Duality relations for elastic constants of the classical Gaussian core model

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The many-body Gaussian core model involves a potential energy function that consists of a sum of repelling pair interactions, each of which is a simple Gaussian function of distance. This paper examines the linear elastic response of the model for its stable lattices at absolute zero temperature, in $D=1$, 2, and 3 dimensions. Owing to the fact that the Gaussian function is self-similar under Fourier transformation, exact relations exist connecting each elastic constant at number density ρ to a partner at dual density ρ' in the reciprocal lattice, where $\rho\rho'=\pi^{-D}$. By using these identities, it has been possible to show that shear elastic constants in $D=2$ and 3 tend strongly to zero in the asymptotic high density limit.

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I. INTRODUCTION

The classical Gaussian core model (GCM) consists of a set of N identical structureless particles subject to the following interaction potential:

$$\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\sum_{i<j}\exp(-r_{ij}^2). \tag{1.1}$$

Here we have chosen to use the height and range of the pair Gaussians as natural energy and length units, and r_{ij} represents the scalar distance between particles i and j. Part of the scientific motivation for considering this model is that it provides a simple representation for the effective interaction operating between polymer coils or flexible dendrimers suspended in suitable solvents [1–4]. However, the GCM also exhibits some unusual mathematical properties [5–8] that generate additional interest, which consequently warrants examination of the model in a broad analytical context, including variable space dimension D.

The ground-state (zero temperature) structures for the GCM are relatively simple, in which all particles are equivalent. For the linear case, $D=1$, it is the elementary periodic array. In the planar version, $D=2$, the ground-state structure is the six-coordinate triangular lattice at all densities. Two distinct structures appear in $D=3$; at low density the face-centered cubic crystal predominates, while at high density the body-centered cubic form takes over [4,5,7,8]. These classical ground states have lattice energies that satisfy duality relations which link pairs of low and high densities. Specifically, let $\phi(\rho)$ denote the lattice energy per Gaussian particle in any one of these cases, where ρ is the number density. Then it has been demonstrated that [7,8]

$$\rho^{-1/2}[1+2\phi(\rho)]=(\rho')^{-1/2}[1+2\phi(\rho')], \tag{1.2}$$

where ρ' is a density dual to ρ satisfying

$$\rho\rho'=\pi^{-D}. \tag{1.3}$$

In particular, Eq. (1.2) connects the lattice energies of the face-centered and body-centered cubic structures for $D=3$, and establishes that these energies are equal at the self-dual density $\pi^{-3/2}$.

The objective of the present paper is to explore extensions of the above duality relation to include uniformly strained versions of the ground-state crystals. The focus remains on the zero temperature limit for the GCM, and strains will be limited to infinitesimal values. Consequently the results concern linear elastic response. Section II provides the necessary background and definitions for the generalization to be exploited. Section III concentrates on the $D=2$ case, the elastically distorted triangular lattice. Section IV analyzes the $D=3$ case, for which elastic constants of the low-density face-centered cubic crystal are linked to the elastic constants of the high-density body-centered cubic crystal. Finally, Sec. V contains some remarks about connections to other aspects of the GCM, including its phonon spectra.

II. PRELIMINARIES

The most basic elastic response is that produced by isotropic (hydrostatic) stress. It can be described in the present context simply by the inverse of the zero-temperature compressibility $\kappa(\rho)$. A connection between low and high density behaviors of this quantity, and of the zero-temperature pressure p, for the GCM's can readily be inferred from the elementary duality relation (1.2) above. These quantities are connected to the lattice energy $\phi(\rho)$ by the relations

$$p(\rho)=\rho^2[d\phi(\rho)/d\rho],$$
$$1/\kappa(\rho)=\rho[dp(\rho)/d\rho]. \tag{2.1}$$

By applying density derivatives to Eq. (1.2), while accounting for the dual-density definition Eq. (1.3), and finally rearranging the results, one finds

$$p(\rho')=\pi^{-3D/2}\{(2\rho^2)^{-1}[1+2\phi(\rho)]-\rho^{-3}p(\rho)\} \tag{2.2}$$

and

$$[\kappa(\rho')]^{-1}=\pi^{-3D/2}\{\rho^{-2}[1+2\phi(\rho)]-4\rho^{-3}p(\rho)+[\rho^3\kappa(\rho)]^{-1}\}. \tag{2.3}$$

These relations offer the benefit of ready evaluation for p and κ^{-1} at high density at which many neighbor particles inter-

act, in terms of the low density properties that enjoy the simplification of weak near-neighbor interactions only.

Before application of a homogeneous linear strain field, the zero-temperature GCM lattice will present a state of isotropic stress, characterized by its pressure p. The strain subsequently causes the initial lattice energy Φ_0 to rise to the higher value Φ [9]:

$$\Phi-\Phi_0=\{-p[u_{ii}+(1/2)(u_{ii}u_{jj}-u_{ii}^2)] +(1/2)\lambda_{ijkl}u_{ij}u_{kl}\}\Omega, \tag{2.4}$$

with neglect of terms with cubic and higher orders in the strain components. Here Ω is the unstrained system content (length, area, or volume), the u_{ij} are elements of the symmetric strain tensor in a Cartesian coordinate system, and the λ_{ijkl} are elements of the corresponding fourth-order elastic tensor [9]. The Einstein summation convention applies to terms with repeated subscripts.

For $D=1$ the strain and elastic tensors have only single elements, u_{xx} and λ_{xxxx}. Furthermore, it is easily shown for this simple case that

$$\lambda_{xxxx}(\rho)=1/\kappa(\rho) \quad (D=1). \tag{2.5}$$

As a result, the earlier Eq. (2.3) permits this single $D=1$ elastic constant at high density to be evaluated in terms of quantities at the dual low density.

On account of its symmetry (hexagonal), the triangular ground state crystal for the GCM in two dimensions has its elastic energy terms in Eq. (2.4) reduced to inclusion of only two distinct elastic constants [9]:

$$\tfrac{1}{2}\lambda_{ijkl}u_{ij}u_{kl}\rightarrow 2\lambda_{\xi\eta\xi\eta}(u_{xx}+u_{yy})^2+\lambda_{\xi\xi\eta\eta} \times[(u_{xx}-u_{yy})^2+4u_{xy}^2]. \tag{2.6}$$

Isotropic compression or expansion involves only the first of the two surviving elastic terms. By comparing that first term to the directly-computed work of compression or expansion, one finds the two-dimensional analog of Eq. (2.5):

$$\lambda_{\xi\eta\xi\eta}(\rho)=1/[4\kappa(\rho)] \quad (D=2). \tag{2.7}$$

Once again, this connection, and the prior Eq. (2.3), permit evaluation of this elastic quantity at high density in terms of the dual low-density quantities. Computation of the second elastic constant in Eq. (2.6) forms the subject of the next Sec. III.

In the case of the cubic lattices (fcc and bcc) that provide the ground-state structures in three dimensions, the elastic energy adopts a form with three independent elastic constants [9]:

$$\tfrac{1}{2}\lambda_{ijkl}u_{ij}u_{kl}\rightarrow\tfrac{1}{2}\lambda_{xxxx}(u_{xx}^2+u_{yy}^2+u_{zz}^2)+\lambda_{xxyy}(u_{xx}u_{yy} +u_{xx}u_{zz}+u_{yy}u_{zz})+2\lambda_{xyxy}(u_{xy}^2+u_{xz}^2+u_{yz}^2). \tag{2.8}$$

Isotropic strain now involves the first two of these, which are then found to have the following relation to the pressure and compressibility of the lattice:

$$\tfrac{1}{2}\lambda_{xxxx}(\rho)+\lambda_{xxyy}(\rho)=3/[2\kappa(\rho)] \quad (D=3). \tag{2.9}$$

Section IV below examines two types of anisotropic strains that, in addition to this last result, offer separate expressions for all three cubic-symmetry elastic constants.

The high-density behaviors of Eqs. (2.5), (2.7), and (2.9) depend upon that of the compressibility function. It is straightforward to show from Eqs. (1.2) and (2.1) that

$$1/\kappa(\rho)\sim\pi^{D/2}\rho^2 \quad (\rho\rightarrow\infty). \tag{2.10}$$

III. TRIANGULAR LATTICE, $D=2$

One elastic constant, $\lambda_{\xi\xi\eta\eta}$, remains to be examined for the triangular lattice. For this purpose, the system will be subjected to a uniform area-preserving strain that stretches the lattice along one direction, while compressing it along the perpendicular direction. Particle positions in the strained configuration are determined by integer multiples of two basis vectors $\mathbf{b}_1(\varepsilon)$ and $\mathbf{b}_2(\varepsilon)$,

$$\mathbf{r}_j(\varepsilon)=n_1(j)\mathbf{b}_1(\varepsilon)+n_2(j)\mathbf{b}_2(\varepsilon). \tag{3.1}$$

Here ε is a measure of the imposed strain. Specifically, we choose the basis vectors to be the following:

$$\mathbf{b}_1(\varepsilon)=a(1+\varepsilon)\mathbf{u}_x,$$
$$\mathbf{b}_2(\varepsilon)=a\left[\frac{(1+\varepsilon)}{2}\mathbf{u}_x+\frac{3^{1/2}}{2(1+\varepsilon)}\mathbf{u}_y\right], \tag{3.2}$$

where a is the nearest-neighbor separation in the unstrained lattice,

$$a(\rho)=[2/(3^{1/2}\rho)]^{1/2}, \tag{3.3}$$

and where $\mathbf{u}_x$ and $\mathbf{u}_y$ are unit vectors along the x and y directions, respectively. Notice that the choice (3.2) orients the lattice, regardless of strain, so that one of its principal directions (lines of particles) is parallel to the x axis.

The strain tensor corresponding to the basis vectors (3.2) has the elements

$$u_{xx}=\varepsilon,$$
$$u_{yy}=-\varepsilon+O(\varepsilon^2), \tag{3.4}$$
$$u_{xy}=0.$$

Equations (2.4) and (2.6) then assign the following expression to the energy rise due to strain:

$$[\Phi(\varepsilon)-\Phi_0]/N=\phi(\rho,\varepsilon)-\phi(\rho,0) =4\lambda_{\xi\xi\eta\eta}(\rho)\varepsilon^2/\rho+O(\varepsilon^3). \tag{3.5}$$

Present interest focuses on the leading term describing linear elastic response, but it should be noted in passing that sub-

sequent terms with odd orders in ε can arise in principle, because nonzero strains ε and $-\varepsilon$ are not equivalent.

By formally including a self-interaction term, $\phi(\rho,\varepsilon)$ may be expressed simply as the integral of the product of the Gaussian interaction and the periodic lattice density function $\rho^{(1)}(\mathbf{r},\varepsilon)$:

$$1+2\phi(\rho,\varepsilon)=\int \exp(-r^2)\rho^{(1)}(\mathbf{r},\varepsilon)d\mathbf{r}, \tag{3.6}$$

$$\rho^{(1)}(\mathbf{r},\varepsilon)=\sum_{n_1,n_2}\delta[\mathbf{r}-n_1\mathbf{b}_1(\varepsilon)-n_2\mathbf{b}_2(\varepsilon)]. \tag{3.7}$$

Because it is periodic, $\rho^{(1)}$ can alternatively be expressed as a Fourier sum [after representing delta functions in Eq. (3.7) temporarily as narrow normalized Gaussians]:

$$\rho^{(1)}(\mathbf{r},\varepsilon)=\rho\lim_{\alpha\to\infty}\sum_{\mathbf{K}(\varepsilon)}\exp[i\mathbf{K}(\varepsilon)\cdot\mathbf{r}-\mathbf{K}^2(\varepsilon)/(4\alpha)]. \tag{3.8}$$

The sum in this last expression spans the lattice that is reciprocal to that generated by $\mathbf{b}_1(\varepsilon)$ and $\mathbf{b}_2(\varepsilon)$:

$$\mathbf{K}(\varepsilon)=m_1\mathbf{K}_1(\varepsilon)+m_2\mathbf{K}_2(\varepsilon). \tag{3.9}$$

Here m_1 and m_2 cover positive and negative integers, and zero, and $\mathbf{K}_1(\varepsilon)$ and $\mathbf{K}_2(\varepsilon)$ are the basis vectors for that reciprocal lattice, and therefore satisfy the relations [10]

$$\mathbf{K}_i(\varepsilon)\cdot\mathbf{b}_j(\varepsilon)=2\pi\delta_{ij}. \tag{3.10}$$

One readily finds

$$\mathbf{K}_1(\varepsilon)=\left(\frac{4\pi}{3^{1/2}a}\right)\left[\left(\frac{3^{1/2}}{2(1+\varepsilon)}\right)\mathbf{u}_x-\left(\frac{1+\varepsilon}{2}\right)\mathbf{u}_y\right],$$

$$\mathbf{K}_2(\varepsilon)=\left(\frac{4\pi}{3^{1/2}a}\right)(1+\varepsilon)\mathbf{u}_y. \tag{3.11}$$

Upon substituting expression (3.8) for $\rho^{(1)}$ into the right member of Eq. (3.6), one finds

$$1+2\phi(\rho,\varepsilon)=\pi\rho\lim_{a\to\infty}\sum_{\mathbf{K}(\varepsilon)}\exp[-(1+1/\alpha)K^2(\varepsilon)/4]$$

$$=\pi\rho\sum_{m_1,m_2}\exp\{-[m_1\mathbf{K}_1(\varepsilon)+m_2\mathbf{K}_2(\varepsilon)]^2/4\}. \tag{3.12}$$

Notice that this is also a lattice sum for a Gaussian interaction, but with an extra divisor 4 in the exponent. Formally this is equivalent to the simple Gaussian summed over a lattice with half the spacing, i.e., with basis vectors

$$\mathbf{K}_1(\varepsilon)/2,\quad \mathbf{K}_2(\varepsilon)/2. \tag{3.13}$$

One easily sees from Eqs. (3.11) that this latter pair of basis vectors generates a lattice with number density equal to

$$\rho'=(\pi^2\rho)^{-1}, \tag{3.14}$$

the density that is dual to ρ, Eq. (1.3). Furthermore, the rescaled reciprocal lattice generated by basis vectors (3.13) is itself a triangular lattice subject to homogeneous strain, with

$$u_{xx}=-\varepsilon+O(\varepsilon^2),$$

$$u_{yy}=\varepsilon, \tag{3.15}$$

$$u_{xy}=0.$$

In spite of the fact that the strain direction has been rotated by $\pi/2$ compared to that initially imposed on the starting lattice, Eq. (3.4), the linear elastic response is similar. As a result, within the linear response regime Eq. (3.12) is equivalent to

$$\rho^{-1/2}[1+2\phi(\rho,\varepsilon)]=(\rho')^{-1/2}[1+2\phi(\rho',\varepsilon)], \tag{3.16}$$

a straightforward extension of the original duality relation (1.2). Equation (3.5) above allows this last expression to be recast in terms of the elastic constants at the dual densities:

$$\rho^{-3/2}\lambda_{\xi\xi\eta\eta}(\rho)=(\rho')^{-3/2}\lambda_{\xi\xi\eta\eta}(\rho'). \tag{3.17}$$

Equation (3.17) of course reduces to a triviality at the self-dual density π^{-1}. However, it produces a nontrivial insight when one of the densities, say ρ, is very low, and its dual ρ' is very high. In that circumstance, the shear elastic constant $\lambda_{\xi\xi\eta\eta}(\rho)$ will be determined solely be the weak Gaussian tail of widely separated nearest neighbors in the sparse triangular lattice, and consequently will vanish exponentially as $\rho\to 0$. A straightforward calculation shows that in this low-density limit

$$\lambda_{\xi\xi\eta\eta}(\rho)\sim\left(\frac{1}{\rho}-3^{1/2}\right)\exp\left[-\frac{2}{3^{1/2}\rho}\right]\quad(\rho\to 0). \tag{3.18}$$

By subsequently applying the duality relation (3.17), one finds that in the high-density asymptotic regime

$$\lambda_{\xi\xi\eta\eta}(\rho')\sim(\pi\rho')^3(\pi^2\rho'-3^{1/2})\exp\left[-\frac{2\pi^2\rho'}{3^{1/2}}\right]$$

$$(\rho'\to\infty), \tag{3.19}$$

implying a remarkable mechanical weakness of the triangular lattice under high compression. On account of the fact that $\lambda_{\xi\xi\eta\eta}$ vanishes in both limits, it is evident that it must pass through at least a single maximum at intermediate density.

IV. CUBIC LATTICES, $D=3$

To begin the analysis in the three-dimensional context, let a uniformly strained face-centered cubic lattice be generated by the following combination of basis-vector integer multiples:

$$\mathbf{r}_j(\varepsilon)=n_1(j)\mathbf{b}_1(\varepsilon)+n_2(j)\mathbf{b}_2(\varepsilon)+n_3(j)\mathbf{b}_3(\varepsilon), \tag{4.1}$$

where, as before, ε measures the strain. The corresponding energy per particle $\phi(\rho,\varepsilon)$ can then be expressed in the same manner as was used for the two-dimensional case, Eqs. (3.6) and (3.7):

$$1+2\phi(\rho,\varepsilon)=\int \exp(-r^2)\rho^{(1)}(\mathbf{r},\varepsilon)d\mathbf{r}, \tag{4.2}$$

$$\rho^{(1)}(\mathbf{r},\varepsilon)=\sum_{n_1,n_2,n_3}\delta[\mathbf{r}-n_1\mathbf{b}_1(\varepsilon)-n_2\mathbf{b}_2(\varepsilon)-n_3\mathbf{b}_3(\varepsilon)]. \tag{4.3}$$

Also, as before [Eq. (3.8)], the periodic singlet density distribution $\rho^{(1)}(\rho,\varepsilon)$ can be written as a Fourier series involving terms from the appropriate reciprocal lattice,

$$\rho^{(1)}(\mathbf{r},\varepsilon)=\rho\lim_{\alpha\to\infty}\sum_{\mathbf{K}(\varepsilon)}\exp[i\mathbf{K}(\varepsilon)\cdot\mathbf{r}-\mathbf{K}^2(\varepsilon)/(4\alpha)], \tag{4.4}$$

$$\mathbf{K}(\varepsilon)=m_1\mathbf{K}_1(\varepsilon)+m_2\mathbf{K}_2(\varepsilon)+m_3\mathbf{K}_3(\varepsilon), \tag{4.5}$$

where the $\mathbf{K}_i(\varepsilon)$ are determined by the basic Eq. (3.10). After substituting Eq. (4.4) into Eq. (4.2), and carrying out the $\mathbf{r}$ integration, the result is the three-dimensional analog of the prior Eq. (3.12) for the strained triangular lattice:

$$1+2\phi(\rho,\varepsilon)=\pi^{3/2}\rho\sum_{m_1,m_2,m_3}\exp\{-[m_1\mathbf{K}_1(\varepsilon)+m_2\mathbf{K}_2(\varepsilon)+m_3\mathbf{K}_3(\varepsilon)]^2/4\}. \tag{4.6}$$

The right member of this last equality amounts to a sum of the simple Gaussian pair interaction over all relative positions in a lattice whose basis vectors are $\mathbf{K}_i(\varepsilon)/2$, and whose number density is just the dual density

$$\rho'=(\pi^3\rho)^{-1}. \tag{4.7}$$

Consequently we can write

$$\rho^{-1/2}[1+2\phi(\rho,\varepsilon)]=(\rho')^{-1/2}[1+2\phi^{(\mathrm{rec})}(\rho',\varepsilon)], \tag{4.8}$$

the three-dimensional version of the former Eq. (3.16), now generally involving energies per particle for distinct structures, the direct and reciprocal (rec) lattices.

In order to exploit this last identity for elastic properties, we shall first examine the constant-volume deformation that dilates the face-centered cubic lattice in the x direction, while contracting it by a compensating amount in the y direction; the z direction will remain unstrained. If the number density of the lattice is ρ, the corresponding forms assigned to the $\mathbf{r}$-space basis vectors will be

$$\begin{aligned}\mathbf{b}_1(\varepsilon)&=(2\rho)^{-1/3}[(1+\varepsilon)\mathbf{u}_x+(1+\varepsilon)^{-1}\mathbf{u}_y],\\ \mathbf{b}_2(\varepsilon)&=(2\rho)^{-1/3}[(1+\varepsilon)\mathbf{u}_x+\mathbf{u}_z],\\ \mathbf{b}_3(\varepsilon)&=(2\rho)^{-1/3}[(1+\varepsilon)^{-1}\mathbf{u}_y+\mathbf{u}_z].\end{aligned} \tag{4.9}$$

The reciprocal lattice basis vectors then follow from Eq. (3.10):

$$\begin{aligned}\mathbf{K}_1(\varepsilon)&=\pi(2\rho)^{1/3}[(1+\varepsilon)^{-1}\mathbf{u}_x+(1+\varepsilon)\mathbf{u}_y-\mathbf{u}_z],\\ \mathbf{K}_2(\varepsilon)&=\pi(2\rho)^{1/3}[(1+\varepsilon)^{-1}\mathbf{u}_x-(1+\varepsilon)\mathbf{u}_y+\mathbf{u}_z],\\ \mathbf{K}_3(\varepsilon)&=\pi(2\rho)^{1/3}[-(1+\varepsilon)^{-1}\mathbf{u}_x+(1+\varepsilon)\mathbf{u}_y+\mathbf{u}_z].\end{aligned} \tag{4.10}$$

This latter set generates a body-centered cubic lattice subject to a volume-preserving uniform strain that contracts along the along the x direction by factor $(1+\varepsilon)^{-1}$, and expands along the y direction by factor $1+\varepsilon$. The same factors of course apply to the lattice with bases $\mathbf{K}_i(\varepsilon)/2$ that are relevant to Eq. (4.8), and aside from a direction rotation of $\pi/2$, this is the same uniform strain applied to the starting face-centered cubic lattice, Eqs. (4.9). In view of these facts, both members of Eq. (4.8) can be interpreted in terms of the appropriate combination of linear elastic constants, for small ε:

$$\begin{aligned}&\rho^{-3/2}[\lambda^{(f)}_{xxxx}(\rho)-\lambda^{(f)}_{xxyy}\rho)]\\ &\quad=(\rho')^{-3/2}[\lambda^{(b)}_{xxxx}(\rho')-\lambda^{(b)}_{xxyy}(\rho')].\end{aligned} \tag{4.11}$$

Here the superscripts f and b refer respectively to the face-centered cubic and body-centered cubic lattices. By applying the earlier relation (2.9) both at ρ and at ρ', individual duality relations (with identical forms) for each of the two elastic constants in Eq. (4.11) can be obtained:

$$\begin{aligned}&\rho^{-3/2}[\lambda^{(f)}_{xxxx}(\rho)-1/\kappa^{(f)}(\rho)]\\ &\quad=(\rho')^{-3/2}[\lambda^{(b)}_{xxxx}(\rho')-1/\kappa^{(b)}(\rho')],\end{aligned} \tag{4.12}$$

$$\begin{aligned}&\rho^{-3/2}[\lambda^{(f)}_{xxyy}(\rho)-1/\kappa^{(f)}(\rho)]\\ &\quad=(\rho')^{-3/2}[\lambda^{(b)}_{xxyy}(\rho')-1/\kappa^{(b)}(\rho')].\end{aligned} \tag{4.13}$$

One cubic-symmetry elastic constant remains to be investigated, namely λ_{xyxy}. For that purpose, consider the face-centered cubic lattice at density ρ subject to a pure shear deformation. The following set of basis functions satisfies that objective, where the only nonzero element of the strain tensor is $u_{xy}=\varepsilon/2$:

$$\begin{aligned}\mathbf{b}_1(\varepsilon)&=(2\rho)^{-1/3}[(1+\varepsilon)\mathbf{u}_x+\mathbf{u}_y],\\ \mathbf{b}_2(\varepsilon)&=(2\rho)^{-1/3}[\mathbf{u}_x+\mathbf{u}_z],\\ \mathbf{b}_3(\varepsilon)&=(2\rho)^{-1/3}[\varepsilon\mathbf{u}_x+\mathbf{u}_y+\mathbf{u}_z].\end{aligned} \tag{4.14}$$

These lead to reciprocal-lattice basis vectors:

$$\begin{aligned}\mathbf{K}_1(\varepsilon)&=\pi(2\rho)^{1/3}[\mathbf{u}_x+(1-\varepsilon)\mathbf{u}_y-\mathbf{u}_z],\\ \mathbf{K}_2(\varepsilon)&=\pi(2\rho)^{1/3}[\mathbf{u}_x-(1+\varepsilon)\mathbf{u}_y+\mathbf{u}_z],\\ \mathbf{K}_3(\varepsilon)&=\pi(2\rho)^{1/3}[-\mathbf{u}_x+(1+\varepsilon)\mathbf{u}_y+\mathbf{u}_z],\end{aligned} \tag{4.15}$$

corresponding to a body-centered cubic lattice subject to the pure shear $u_{xy}=-\varepsilon/2$. Then as a deduction from the general duality relation (4.8), and the definition (2.8) of the elastic constant, one finally has

$$\rho^{-3/2}\lambda^{(f)}_{xyxy}(\rho)=(\rho')^{-3/2}\lambda^{(b)}_{xyxy}(\rho'), \tag{4.16}$$

a result directly analogous to that for the triangular lattice shear constant, Eq. (3.17).

At low density, $\lambda^{(f)}_{xyxy}$ depends only on nearest-neighbor interactions. Owing to this simplification, it is an easy matter to show that

$$\lambda^{(f)}_{xyxy}(\rho)\sim(A\rho^{-1/3}-B\rho^{1/3})\exp(-2^{1/3}\rho^{-2/3}) \quad (\rho\to 0),$$
$$A=2^{5/3}, \tag{4.17}$$
$$B=2^{7/3}.$$

The elastic-constant duality relation (4.16) then allows assignment of the high-density asymptote:

$$\lambda^{(b)}_{xyxy}(\rho')\sim[A'(\rho')^{10/3}-B'(\rho')^{8/3}] \times\exp[-2^{1/3}\pi^2(\rho')^{2/3}] \quad (\rho'\to\infty),$$
$$A'=2^{5/3}\pi^{11/2},$$
$$B'=2^{7/3}\pi^{7/2}. \tag{4.18}$$

An exactly analogous calculation can be carried out for the elastic constant difference $\lambda^{(f)}_{xxxx}-\lambda^{(f)}_{xxyy}$ in the asymptotic low-density limit:

$$\lambda^{(f)}_{xxxx}(\rho)-\lambda^{(f)}_{xxyy}(\rho)\sim 2(A\rho^{-1/3}-B\rho^{1/3})\exp(-2^{1/3}\rho^{-2/3}) \quad (\rho\to 0), \tag{4.19}$$

i.e., twice the corresponding result in Eq. (4.17). Duality relation (4.11) then leads in turn to the high-density asymptote:

$$\lambda^{(b)}_{xxxx}(\rho')-\lambda^{(b)}_{xxyy}(\rho')\sim 2[A'(\rho')^{10/3}-B'(\rho')^{8/3}] \times\exp[-2^{1/3}\pi^2(\rho')^{2/3}] \quad (\rho'\to\infty). \tag{4.20}$$

These results (4.18) and (4.20) indicate that the body-centered cubic array for the Gaussian core model manifests extraordinary weakness toward shear strain in the high-density regime, analogous to that revealed earlier for the two-dimensional triangular lattice.

V. DISCUSSION

The principal objective of the present paper has been to examine a generalization of a previously-derived duality relation for the classical Gaussian core model. Specifically, this generalization considers uniformly strained versions of the zero-temperature crystals for this model in one, two, and three dimensions, and thus concerns elastic properties. In the regime of linear elastic response, the extended duality relations provide exact connections, for the linear array ($D=1$) and for the triangular lattice ($D=2$), between the values of elastic constants at dual-density pairs defined by Eq. (1.3) above. For $D=3$, the most stable crystal structures at low and at high density respectively, are face-centered cubic, and body-centered cubic, and it is identities between corresponding linear elastic constants in these reciprocal lattices that emerge from the analysis. In each of these cases, the elastic constant dualities offer a straightforward way to evaluate the high-density quantities (nominally involving particle interactions with many neighbors) in terms of their low-density partners (dominated by first-neighbor interactions). A direct implication of the dualities is that elastic constants for pure shear in the $D=2$ triangular lattice and the $D=3$ body-centered cubic lattice both tend strongly toward zero with increasing density.

Although the focus of the present study has been the linear elastic regime, this is not an intrinsic limitation. In principle it is possible to recast the development presented above so as to relate nonlinear homogeneous deformation energies at dual density pairs. In this connection, one can observe that in three dimensions a continuous uniaxial deformation path at constant density exists that smoothly transforms the face-centered-cubic array into the body-centered-cubic form. The approach followed above relates this deformation to the same continuous deformation, traversed in the opposite direction, at the dual density. This process then links nonlinear elastic energies for those lattice pairs. At the midpoint of the connecting path, there exists a single lattice structure whose elastic properties at dual low and high densities consequently become related.

A key attribute of the Gaussian pair interaction for the derivation of duality relations is that of self-similarity under Fourier transformation. The single Gaussian is the simplest example of the wider function class that possesses this attribute. Members of that class can generally be represented in the form (assuming proper integral convergence)

$$\nu(r)=\int_0^\infty w(\alpha)\exp(-\alpha r^2)d\alpha, \tag{5.1}$$

provided that the weight function $w(\alpha)$ satisfies the condition

$$\alpha^{-1/2}w(\alpha^{-1})\equiv Aw(B\alpha), \tag{5.2}$$

where A and B are positive constants. Some members of this class will display relatively simple crystal forms at absolute zero, and will qualify for study by means of an appropriately generalized duality analysis. This is a direction for extension of the present work that should be profitable to follow in the near future.

Elastic constants determine the long-wavelength portions of phonon spectra. The unusual dropoff of the two- and three-dimensional shear constants with increasing density discussed above implies a remarkable slowdown of long-wavelength transverse phonons. A full description of Gaussian core model phonon spectra is beyond the scope of the present study, but will be examined in detail in a forthcoming publication [11].

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