On the Ground State of Electron Gases at Negative Compressibility

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Two- and three-dimensional electron gases with a uniform neutralizing background are studied at negative compressibility. Parametrized expressions for the dielectric function are used to access this strong-coupling regime, where the screened Coulomb potential becomes overall attractive for like charges. Closely examining these expressions reveals that the ground state with a periodic modulation of the charge density, albeit exponentially damped, replaces the homogeneous one at positive compressibility. The wavevector characterizing the new ground state depends on the density and is complex, having a positive imaginary part, as does the homogeneous ground state, and real part, as does the genuine charge density wave.

I. INTRODUCTION

The nature of the metallic state of a dilute two-dimensional electron gas (2DEG) in high-mobility silicon MOSFETs, first observed by Kravchenko et al. nearly a decade ago, has still not been established. Various scenarios have been proposed to explain the new conducting state, ranging from superconducting, to non-Fermi liquid, to percolation, to classical (see Refs. 1,2 for overviews and references to the original literature). The unique character of this state is reflected by its thermodynamic signatures of both negative pressure and compressibility.

Although recognized as a theoretical possibility for quite some time—at least in three dimensions—an electron gas with a uniform neutralizing background was expected to be unstable at negative compressibility, and the model meaningless. Later theoretical and also numerical studies nevertheless considered both the region with positive and negative compressibility without encountering conceptual difficulties.

Eisenstein, Pfeiffer, and West recently concluded that the global features of their 2DEG compressibility data to very low densities, where the system appears to undergo a quantum phase transition to an insulating state, could be explained simply using the Hartree-Fock approximation, which consists of including the electron exchange contribution to the ground-state energy of a free fermion gas. Their analysis does not account for impurities, which are of paramount importance at and beyond the metal-insulating (MI) transition.

Ilani et al. reached similar conclusions based on their compressibility data of a dilute two-dimensional hole gas (2DHG). By placing several single electron transistors directly above the 2DHG, they could in addition determine possible spatial variations in the system. They concluded that the metallic state at negative compressibility is homogeneous in space and well described by the Hartree-Fock approximation. As the system crosses to the insulating state and the Hartree-Fock approximation ceases to be applicable, they found the system to become spatially inhomogeneous. They interpreted this observation as supporting scenarios in which the MI transition is described as a percolation process.

Using density functional theory in the local density approximation, Shi and Xie recently investigated the spatial distribution of the electron number density of a 2DEG in the presence of impurities. As usual, impurities were included by coupling the particle number density to a fluctuating potential with a random distribution. The parameter characterizing the Gaussian distribution, which we will refer to as the impurity strength, determines the roughness of the impurity landscape. Their numerical study incorporates the Monte Carlo data on the ground-state energy of a clean system by Tanatar and Ceperly. For given impurity strength, the study shows that at some average density \( n \) islands of very low densities form in a metallic sea of high densities. At higher average densities, the sea level is high enough to fill all of the valleys of the impurity landscape, and the system is homogeneous. With decreasing \( n \), the sea level drops and the insulating islands grow. At a critical value, the islands percolate the system, which at this percolation threshold becomes insulating. The sea level now dropped to the extent that the electrons are confined to the valleys of the impurity landscape. According to this picture, the transition to the insulating state takes place at lower densities for cleaner systems. This is in accord with experiments, where the lowest critical density, \( n_c = 7.7 \pm 0.2 \times 10^{11} \text{cm}^{-2} \), was observed in an exceptionally clean 2DHG. Shi and Xie also studied the importance of the Coulomb interaction by comparing with the case where this interaction is turned off. They found that at an average density where the interacting system was still metallic, the free electron gas, which is insulating, had formed a few isolated lakes of high density at valleys of the impurity landscape.

In this paper, we postulate on the nature of the ground state of electron gases at negative compressibility. In doing so, we ignore impurities, as justified by the experimental findings that this metallic state is homogeneous in space and that the compressibility data is already well described by the Hartree-Fock approximation of a clean electron gas. The study emphasizes the three-dimensional electron gas (3DEG) as much more informative from theoretical studies is available than for the 2DEG. Most of the 3D conclusions, however, also apply to the 2D case discussed in Sec. 1. The following two sections focus on the changes brought about when going from positive to negative compressibility. One of the most surprising changes is that a test particle acquires a screening cloud in its immediate vicinity which overcompensates the test charge, so that the Coulomb interaction becomes attractive for like charges. The changes are also discussed from the perspective of Fermi liquid theory, describing the electron gas after the screening mechanism has taken effect and resulted in only short-range interactions. The main result of this paper is contained in Sec...
where it is argued that the ground state of an electron gas at negative compressibility is a charge density wave (CDW), although exponentially damped. The phenomena considered here are by no means specific to an electron gas, but also appear in a charged Bose gas as discussed in Sec. IV.

II. SCREENING VS. OVERSCREENING

A 3DEG is characterized by the screening of charges. When a test particle of charge $Z$ is placed at the origin, $\rho(x) = Z\delta(x)$, the system responds by rearranging its charge distribution to screen the external charge. The charge density $\rho_{\text{ind}}$ thus determined,

$$\rho_{\text{ind}}(x) = Z \int \frac{d^3 q}{(2\pi)^3} \left[ \frac{1}{\epsilon(q, 0)} - 1 \right] e^{i q \cdot x}, \quad (1)$$

is determined by the dielectric function $\epsilon(q,0)$ at zero frequency, which encodes the static screening effects of the 3DEG. The total induced charge

$$Q_{\text{ind}} = \int d^3 x \rho_{\text{ind}}(x) = \rho_{\text{ind}}(q = 0) = -Z \quad (2)$$

cancels the charge of the test particle since the screening factor $1/\epsilon(q, 0)$ vanishes at zero wavevector $q = |q|$. The test charge is therefore always perfectly screened. However, the induced charge density differs in how it is distributed, depending on the electron number density $n$, or, equivalently, the ratio $r_s = a/a_0$ of the average interparticle distance $a = (3/4\pi n)^{1/3}$ to the Bohr radius $a_0 = \hbar^2/m e^2$. (For valence electrons in 3D metals, $r_s$, characterizing the strength of the Coulomb interaction, ranges from 1.8 to 5.6.)

At weak coupling ($r_s < 1$), corresponding to high electron number densities, a screening cloud of opposite charge surrounds the test charge, and the screened Coulomb potential decreases exponentially with increasing distance. On its tail, far away from the test charge, the potential has superimposed a small oscillatory modulation of wavevector $q = 2k_F$, with $k_F$ the Fermi wavevector. These Friedel oscillations, leading to a periodic change in sign of the Coulomb potential, originate from a singularity in the dielectric function at $q = 2k_F$, where electron-hole excitations start to develop an energy gap.

A 3DEG’s response to a test charge fundamentally changes at larger values of the coupling constant $r_s$, because of a qualitative change in the dielectric function. Namely, at some value $r_s = r_s^*$, the dielectric function becomes negative for small wavevectors. Rather than surrounded by a screening cloud of opposite charge in its immediate vicinity, the test charge now becomes overscreened. The Coulomb potential rapidly drops below zero with increasing distance and becomes attractive for like charges. Further away from the test charge, the potential exhibits an exponentially damped oscillatory behavior and periodically changes sign similar to Friedel oscillations. The initial drop of the Coulomb potential to negative values and the resulting overscreening is, however, unrelated to Friedel oscillations. Overscreening in a plasma was first noted in a 2D Bose gas with a $1/x$ Coulomb potential.

The fundamental change in the screening behavior of a 3DEG is paralleled by a modification of its ground state. At the critical electron number density, where the dielectric function becomes negative for small wavevectors and a test charge overscreened, the compressibility changes sign as well. As argued in the following, the homogeneous ground state of the regime with positive compressibility then gives way to a ground state with a periodic modulation of the charge density, which is, however, exponentially damped.

III. NEGATIVE COMRESSIBILITY

At weak coupling, the dielectric function can be written for small wavevectors as

$$\lim_{q \to 0} \epsilon(q,0) = 1 - v(q) \chi_{\text{sc}}(0,0), \quad (3)$$

with $v(q) = 4\pi e^2/q^2$ the Fourier transform of the (unscreened) Coulomb potential, and $\chi_{\text{sc}}(0,0)$ the screened density-density response function at zero wavevector and frequency. The screened response function, a theoretic construct to be distinguished from the physical one, measures the response to a screened external field rather than the external field itself. Physically, this function describes a fictitious system with only short-range interactions that are remnants of the long-range Coulomb interaction after the screening mechanism of the 3DEG has taken effect. Derived from the Coulomb interaction, the short-range interactions of the fictitious system vanish in the limit $r_s \to 0$.

In writing Eq. (5), the $O(q^2)$ term in the Taylor expansion of $\chi_{\text{sc}}(q,0)$ is assumed to be substantially smaller than 1. This is true only at weak coupling. For example, when $r_s = 1$, the value of the constant term in Eq. (6) is reduced already by about 6 %.

The compressibility sum rule relates the screened response function to the compressibility $\kappa$ of the 3DEG via

$$\lim_{q \to 0} \chi_{\text{sc}}(q,0) = -\frac{\partial n}{\partial \mu} = n^2 \kappa, \quad (4)$$

with $\mu$ the chemical potential. If positive, the compressibility can be expressed in terms of the speed of sound $c$ in the fictitious system with only short-range interactions as

$$n \kappa = 1/m c^2. \quad (5)$$

Equation (5) can then be cast in the equivalent form

$$\lim_{q \to 0} \epsilon(q,0) = 1 + \frac{\omega_{\text{pl}}^2}{c^2 q^2}, \quad (6)$$

corresponding to the spectrum $\omega^2 = \omega_{\text{pl}}^2 + c^2 q^2$ of the plasma mode, where $\omega_{\text{pl}}$ denotes the plasma frequency, $\omega_{\text{pl}}^2 = 4\pi n e^2/m$. The plasmon spectrum differs from the gapless spectrum $\omega^2 = c^2 q^2$ of the sound mode of the fictitious system in that, due to the long range of the Coulomb interaction, the former has an energy gap. At short wavelengths ($c q > \omega_{\text{pl}}$), the difference is negligible, thereby allowing use
of the plasmon to access, via $c$, the screened interaction as a function of the coupling constant—at least for $r_s < 1$.

In the limit $r_s \to 0$, the screened response function reduces to (minus) the density of states $\nu_0 = m \hbar k_F / \pi^2$ at the Fermi surface. Simultaneously, $\epsilon^2 = \epsilon_0^2 = v_F^2 / 3$, with $v_F = \hbar k_F / m$ the Fermi velocity, and the Thomas-Fermi approximation for the dielectric function is recovered.

Owing to its short-range interactions, the fictitious system can be described by Fermi liquid theory. The elementary excitations are fermionic quasiparticles of mass $m^*$, with an interaction characterized by spin symmetric $(s)$ and spin antisymmetric $(a)$ Landau parameters $F_{\ell}^{s,a}$, where $\ell$ denotes the angular momentum channel. The Landau parameters depend on $r_s$ and vanish in the limit $r_s \to 0$, where also $m^* \to m$.

The speed of sound in the fictitious system can be expressed in these parameters as follows

$$c^2 = (1 + F_0^2)(m/m^*)\epsilon_0^2. \quad (7)$$

Due to the Pauli exclusion principle, even with an attractive interaction, a Fermi liquid can still support a sound mode, provided that $F_0^2 > -1$.

Approximate calculations indicate that the effective mass is comparable to the free electron mass, while the Landau parameter $F_0^2$ is negative. The latter implies an attractive quasiparticle interaction in the spin-symmetric $(s)$ or spin antisymmetric $(a)$ Landau parameter.

At the level of the first-order correction to the ground-state energy of a free Fermi gas, which itself is a 1-loop result, the origin can be understood as follows. Two Feynman diagrams contribute to the 2-loop, or Hartree-Fock correction: the direct, or Hartree term containing two fermion loops, and the exchange term containing only one fermion loop. The latter implies an attractive quasiparticle interaction in the spin-symmetric $(s)$ or spin antisymmetric $(a)$ Landau parameter.

The unique character of the point $r_s = r_s$ can also be noted when considering the spatial average of the electrostatic potential generated by the static test charge at the origin

$$\int d^3x \varphi(x) = \varphi(q = 0) = \frac{Z}{e^2\pi \kappa^2}. \quad (10)$$

where $\varphi(q) = 4\pi Z/c(q,0)q^2$. When the inverse compressibility becomes negative, the overall potential changes sign as well.

To investigate the strong-coupling regime, we use a parametrized expression for the local-field correction $G(q)$ as it appears in the generalized random phase approximation of the screened response function

$$\chi_{sc}(q,0) = \frac{\chi_0(q,0)}{1 + v(q)G(q)\chi_0(q,0)} \quad (11)$$

proposed by Ichimaru and Utsumi. Here, $\chi_0(q,0)$ denotes the response function of a free Fermi gas at zero frequency. The random phase approximation is recovered by setting $G(q)$ to unity. Since only the zero-frequency response function is required to study the condition (8), we can sidestep the difficulties which arise when the frequency dependence is included in $G(q)$ to arrive at the dynamic correction. The parametrized expression, which applies to the range $0 < r_s < r_s$ incorporates Monte Carlo data on the ground-state energy as well as the ladder diagram calculation of the pair...
distribution function at zero separation. Importantly, the resulting dielectric function satisfies a number of exact boundary conditions and sum rules, including the compressibility sum rule. As noted in the overview, these features and its simplicity makes the parametrized expression proposed in Ref. 4 convenient for applications.

The compressibility sum rule determines the behavior of the local-field correction at long wavelengths. With the definition

$$\lim_{q \to 0} G(q) = \gamma_0(r_s) q^2,$$

(12)

where $\hat{q} = q/k_F$, it follows from Eq. (6) and a similar expression for the noninteracting system with compressibility $\kappa_0$, that the coefficient $\gamma_0(r_s)$ is related to the compressibility via

$$\frac{\kappa_0}{\kappa} = 1 - \frac{4\alpha}{\pi} \gamma_0(r_s) r_s.$$

(13)

The compressibility of a 3DEG can be extracted from the Monte Carlo data of Ceperly and Alder, thus fixing $\gamma_0(r_s)$. In particular, when the inverse compressibility changes sign it becomes

$$\gamma_0(\bar{r}_s) = \frac{\pi}{4\alpha} \frac{1}{r_s}.$$

(14)

Because the compressibility sum rule is satisfied, the parametrized expression for the dielectric function,

$$\epsilon(q, 0) = 1 - v(q)\chi_{\text{sc}}(q, 0),$$

(15)

with $\chi_{\text{sc}}$ given by Eq. (14), becomes negative for small wavevectors also at $r_s = \bar{r}_s$, as it should.

With the expression (15) substituted and the left hand expanded in a Taylor series to order $q^4$, Eq. (8) leads to the condition:

$$a_0 + a_2 \hat{q}^2 + a_4 \hat{q}^4 = 0,$$

(16)

valid at long wavelengths. The quartic term is included because the first term in the expansion,

$$a_0 = \frac{(4\alpha/\pi)r_s}{1 - (4\alpha/\pi)\gamma_0(r_s)r_s},$$

(17)

changes sign at $r_s = \bar{r}_s$. The coefficients $a_2$ and $a_4$ have no simple analytic representation, depending on the specific parametrization of the local-field correction $G(q)$. They are best represented simply by their numerical values for each $r_s$. The coefficients diverge at $r_s = \bar{r}_s$. As a result of which, a small region just below $\bar{r}_s$ is numerically inaccessible.

The physical solution $q(r_s)$ of the condition (16), which is a quadratic equation in $q^2$, remains purely imaginary in the entire regime where $1/\kappa > 0$, as it is at weak coupling (see Fig. 2). The corresponding screening length $\lambda = i/q(r_s)$, being infinite at $r_s = 0$, decreases with increasing coupling constant until it reaches a minimum $\lambda/a \approx 0.30$ at $r_s \approx 3.2$. Further increasing $r_s$ surprisingly increases $\lambda/a$ again until it becomes infinite once more at $r_s = \bar{r}_s \approx 5.25$, where the inverse compressibility changes sign and the sound mode of the

![FIG. 1: Real (Re) and imaginary (Im) part of the wavevector $q(r_s)$ solving the condition (16). The grey region just below $r_s = \bar{r}_s \approx 5.25$ could not be accessed because of numerical instabilities in the expansion coefficients.](image)
The plasma frequency,\footnote{The plasma frequency in 3D is \( \omega_{pl} = (4\pi e^2/\varepsilon_{0}m)^{1/2} \).} the deviation of the screened from the unscreened Coulomb potential is measured at short distances from a test charge.\footnote{A test charge is a particle of charge \( q \) at a distance \( r \) from a charged system.} It is defined by writing the electrostatic potential generated by a static test charge at the origin [see below Eq. (10)] as
\[
\varphi(x) = \frac{Z}{x} \left[ 1 + \frac{2}{\pi} \int_0^\infty dq \left( \frac{1}{\epsilon(q,0)} - 1 \right) \sin(qx) \right], \tag{18}
\]
and expanding the right side in a Taylor series for small \( x \),
\[
\varphi(x) = \frac{Z}{x} \left( 1 - \frac{x}{\lambda_s} + \cdots \right), \tag{19}
\]
with
\[
\frac{a}{\lambda_s} = \left( \frac{18}{\pi^2} \right)^{1/3} \int_0^\infty dq \left[ 1 - \frac{1}{\epsilon(q,0)} \right]. \tag{20}
\]
Since \( 1/\epsilon(q,0) < 1 \), \( \lambda_s \) is always positive. The short-range screening length coincides with the Thomas-Fermi screening length in the limit \( r_s \to 0 \). As expected for a system coupling with an interaction that becomes increasingly stronger, \( \lambda_s \) monotonically decreases (roughly as \( r_s^{-1/2} \)) with increasing coupling constant in the entire range \( 0 < r_s < 15 \) where the parametrized expression for \( \epsilon(q,0) \) applies. The ratio \( \lambda_s/a \) is unity around \( r_s = 0.78 \). Whereas at \( r_s = r_s^* \), its value is reduced to \( \lambda_s/a \approx 0.39 \).

The exponentially damped CDW in a 3DEG arises in the nonperturbative, strong-coupling regime. It is worth considering an example where a similar ground state arises at weak coupling, to access it in perturbation theory. Such an example is provided by a charged Bose gas.

V. CHARGED BOSE GAS

A free Bose and Fermi gas differ in that, owing to the Pauli exclusion principle, the latter can support a sound mode at zero temperature, whereas the former cannot. The single-particle excitation with the spectrum \( \omega = \hbar q^2/2m \) is therefore the only gapless mode available. By repeating the argument leading to the plasmon spectrum of a 3DEG at weak coupling, we obtain the spectrum \( \omega^2 = \omega_{pl}^2 + 4\pi^2 q^2/\lambda_s^2 \) of a charged Bose gas in the limit \( r_s \to 0 \), with the same expressions for the plasma frequency, \( \omega_{pl}^2 = 4\pi ne^2/m \), and \( r_s \) as for a 3DEG. The plasma spectrum of the charged Bose gas at weak coupling corresponds to the dielectric function
\[
\lim_{q \to 0} \epsilon(q,0) = 1 + \frac{\omega_{pl}^2}{\hbar^2 q^2/4m^2}. \tag{21}
\]
These formulas agree with the perturbative results first obtained in Ref.\cite{landau} and Ref.\cite{landau2} respectively, using Bogoliubov’s method.

A solution of the condition \( \lim_{q \to 0} \epsilon(q,0) = 1 + \omega_{pl}^2/\hbar^2 q^2/4m^2 \) with the dielectric function \( \epsilon(q,0) \) is given by
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\]

The resulting ground state is an exponentially damped CDW with both the wavelength and screening length expressed as
\[
\lambda/a = 1/(3r_s)^{1/4}, \tag{23}
\]
cf. the analogous expression \( \lambda/a = 1/(3r_s)^{1/4} \) for a 3DEG.

As for a 3DEG, the exponentially damped CDW of a charged Bose gas in 3D has a negative compressibility as well. Specifically, the energy per particle given by
\[
\frac{E}{N} = -A \epsilon^2 \frac{1}{2\lambda_0} \frac{1}{r_s^3} \tag{24}
\]
to the lowest order in the loop expansion leads to
\[
\frac{1}{\kappa} = -5A \frac{\epsilon^2}{16} \frac{n}{2\lambda_0} \frac{1}{r_s^3}. \tag{25}
\]
with \( A \approx 0.8031 \). A negative compressibility is possibly a generic characteristic of an exponentially damped CDW.

VI. 2DEG

Next, 2DEGs with a \( 1/\pi \) Coulomb potential and average interparticle distance \( a = (\pi/n)^{1/2} \) are considered. The shift to 2D is facilitated by replacing the 3D Fourier transform \( 4\pi^2 q^2/\lambda_s^2 \) of the \( 1/\pi \) potential with \( 2\pi^2 q^2/\lambda_s^2 \) in the above equations. Doing so leads to a plasma frequency
\[
\omega_{pl}^2 = 2\pi ne^2/m, \tag{26}
\]
which depends on \( q \) and tends to zero for vanishing wavevectors. That is, although harder than the gapless modes of the corresponding fictitious fermionic and bosonic systems, the resulting plasma modes are, unlike their 3D counterparts, gapless. Most of the striking features of the 3D systems, such as negative compressibility\footnote{Negative compressibility \( \kappa = -5A \epsilon^2/n \pi^2(\pi/n)^{1/2} \) in 3D is also found.} and the Landau parameter \( \ell_n^2 \) taking the value \( -1 \) at the point where the inverse compressibility changes sign\footnote{In 3D, \( \ell_n^2 \) is found to be negative.} and overscreening\footnote{In 3D, \( \ell_n^2 \) is found to be positive.} are nevertheless also found in 2D.

One noteworthy difference is that the condition \( \epsilon(q,0) = 1 + \omega_{pl}^2/\hbar^2 q^2/4m^2 \) for a 2DEG with the weak-coupling expression for the dielectric function \( \epsilon(q,0) \) and the plasma frequency \( \omega_{pl}^2 \)
\[
q^2 + 2\pi ne^2/mc^2 = 0, \tag{27}
\]
has no physical solution. In accordance with the gapless plasmon spectrum, this implies the absence of Thomas-Fermi screening.

The 2DEG’s dielectric function \( \epsilon(q,0) \) has not been determined to the extent the 3DEG’s functions have. However, the local-field correction proposed in Ref.\cite{landau3} incorporating the variational Monte Carlo data on the ground-state energy and the compressibility by Tanatar and Ceperley\cite{tanatar} serves our purposes as the corresponding dielectric function satisfies the compressibility sum rule. Specifically, with the definition
\[
\lim_{q \to 0} G(q) = \gamma_0(r_s)q \tag{28}
\]
appropriate for 2D, it follows from the compressibility sum rule (3), with $\chi_{sc}(q, 0)$ given by Eq. (11), that the coefficient $\gamma_0(r_s)$ is fixed by the compressibility via

$$\frac{\kappa_0}{\kappa} = 1 - \frac{\sqrt{2}}{\pi} \gamma_0(r_s) r_s.$$  

(29)

The local-field correction was determined in Ref. 13 only at discrete values of $r_s$. We use a simple interpolating procedure to obtain $G(q)$ for arbitrary values of $r_s$ in the entire interval $0 \leq r_s \leq 40$.

At the value $r_s = \bar{r}_s$ where the inverse compressibility changes sign, with $r_s \approx 2.03$ according to the Monte Carlo data, the dielectric function becomes negative for small wavevectors. As for a 3DEG, the long-wavelength solution of the condition (3), with a factor $q$ included instead of $q^2$, changes here qualitatively. The resulting equation is quadratic in $q$ rather than $q^2$,

$$a_0 + a_1 q + a_2 q^2 = 0,$$  

(30)

with

$$a_0 = \frac{(\sqrt{2}/\pi) r_s}{1 - (\sqrt{2}/\pi) \gamma_0(r_s) r_s},$$  

(31)

while the two remaining coefficients are again best represented by their numerical values.

For $r_s < \bar{r}_s$, no physical solution is found, implying that in this entire regime screening is absent and the plasmon mode gapless, as in the weak-coupling limit [see below Eq. (27)]. For $r_s > \bar{r}_s$, a complex solution with positive real and imaginary parts emerges, signalling an exponentially damped CDW in a 2DEG (see Fig. 2). Contrary to the 3D case, the imaginary part of the solution is larger than the real part in the entire regime where the parametrization applies.

In conclusion, 2DEGs and 3DEGs at negative compressibility, where test charges are overscreened, were argued to have an exponentially damped CDW as ground state. The wavevector characterizing this state is complex and varies with the electron number density. The real part vanishes above the critical density, where the inverse compressibility changes sign and the system becomes homogeneous.

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