First-principles calculations of shear moduli for Monte Carlo–simulated Coulomb solids

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First-principles calculations of the shear modulus tensor are presented for the bcc crystalline and rapidly quenched Coulomb solids produced by the Monte Carlo simulation method. The shear moduli are calculated for temperatures up to the melting conditions, including the effects of thermal fluctuations. An effective shear modulus appropriate to an approximate "isotropic" body is introduced through averages over directions.

I. INTRODUCTION

McDermott, Hansen, Van Horn, and Buland[1] first analyzed nonradial oscillations of neutron stars, modeled as three-component stars consisting of fluid interiors, solid crusts, and fluid "oceans." Novel features in the analyses were the predictions of the bulk and interfacial modes, associated with the nonvanishing shear modulus of the crustal solid, with characteristic periodicity on the order of milliseconds.

The value of the shear modulus used for the crust was one of the "Fuchs values"[2] appropriate to the body-centered-cubic (bcc) Coulomb crystal at zero temperature and a specific mode of deformation. Generally, however, the stress-strain relations in solids should be expressed through tensors of higher order.[2,3] The shear modulus tensor should depend sensitively on the temperature, as the melting transition is approached. The value used in the calculations,[1] in fact, corresponded to the largest possible value in the tensorial shear moduli of the bcc Coulomb solids. Elucidation of the temperature dependence of the shear modulus tensor has been an outstanding problem in condensed-plasma physics and astrophysics.

In this paper we present a first-principles study of the shear modulus tensor for Coulomb solids with inclusion of temperature-dependent effects. The Coulomb solids at finite temperatures are created by the Monte Carlo (MC) simulation method in two ways: crystalline[4,5] and quenched[5,6] simulations. The free-energy increments[3,7] stemming from virtual deformations of the resultant solids are then evaluated by MC samplings of the relevant Ewald sums; these evaluations lead to determination of the temperature-dependent shear modulus tensors. Finally, we show a way to approximate the solid as an "isotropic" body by introducing an effective shear modulus through averages over directions. Application of the results to analyses of the nonradial oscillations of neutron stars will be reported elsewhere.[8]

II. MC-SIMULATED COULOMB SOLIDS

We have investigated the microscopic structures of the Coulomb solids at finite temperatures T by the MC simulation method[4–6] with the number of the MC particles, $N=1458$, distributed in the MC cell volume L^3 with the periodic boundary conditions; $n=N/L^3$ is the number density. The Coulomb coupling parameter Γ and the ion-sphere radius a are then given by

$$\Gamma=(Ze)^2/ak_BT\ , \tag{1}$$

$$a/L=(3/4\pi N)^{1/3}\ , \tag{2}$$

where Ze is the electric charge and k_B is the Boltzmann constant. The thermodynamic melting condition has been assessed[4] as $\Gamma\simeq 180$.

In the crystalline simulations, the particles were placed initially at the bcc lattice points in the cell, and $(1\sim 2)\times 10^6$ MC configurations were generated subsequently at $\Gamma=200$, 300, 400, or 800. In each case thermalization was ensured. The final states of the simulations maintain the cubic symmetry of the bcc lattice.

In the quenched simulations, starting with an equilibrated fluid state at $\Gamma=160$, we applied gradual quenches in stepwise decreases of the temperature until $\Gamma=300$, 400, or 800 was reached. Each quenched state was observed over a few times 10^8 MC configurations to ensure a metastable state. The salient feature in the ensuing freezing transition was a formation of layered structures in finite angles with respect to the MC cell axes.[6,9] It has been concluded[5,6] that the final states of the quenched Coulomb solids are bcc monocrystalline states with an admixture of a few imperfections; to a degree the cubic symmetry has been destroyed. Finally, we have a case of fluid simulation, in which a quench from $\Gamma=160$ to 200 results in a supercooled fluid state.[5,6]

III. ELASTIC-CONSTANT TENSORS

The free-energy increment δF resulting from the application of a strain u_{ij} is expressed as[3]

$$\delta F=\tfrac{1}{2}S_{ij,kl}u_{ij}u_{kl}\ . \tag{3}$$

Here $S_{ij,kl}$ is the elastic modulus tensor, the subscripts i, j, k, and l designate the Cartesian components x, y, and z, and we adopt the summation convention for repeated subscripts. For an isotropic body, Eq. (3) reduces to

$$\delta F=\tfrac{1}{2}\lambda u_{ii}^2+\mu u_{ik}u_{ik}\ . \tag{4}$$

The quantities λ and μ are Lamé coefficients.

The usual elastic constants,[2] c_{rs} $(r,s=1,2,\ldots,6)$, are derived from the elastic modulus tensor through the

transformation $(ij,kl)\rightarrow(r,s)$ of the subscripts $(xx,yy,zz,xy,yz,zx)\rightarrow(1,2,3,4,5,6)$, such that

$$c_{rs}=S_{ij,kl} \ . \tag{5}$$

For a solid with cubic symmetry, only three elastic constants remain:[3] $c_{11}=c_{22}=c_{33}$, $c_{12}=c_{21}=c_{23}=c_{32}=c_{31}=c_{13}$, and $c_{44}=c_{55}=c_{66}$. When such a solid is deformed without a change in the volume (i.e., $\sum_i u_{ii}=0$), one finds

$$\delta F=\tfrac{1}{2}(c_{11}-c_{12})u_{ii}^2+c_{44}u_{ik}u_{ik} \quad (i\neq k) \ . \tag{6}$$

The first term on the right-hand side represents a differential between two compressional deformations.

If the cubic symmetry is destroyed, as in the case of the quenched solids, more independent elements should appear. In conjunction with the first term on the right-hand side of Eq. (6), it is useful to define and introduce

$$\begin{aligned} b_{11}&=(2c_{11}-c_{12}-c_{31})/4 \ , \\ b_{22}&=(2c_{22}-c_{23}-c_{12})/4 \ , \\ b_{33}&=(2c_{33}-c_{31}-c_{23})/4 \ . \end{aligned} \tag{7}$$

The shear modulus tensor is then represented by the elements $b_{11},b_{22},b_{33},c_{44},c_{55},c_{66}$. For an isotropic body, all of these elements take on the same value that coincides with the shear modulus μ in Eq. (4).

IV. MC CALCULATIONS OF THE SHEAR MODULI

The following steps have been taken in the calculations of the shear moduli for the MC-simulated Coulomb solids. Since the crustal matter under consideration is virtually incompressible owing to the high Fermi pressure of dense electrons, we choose deformations which induce no changes in volume elements to the desired second order in the infinitesimal displacement ϵ [cf. (b) below].

(a) For the crystalline-simulated solids, we choose the Cartesian axes along the MC cell. For those solids produced in the quenched simulations, we perform rotational transformations of the coordinate axes so that the resultant Cartesian axes coincide with those close to the symmetry axes defined in terms of the layered structures. Figure 1 displays an example of such Cartesian axes chosen along a layer of particles (with interstitials B) for a quenched solid.

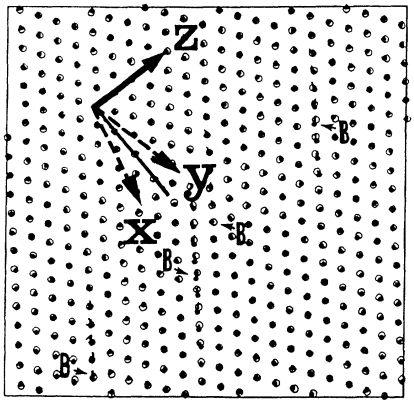

FIG. 1. A layered configuration of particles in a MC quenched Coulomb solid (Ref. 6). The Cartesian axes are chosen so that the x and y axes penetrate the layer at angles by a half of the $\pi/2$ radians while the z axis is on the layer along one of the axes for the resultant quasi-bcc structure.

(b) In each case of the Coulomb solids, the following set of deformations is applied:

$$D_1\text{:}\quad u_{xx}=\epsilon+\tfrac{3}{2}\epsilon^2, \quad u_{yy}=u_{zz}=-\frac{\epsilon}{2} \ .$$

$$D_2\text{:}\quad (x,y,z)\rightarrow(y,z,x), \quad \text{to } D_1 \ .$$

$$D_3\text{:}\quad (x,y,z)\rightarrow(z,x,y), \quad \text{to } D_1 \ .$$

$$D_4\text{:}\quad u_{xy}=u_{yx}=\frac{\epsilon}{2}, \quad u_{zz}=\frac{\epsilon^2}{4} \ .$$

$$D_5\text{:}\quad (x,y,z)\rightarrow(y,z,x), \quad \text{to } D_4 \ .$$

$$D_6\quad (x,y,z)\rightarrow(z,x,y), \quad \text{to } D_4 \ .$$

In these deformations, an elementary volume is kept invariant up to order ϵ^2, so that the derivatives $dv/d\epsilon$ and $d^2v/d\epsilon^2$ [cf. (d) below] may be calculated through Ewald sums without changing the MC cell volume ($=L^3$). The deformations D_1 and D_4 are depicted in Figs. 2(a) and 2(b).

(c) Let v be defined by

$$v(u_{lm})=\tfrac{1}{2}\sum_{p\neq q=1}^{N}\Phi[\mathbf{r}_p(u_{lm})-\mathbf{r}_q(u_{lm})]+U_0(u_{lm}) \ , \tag{8}$$

where $\mathbf{r}_p$ denotes the position vector of the pth MC particle. The potentials in (8) are defined and calculated as

$$\begin{aligned} \Phi(\mathbf{r}(u_{lm}))=&\frac{a}{L}\sum_i\sum_{\substack{t=-\infty\\ t\neq 0}}^{+\infty}\frac{\exp[-\pi|t\boldsymbol{\alpha}^i(u_{lm})|^2]}{\pi|t\boldsymbol{\alpha}^i(u_{lm})|^2}\cos\left[\frac{2\pi}{L}t\boldsymbol{\alpha}^i(u_{lm})\cdot\mathbf{r}(u_{lm})\right] \\ &+\frac{a}{L}\sum_i\sum_{t=-\infty}^{+\infty}\frac{\operatorname{erfc}[\sqrt{\pi}|t\boldsymbol{\alpha}^i(u_{lm})-\mathbf{r}(u_{lm})/L|]}{|t\boldsymbol{\alpha}^i(u_{lm})-\mathbf{r}(u_{lm})/L|}-\frac{a}{L} \ , \end{aligned} \tag{9}$$

$$U_0(u_{lm})=\frac{Na}{2L}\sum_i\sum_{\substack{t=-\infty\\ t\neq 0}}^{+\infty}\frac{\exp[-\pi|t\boldsymbol{\alpha}^i(u_{lm})|^2]}{\pi|t\boldsymbol{\alpha}^i(u_{lm})|^2}+\frac{Na}{2L}\sum_i\sum_{\substack{t=-\infty\\ t\neq 0}}^{+\infty}\frac{\operatorname{erfc}[\sqrt{\pi}|t\boldsymbol{\alpha}^i(u_{lm})|]}{|t\boldsymbol{\alpha}^i(u_{lm})|}-\frac{3Na}{2L} \ . \tag{10}$$

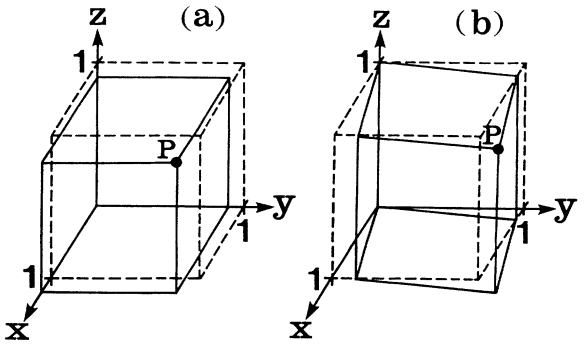

FIG. 2. Schematic views of the deformations: (a) D_1; (b) D_4.

Here t is an integer, u_{lm} are the elements of the strain tensors specified in (b),

$$r_i(u_{lm})=(\delta_{ik}+u_{ik})r_k \ , \tag{11}$$

with δ_{ik} representing Kronecker's delta, the unit Cartesian vectors $\mathbf{a}^i$ are analogously transformed as

$$a_j^i(u_{lm})=(\delta_{jk}+u_{jk})a_k^i \ , \tag{12}$$

the vectors $\boldsymbol{\alpha}^i(u_{lm})$ orthogonal to $\mathbf{a}^j(u_{lm})$ are then defined as $(i\neq j\neq k)$

$$\boldsymbol{\alpha}^i(u_{lm})=\mathbf{a}^j(u_{lm})\times\mathbf{a}^k(u_{lm}) \ , \tag{13}$$

and the error function complement is

$$\mathrm{erfc}(x)=1-\frac{2}{\sqrt{\pi}}\int_0^x \exp(-t^2)dt \ . \tag{14}$$

(d) In each case of the deformations D_m $(m=1,2,\ldots,6)$, we calculate the MC averages:

$$f_m\equiv\left\langle\frac{d^2v}{d\epsilon^2}\right\rangle-\Gamma N\left[\left\langle\left[\frac{dv}{d\epsilon}\right]^2\right\rangle-\left\langle\frac{dv}{d\epsilon}\right\rangle^2\right] \ , \tag{15}$$

where $d/d\epsilon=(\partial u_{ij}/\partial\epsilon)(\partial/\partial u_{ij})$. In the absence of thermal fluctuations (i.e., $T=0$), only the first term on the right-hand side remains in Eq. (15).

(e) The shear moduli are finally obtained as

$$\begin{aligned} b_{11}&=(5f_1-f_2-f_3)/9 \ , \\ b_{22}&=(5f_2-f_3-f_1)/9 \ , \\ b_{33}&=(5f_3-f_1-f_2)/9 \ ; \end{aligned} \tag{16}$$

$$c_{44}=f_4, \quad c_{55}=f_5, \quad c_{66}=f_6 \ . \tag{17}$$

We have accordingly evaluated the shear moduli at different values of Γ in the various cases (crystalline, quenched, and fluid in Sec. II) of Coulombic systems. The results are listed in Table I. We observe significant dependence of the shear moduli on temperatures and on the modes of deformations.

At $T=0$ (i.e., $\Gamma=\infty$) the shear moduli are calculated from the first term of Eq. (15). The bcc crystalline values so calculated are also in Table I; for the face-centered-cubic (fcc) crystal, we find $b_{11}=b_{22}=b_{33}=0.02066$ and $c_{44}=c_{55}=c_{66}=0.1852$ in units of $n(Ze)^2/a$. These are identical to the Fuchs values cited in Ref. 2.

V. EFFECTIVE SHEAR MODULUS

Though the elastic properties of crystalline solids are known to be anisotropic, it is sometimes convenient and useful for practical purposes if an effective shear modulus μ_{eff} may be introduced approximately in the sense of Eq. (4). We have approached this problem from two directions: by performing the directional averages of f_4 in Eq. (15) over all the rotations of the Cartesian axes, and through averages of the dispersion relations for the transverse shear modes with respect to the polarizations and the directions of propagation. (See the Appendix for the latter approach.) Both naturally have led to the same expression, which is

$$\mu_{\text{eff}}=[2(b_{11}+b_{22}+b_{33})+3(c_{44}+c_{55}+c_{66})]/15 \ . \tag{18}$$

The values of μ_{eff} are likewise entered in Table I.

It is instructive to note that the values of μ_{eff} for the quenched solids remain approximately the same as those with the corresponding bcc crystals, although the shear moduli of the former solids deviate considerably from the cubic-symmetry values of the latter. Analogous observation can be made also between the bcc and fcc crystals at

TABLE I. Elements of the shear modulus tensor [in units of $n(Ze)^2/a$]. In the Cases column, C denotes crystalline, Q quenched, and F fluid. The numbers in the parentheses denote possible errors in the last digits. Only the common values are entered when b's or c's are equal.

Γ	Case	b_{11}	b_{22}	b_{33}	c_{44}	c_{55}	c_{66}	μ_{eff}
∞	C		0.024 54			0.1827		0.1194
800	C		0.024(2)			0.174(1)		0.114(2)
800	Q	0.053(2)	−0.007(1)	0.057(1)	0.181(2)	0.171(2)	0.133(1)	0.111(2)
400	C		0.025(2)			0.167(1)		0.110(2)
400	Q	0.059(3)	−0.009(3)	0.062(3)	0.170(2)	0.169(1)	0.121(4)	0.107(4)
300	C		0.025(3)			0.157(4)		0.104(4)
300	Q	0.053(1)	0.025(2)	0.014(3)	0.141(3)	0.167(2)	0.149(3)	0.104(3)
200	C		0.019(3)			0.12(1)		0.08(1)
200	F		−0.004(16)			0.05(2)		0.03(2)

$T=0$. The reason for these may be attributed to the relative insensitivity of Coulombic Ewald sums such as Eq. (8) to details of the microscopic particle configurations after averages over directions are carried out. We recall in these connections that the internal energies of Coulombic systems, involving analogous Ewald sums, are approximately the same for the bcc, fcc, and even isotopic ion-sphere configurations.

The values in Table I suggest a possibility that the supercooled fluid at $\Gamma=200$ may sustain a nonvanishing shear modulus of small magnitude. A definite conclusion on this issue, however, should be deferred until the nature of the equilibrium ensemble of the MC configurations generated in the supercooled fluid state is more carefully assessed.

VI. CONCLUDING REMARKS

We have thus presented an accurate evaluation of the shear modulus tensor for perfect and imperfect Coulomb solids, including the effects of thermal fluctuations for temperatures up to the melting conditions. All the values of the shear moduli calculated here are new, except for the bcc and fcc cases without thermal fluctuations, where the conventional Fuchs values[2] have been available.

The effects of the fluctuations on the elastic constants were formulated by Squire, Holt, and Hoover[10] for a classical ensemble of particles interacting through a central potential. Fluctuation effects in the screened metallic systems were subsequently studied.[11] The present theory treats the cases of the long-range Coulomb interaction, where volume fluctuations should be avoided in the Ewald sums.

In a separate contribution,[8] we have shown how the new values of the effective shear modulus would influence predictions on the nonradial oscillation spectra of the neutron stars. It has also been commented that the new values for the shear modulus may be important for investigations of the glitch phenomena in pulsars. These will make outstanding future problems in condensed-matter astrophysics.

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APPENDIX

In this appendix, we describe a derivation of Eq. (18) through directional averages of the dispersion relations for the shear waves. Let $\mathbf{u}$ be a displacement vector so that the strains are written as

$$u_{ij}=\frac{1}{2}\left[\frac{\partial u_i}{\partial r_j}+\frac{\partial u_j}{\partial r_i}\right] . \tag{A1}$$

Its equations of motion are then given by[3]

$$\rho\frac{\partial^2 u_i}{\partial t^2}=\tfrac{1}{2}S_{ij,ij}\left[\frac{\partial^2 u_i}{\partial r_j\partial r_j}+\frac{\partial^2 u_j}{\partial r_i\partial r_j}\right] , \tag{A2}$$

where ρ is the mass density. Assuming plane-wave displacements $u_i=a_i\exp(ik_l r_l-i\omega t)$ and multiplying (A2) by a_i (with the summation convention), we find

$$\rho\omega^2 a^2=\tfrac{1}{2}S_{ij,ij}(a_i^2k_j^2+a_ia_jk_ik_j) . \tag{A3}$$

Averages of $\rho\omega^2/k^2$ over the directions of $\mathbf{k}$ and $\mathbf{a}$ (polarizations) with the constraint $\mathbf{a}\cdot\mathbf{k}=0$ yield Eq. (18).

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