ law can be replaced. For instance, if $P_\lambda(\varepsilon) \sim A\varepsilon^{-\alpha}$ for small $\varepsilon$ and $\lambda$, a similar calculation as that used in Eq. (6) leads to $\rho(\lambda) \sim A\lambda^{5/2-\alpha}$. This implies that $D(\omega) \sim A\omega^{4-2\alpha}$. Interestingly, for amorphous solids prepared by instantaneous quenching without inertia, Lerner and Bouchbinder [60] observed $D(\omega) \sim \omega^3$ with $\beta < 4$ suggesting that $\alpha > 0$. Also, some spring models for amorphous solids on the scale-free network [61] and random graph [62] show that $\beta$ can change depending on the spatial dimensions and distribution of the coordination number. Further investigations are required to identify
what physical mechanisms control $\alpha$ and $\beta$.

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Supplemental information for “Universal non-mean-field scaling in the density of state of amorphous solids”

Here we briefly explain the scaling behavior of the mean-field eigenvalue distribution near the minimal eigenvalue. For more complete and rigorous derivations, see for instance Refs. [63, 64]. We consider a Hessian $H_{ij}$, $i, j = 1, \cdots, N$ of a fully connected model. The eigenvalue distribution function is obtained by using the Edwards and Jones formula [63]:

$$
\rho(\lambda) = \frac{1}{N} \sum_{i=1}^{N} \delta(\lambda - \lambda_i) = \left| \frac{2}{\pi N} \text{Im} \left[ \frac{\partial}{\partial \lambda} \log Z(\lambda) \right] \right|, \tag{19}
$$

where

$$
Z(\lambda) = \int du \exp \left[ -\frac{1}{2} u \cdot (H - \lambda I) u \right]. \tag{20}
$$

Introducing the new variable $q \equiv u \cdot u / N$ and using the saddle point method, $Z(\lambda)$ is calculated as

$$
\log Z(\lambda) \approx N \left( \lambda \frac{q}{2} + G(q) \right), \tag{21}
$$

where

$$
G(q) = \frac{1}{N} \log \int du \delta(u \cdot u - Nq) e^{-\frac{1}{2} u \cdot H u}. \tag{22}
$$

For fully connected models, one can directly calculate this quantity by using the replica method. However, the detailed functional form is not necessary for our purpose. The saddle point value of $q$ is determined by

$$
\lambda = -2G'(q). \tag{23}
$$

Substituting Eq. (21) into Eq. (19), we have a simple result:

$$
\rho(\lambda) = \left| \frac{1}{\pi} \text{Im}[q(\lambda)] \right|. \tag{24}
$$

$\rho(\lambda)$ would have a small value near the edge of the distribution. Eq. (24) implies that $|\text{Im}[q(\lambda)]|$ is also small near that point. We expand the real and imaginary parts of Eq. (23) for $|q|$:

$$
\lambda = -2G'(\text{Re}[q(\lambda)]) + \text{Im}[q(\lambda)]^2 G'''(\text{Re}[q(\lambda)]) + \cdots, \tag{25}
$$

$$
0 = \text{Im}[q(\lambda)] G''(\text{Re}[q(\lambda)]) + \cdots. \tag{26}
$$

Then, $\text{Im}[q(\lambda)]$ is calculated as

$$
\text{Im}[q(\lambda)] \sim \sqrt{\frac{\lambda + 2G'(\text{Re}[q])}{G'''(\text{Re}[q])}} \sim \sqrt{\lambda - \varepsilon}, \tag{26}
$$

where $\varepsilon = -2G'(\text{Re}[q])$ and $\text{Re}[q]$ is determined by $G''(\text{Re}[q]) = 0$. From Eqs. (24) and (26), one can see that $\rho(\lambda)$ shows the square root singularity near the minimal eigenvalue $\rho(\lambda) \sim \sqrt{\lambda - \varepsilon}$. 

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