Partial Screening in Dense Lattice-Configuration Suspensions

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Hydrodynamically mediated particle interactions in creeping flows of suspensions are investigated to address the open question as to whether they are screened. A numerical study of lattice configurations, over the full range of volume fractions, reveals that only the longitudinal part (in wave vector space) of the force-velocity interaction is unscreened, and the general lattice form of the long-range interaction is found to be in qualitative but not quantitative agreement with a mean field result.

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The screening of the bare long-range Coulomb field of an electric charge by charges of opposite sign, also known as Debye screening, is an important many-body effect in numerous physical systems such as metals and electrolyte solutions. This Letter addresses another class of systems in which the bare interaction is long ranged, and asks whether many-body effects can screen it. Unlike in systems of charges, the main entities discussed here, in a system of solid particles suspended in an incompressible fluid in creeping flow, are vectorial and/or tensorial in nature.

The velocity and pressure fields induced in an incompressible fluid by a single slowly moving solid particle decay, at large distances from the particle, as small powers of that distance [1], so the bare effect of the particle motion is long ranged. Determining whether the presence of other particles can screen this influence, i.e., whether the effective hydrodynamic interaction is screened by many-body effects, is important from the basic physics point of view, and may have practical ramifications as it may enable the simulation of greater numbers of particles [2] and the development of improved macroscopic descriptions of suspensions (see, e.g., [3]).

Screening in suspensions has been studied before in the context of sedimentation [4], the relevant quantities there being velocity correlations. In this Letter we do not address the specific case of sedimentation; rather, we investigate the possibility of screening in suspensions due to many-body effects as a matter of principle. To this end, we specialize mostly in infinite monodisperse suspensions of rigid spherical particles instantaneously positioned at lattice points, so that we can employ lattice Fourier transforms. We do not assume that the particle velocities (and angular velocities) are periodic, only that the instantaneous particle configuration is. We do also consider random configurations, especially in dilute systems. Physical boundaries, as well as possible body forces such as gravity, are ignored here for the sake of simplicity, though they can be included in the formalism and calculations. Our approach to the problem is in principle exact, though we do employ high-order truncations of the equations to obtain numerical solutions.

The main qualitative result presented in this Letter is that there is partial screening of the bare hydrodynamic interactions in the sense that the effective two-particle interactions (as defined below) can be decomposed into a pressure-like part which decays like $\mathcal{O}(r^{-3})$ [faster than the bare $\mathcal{O}(r^{-1})$ decay, yet still not absolutely integrable], whereas the remaining parts are strongly screened. A similar result can be obtained in the framework of Brinkman's phenomenological effective medium theory, the differences being the following: (i) Our results are valid for *all physically allowed volume fractions.* (ii) They have been obtained from analysis of the many-body discrete-particle problem. (iii) They differ in detail from the Brinkman result, with configuration-dependent multiplicative prefactors and anisotropic forms. (iv) They provide detailed information on the short-range parts of the interaction. In addition, the long-range part of the interaction is asymptotically given by a universal formula for general Bravais lattices which relates it to the permeability of the lattice regarded as a model porous medium. In order to test whether our results are specific to lattice configurations, we performed several random configuration simulations, obtaining similar results. We therefore conjecture that our main results are of general validity.

The definition of screening used here is motivated by similar definitions in charged systems. Since the Stokes equations for creeping flows are linear, one can utilize superposition. Consequently, when one seeks the force on a particle given the *velocities* of the other particles, it is sufficient to find the force on that particle given only one other particle in motion with the others at rest, and sum over such solutions in an obvious way. If, rather, the *forces* are given, one can use a similar procedure to find the particle velocities. Thus, the problem reduces to that of computing a Green's function tensor which gives $F_\alpha^{(i)} = \sum_j (G_{\alpha\beta}^{[F/V](ij)} V_\beta^{(j)} + G_{\alpha\beta}^{[F/\Omega](ij)} \Omega_\beta^{(j)})$, where Latin indices denote particle identities, Greek indices denote vector

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components, $\mathbf{V}^{(j)}$ and $\mathbf{\Omega}^{(j)}$ are the instantaneous velocity and angular velocity of particle "j," respectively, $\mathbf{F}^{(i)}$ is the instantaneous force on particle "i," and repeated Greek letters imply summation. A similar expression relates the torque $\mathbf{M}^{(i)}$ to the Green's functions $\mathbf{G}^{[M/V]}$ and $\mathbf{G}^{[M/\Omega]}$. By linearity, $\mathbf{G}$ is a function of the instantaneous particle configuration and the external boundary conditions. Note that $\mathbf{G}^{[F/V](ij)}$ is the force on particle i when only particle j has nonzero velocity. When the forces and torques are known, particle velocities are determined by inversion of $\mathbf{G}$, so its properties remain of essential importance. We define the interactions to be screened if $\mathbf{G}$ decays faster than $1/r^3$ for distance r between particles i and j, i.e., if it is absolutely integrable. Below, we specialize for the sake of simplicity to the case of infinite systems with the external boundary condition being the decay of $\mathbf{G}$ to zero at infinite distances, and no external flows imposed. This restriction allows the study of the many-body effect without the extra modifications introduced by specific finite boundaries. The naive application of the Green's function to infinite systems in which the norms of the velocities do not decay at large distances may lead to diverging sums. The source of this problem and its resolution were explained by Hasimoto [5].

It is instructive to first consider the dilute case. Keeping only the leading order in $1/|\mathbf{R}^{(ij)}|$, $\mathbf{R}^{(ij)} \equiv \mathbf{R}^{(i)} - \mathbf{R}^{(j)}$, where $\mathbf{R}^{(j)}$ is the position of particle j, the flow field given by Stokeslet field sources, $\mathbf{w}^{(j)}$, yields [1]

$$V_\alpha^{(j)} = w_\alpha^{(j)} + \sum_{i\neq j} \frac{3a}{4} \frac{w_\beta^{(i)}}{|\mathbf{R}^{(ij)}|} \left[\delta_{\alpha\beta} + \frac{R_\alpha^{(ij)} R_\beta^{(ij)}}{|\mathbf{R}^{(ij)}|^2} \right] \quad (1)$$

for particle radius a. The hydrodynamic force on particle j is $\mathbf{F}^{(j)} = -6\pi\mu a \mathbf{w}^{(j)} \equiv C_0 \mathbf{w}^{(j)}$, in a suspending fluid of dynamic viscosity μ. The sum in (1) can diverge if the $\mathbf{w}$'s decay sufficiently weakly with position; however, for the Green's function, with, e.g., $V_\alpha^{(j)} = V_\alpha^{(0)} \delta_{j0}$, it can be shown (see also below) that $\mathbf{w}^{(i)}$ decays like $\mathcal{O}(|R^{(i)}|^{-3})$. Hence the above sum is absolutely convergent.

For the sake of demonstration, consider a mean field analysis of (1). To this end, define the particle momentum (per unit mass) field by $\mathbf{V}(\mathbf{r}) \equiv \sum_j \mathbf{V}^{(j)} \delta(\mathbf{r} - \mathbf{R}^{(j)})$, with similar definitions for the particle number density $n(\mathbf{r})$, and the force density $\mathbf{F}(\mathbf{r})$. With $\mathbf{R} \equiv \mathbf{r}' - \mathbf{r}$, Eq. (1) becomes

$$C_0 V_\alpha(\mathbf{r}) = F_\alpha(\mathbf{r}) + \frac{3a}{4} n(\mathbf{r}) \int_{|\mathbf{r}'-\mathbf{r}|>\Lambda} d\mathbf{r}' \, \frac{F_\beta(\mathbf{r}')}{|\mathbf{R}|} \left[\delta_{\alpha\beta} + \frac{R_\alpha R_\beta}{|\mathbf{R}|^2} \right]. \quad (2)$$

The mean field approximation consists of replacing $n(\mathbf{r})$ by a space-independent constant, $\bar{n}$ (say, the bulk average density in a large but finite system). The cutoff Λ is set to zero since no incurable divergences occur. The Fourier transform of (2) is then $V_\alpha(\mathbf{k}) = H_{\alpha\beta}(\mathbf{k}) F_\beta(\mathbf{k})$, where

$$C_0 H_{\alpha\beta}(\mathbf{k}) = \delta_{\alpha\beta} + \frac{\zeta^2}{k^2} \left(\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} \right), \quad (3)$$

with $\zeta^2 \equiv 6\pi a \bar{n}$. The mean field Green's function, $\mathbf{G} = \mathbf{H}^{-1}$, satisfying $F_\alpha(\mathbf{k}) = G_{\alpha\beta}(\mathbf{k}) V_\beta(\mathbf{k})$, is then

$$G_{\alpha\beta}(\mathbf{k}) = C_0 \frac{k_\alpha k_\beta}{k^2} + C_0 \frac{k^2}{k^2 + \zeta^2} \left(\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} \right). \quad (4)$$

The second term on the right above, the transverse part in $\mathbf{k}$ space (the divergence-free part in real space), corresponds to an exponentially decaying function in $\mathbf{r}$, with screening length ζ^{-1}, plus a short-range Dirac delta function. In contrast, the first term, the longitudinal part in $\mathbf{k}$ space (the curl-free part in real space), gives r^{-3} power law decay: $C_0 \frac{1}{4\pi r^3} (\delta_{\alpha\beta} - \frac{3 r_\alpha r_\beta}{r^2})$. While this is a significant damping of the bare $\mathcal{O}(r^{-1})$ interactions, it remains not absolutely integrable. This result is in conformity with Brinkman's phenomenological study [6] which employed the concept of an effective medium, and is known to be justified for dilute systems (see, e.g., [7]).

In more dense cases, the Stokeslet level truncation (1) is inappropriate and a more accurate scheme must be used. To this end, we employ the generalized Faxén relations developed, e.g., in [8]. Each particle is represented by a multipolar source, which induces a well-defined fluid velocity field, satisfying the Stokes equations in the particle exterior, which is conveniently expanded in solid spherical harmonics. This solution does not automatically satisfy the no-slip boundary conditions at the particle surfaces, only the sum of solutions generated by the particle sources need satisfy the boundary conditions. The free variables in this representation are the coefficients of the spherical harmonic sources corresponding to each particle, and the imposition of the boundary conditions leads to an infinite set of linear equations in these coefficients. The general form of these equations [see, e.g., [2], and cf. (1)] is $\mathcal{V}^{(i)} = \sum_j \mathcal{A}^{(ij)} \mathcal{F}^{(j)}$, where $\mathcal{F}$ represents all source coefficients in the solid spherical harmonics, $\mathcal{V}$ corresponds to the velocities at the particle surfaces, and $\mathcal{A}^{(ij)}$ depends on positions of particles i and j. The hydrodynamic interactions are then obtained by solving for $\mathcal{F}$ given $\mathcal{V}$, that is, by inverting $\mathcal{A}$. Mean field analyses of low-order truncations (beyond Stokeslets) of these equations were performed, yielding $\mathcal{O}(c)$ dilute corrections to (4), but with no qualitative change in the partial screening nature of the interaction.

We find it interesting that the discrete-particle results presented below are in qualitative agreement with (4) at all physically allowed volume fractions, though significant quantitative differences are observed. In particular, unlike in the mean field theory, the Green's functions are anisotropic with particle configuration dependence, and the short-range interactions are not captured correctly by the mean field theory.

Now consider particle arrangements which are instantaneously in primitive lattice configurations, in order to render the full discrete-particle problem tractable. Lattice configurations of suspended particles have been considered previously [5,9,10], with reports of effective properties such as permeabilities and viscosities. However, we believe that no detailed study of Green's functions for lattice or other dense configurations has been previously reported. Since $\mathcal{A}^{(ij)}$ depends on the distance between i and j, the translational invariance of the lattice configuration considered reduces the problem, upon lattice Fourier transformation, to a set of moderate-rank matrix inversions decoupled in $\mathbf{k}$ space. Since some of the transform summations are only conditionally convergent, Ewald-like summation [11] is invoked. Once the sources are fully calculated numerically, the forces and torques on the particles are given in terms of simple formulas [1], hence the Green's function $\mathbf{G}$. In our computations, we have truncated the solid harmonics at 10th order (rank $= 360$) since convergence up to $\mathcal{O}(10^{-7})$ relative error is observed at $c = 20\%$, and up to $\mathcal{O}(10^{-3})$ at $c = 45\%$.

We find that, as $\mathbf{k} \to \mathbf{0}$, the force-velocity Green's function can be expressed, *for all physically allowed volume fractions* and *for all seven Bravais lattice types,* as

$$G^{[F/V]}_{\alpha\beta}(\mathbf{k}) \to -[\hat{\mathbf{k}} \cdot \mathbf{J}(c, \mathcal{L}) \cdot \hat{\mathbf{k}}]^{-1} \frac{k_\alpha k_\beta}{k^2}, \tag{5}$$

where $\hat{\mathbf{k}} \equiv \mathbf{k}/|\mathbf{k}|$ and $\mathbf{J}(c, \mathcal{L})$ depends on the volume fraction c and lattice configuration $\mathcal{L}$ and gives rise to an anisotropic longitudinal Green's function. Interestingly, this tensor is precisely equal to the mobility tensor for a model porous medium having the same lattice configuration. This fact has been checked numerically and a mathematical argument justifying this identification (beyond the scope of this Letter, as the goal here is to characterize the form of the long-range interactions) has been developed. Since we treat lattice configurations, every particle velocity distribution, including that which corresponds to the Green's function, can be represented by its continuous Fourier decomposition inside the first Brillouin zone. The allowed wave vectors are thus bounded, and the small $\mathbf{k}$ properties of $\mathbf{G}$ [cf. (5)] correspond to its large distance behavior. Upon Fourier inverting (5), one obtains the following long-range real-space behavior:

$$G^{[F/V]}_{\alpha\beta}(\mathbf{r}) \sim \frac{-\tau\sqrt{\det \mathbf{K}}}{4\pi(\mathbf{r}\cdot\mathbf{K}\cdot\mathbf{r})^{3/2}} \left(K_{\alpha\beta} - \frac{3K_{\alpha\gamma} r_\gamma K_{\beta\delta} r_\delta}{(\mathbf{r}\cdot\mathbf{K}\cdot\mathbf{r})} \right), \tag{6}$$

where τ is the lattice unit cell volume, and $\mathbf{K} = \mathbf{J}^{-1}$. The above asymptotic form is obtained without indicating the scale at which the screened interactions decay out. "Characteristic lengths" of the short-range interactions are discussed below and found to be of the order of the interparticle separation, except in the most dilute systems. Beyond a few characteristic lengths, the long-range interaction (6) dominates.

For cubic lattices, the mobility is isotropic, and Eqs. (5) and (6) reduce to the mean field form, up to a multiplicative constant equal to the drag correction of the sphere in the corresponding model porous medium (as defined in [10]); cf. small $|\mathbf{k}|$ in Fig. 1. We have compared the drag corrections thus calculated via the $\mathbf{k} \to \mathbf{0}$ limit of $\mathbf{G}^{[F/V]}(\mathbf{k})$ with previous results for the three cubic lattices [10], obtaining excellent agreement.

As a noncubic example, consider the triclinic lattice ("T1") with basis vectors: $\mathbf{e}_1 = \hat{\mathbf{x}}$, $\mathbf{e}_2 = (1/\sqrt{5})\hat{\mathbf{x}} + \frac{\pi}{3}\hat{\mathbf{y}}$, $\mathbf{e}_3 = (1/\sqrt{7})\hat{\mathbf{x}} + \gamma\hat{\mathbf{y}} + \frac{e}{3}\hat{\mathbf{z}}$, where γ is Euler's constant, and π and e are the usual constants. At $c = 2\%$, we find (in Cartesian coordinates)

$$\mathbf{J}^{(\mathrm{T1})}_{2\%} = \frac{\tau J_2}{|C_0|} \begin{pmatrix} 1.013\,359 & 0.006\,221 & 0.000\,506 \\ 0.006\,221 & 0.987\,481 & -0.011\,201 \\ 0.000\,506 & -0.011\,201 & 0.999\,160 \end{pmatrix}, \tag{7}$$

with $J_2 = 0.535\,288$. The mobility tensor becomes more anisotropic for denser systems; e.g., at $c = 40\%$ we find

$$\mathbf{J}^{(\mathrm{T1})}_{40\%} = \frac{\tau J_{40}}{|C_0|} \begin{pmatrix} 1.032\,008 & 0.070\,137 & 0.012\,742 \\ 0.070\,137 & 0.983\,265 & -0.045\,870 \\ 0.012\,742 & -0.045\,870 & 0.984\,726 \end{pmatrix}, \tag{8}$$

with $J_{40} = 0.044\,517\,1$. While this anisotropy is perhaps not very large, it is bigger than at $c = 2\%$.

Greater anisotropy occurs for lattices with larger aspect ratios; in the tetragonal lattice with basis vector lengths

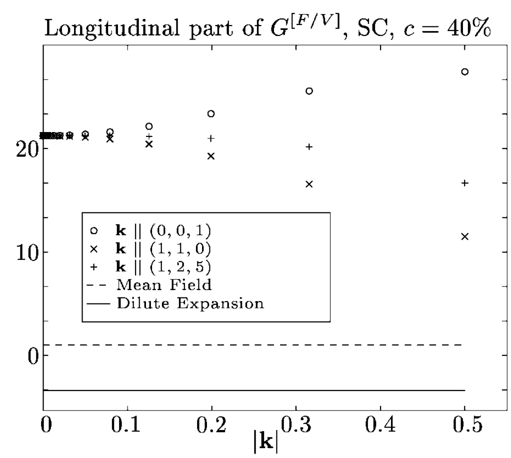

FIG. 1. Multiplicative prefactor to the $(C_0/\tau)(k_\alpha k_\beta/k^2)$ part of $\mathbf{G}^{[F/V]}$ for unit SC lattice at volume fraction $c = 40\%$. Results are compared with mean field (4) and a dilute perturbative expansion [12] that breaks down in this dense system.

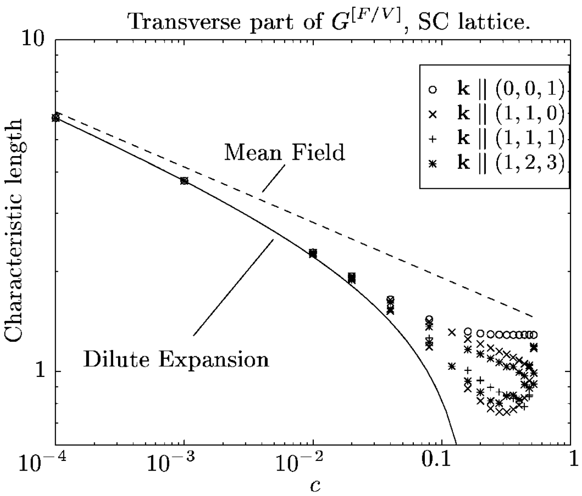

FIG. 2. Characteristic lengths (in units of interparticle separation, $\tau^{1/3}$) of the transverse part of $\mathbf{G}^{[F/V]}$ vs volume fraction c for the unit SC lattice, compared with mean field (4) and a dilute perturbative expansion [12]. For each wave vector direction, $\hat{\mathbf{k}}$, two values are plotted, corresponding to two different components perpendicular to $\hat{\mathbf{k}}$. Characteristic lengths of the other screened parts of the Green's function are similar.

of 0.8, 1.0, and 1.25, the principal mobilities at $c = 2\%$ are $0.6412\tau/|C_0|$, $0.5722\tau/|C_0|$, and $0.4864\tau/|C_0|$, respectively, whereas at $c = 25\%$ they are $0.2058\tau/|C_0|$, $0.1653\tau/|C_0|$, and $0.070\,67\tau/|C_0|$, respectively. For comparison, the mobility of the SC lattice is isotropic with coefficient $0.5222\tau/|C_0|$ at $c = 2\%$, $0.1103\tau/|C_0|$ at $c = 25\%$, and $0.047\,09\tau/|C_0|$ at $c = 40\%$. The mean field prediction is $\tau/|C_0|$ in all cases.

While the longitudinal part of $\mathbf{G}^{[F/V]}$ is directionally dependent as $\mathbf{k} \to \mathbf{0}$, the transverse part of $\mathbf{G}^{[F/V]}$ and the other parts of the Green's function ($\mathbf{G}^{[M/\Omega]}$, $\mathbf{G}^{[M/V]}$, and $\mathbf{G}^{[F/\Omega]}$) are continuous in this limit. Therefore, these Green's functions are screened in that their long range decays faster than $\mathcal{O}(r^{-3})$. Since mean field, perturbative calculations around mean field [12], and numerical results for random dilute suspensions suggest that these screened parts decay exponentially, we conjecture that this is the general case. While it is not easy to determine the analytic structure of the screened parts of the Green's function from numerical data, the screening of the transverse part of $\mathbf{G}^{[F/V]}$ can be described by defining a characteristic length, $r_{\rm char}$, of this part, $\mathbf{G}_T^{[F/V]}(\mathbf{r})$, by $r_{\rm char}^2 \equiv \langle r^4 \mathbf{G}_T^{[F/V]} \rangle / \langle r^2 \mathbf{G}_T^{[F/V]} \rangle$, where $\langle r^{2b} G \rangle \equiv \sum_{\mathbf{r}} r^{2b} G(\mathbf{r})$, summed over all lattice sites. These sums can be evaluated by numerical $\mathbf{k}$ differentiation as $\mathbf{k} \to \mathbf{0}$. In mean field, $r_{\rm char} = (2/\sqrt{5})\zeta^{-1}$. We similarly define directional characteristic lengths by replacing $\mathbf{r}$ in the above moments by its projection in given directions. Figure 2 presents such directional characteristic lengths in several directions, compared with mean field and a dilute perturbative expansion around mean field [12], showing good agreement with the dilute expansion results up to $c \approx 1\%$. Similarly defined characteristic lengths of $\mathbf{G}^{[F/\Omega]}$, $\mathbf{G}^{[M/V]}$, $\mathbf{G}^{[M/\Omega]}$, and the screened part of the longitudinal $\mathbf{G}^{[F/V]}$ are also found to agree well with the same characteristic length predicted by the dilute expansion for small c. For dense systems, as seen in Fig. 2, the characteristic lengths of the screened parts of the interaction display strong anisotropy with values on the order of the interparticle separation.

Partial screening of the hydrodynamic interactions has been demonstrated, wherein the defined Green's function can be decomposed into a pressurelike $\mathcal{O}(r^{-3})$ long-range part and remaining short-range interactions. The work reported here focuses on lattice configurations, the main results being the general form (6) of the long-range part of the interaction, and the characteristic lengths of the short-range interactions. It is obviously important to also study screening in dense random configurations, as well as the effects of physical boundaries and body forces. These and other important problems are relegated to future work.

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