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Coulomb effects in disordered solids. II. A simplified computational method

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We show that Coulomb sums can be truncated in real space in disordered ionic solids, when calculating response functions such as the density of states $\rho(\omega)$ and the dielectric function $\epsilon(\mathbf{k}, \omega)$. The Coulomb forces are treated exactly inside a sphere of radius R_c around each ion. Outside this sphere, the solid is treated as a continuously polarizable medium, which leads to the usual shape-dependent effects. This method is shown to be computationally and conceptually simpler than a previous method used by us on a large periodic random network representing silica. The method is also illustrated on a diluted lattice of polarizable point dipoles. The method works for all quantities, although special care must be taken with $\epsilon(\mathbf{k}, \omega)$ for small $\mathbf{k}$, because of the long-ranged coherence of the eigenstates involved.

I. INTRODUCTION

Disordered ionic solids are an important class of materials, not only for their practical utility but also as systems that exhibit the effects of both nonperiodicity and long-range Coulomb forces. Silica is an example of a structurally disordered solid, and semiconducting alloys are examples of substitutionally disordered ionic crystals. A characteristic feature of these solids in the presence of (time-dependent) macroscopic electric fields generated by the ionic displacements. In crystalline solids, this field acting back on the ions produces a splitting between the zone-center longitudinal- and transverse-optic modes,¹ which in nonionic cubic crystals would be degenerate due to symmetry. In a previous paper² (hereafter referred to as I), we presented a general formulation of the problem of Coulomb forces in a disordered ionic solid. A number of useful sum rules were derived and the results illustrated with a numerical study of an AX_2 ionic glass, using the equation of motion (EOM) technique.³ Coulomb forces were included explicitly via the Ewald method, in which the slowly convergent lattice sums are reexpressed as a combination of rapidly convergent terms in both real and reciprocal space.⁴ In addition, the macroscopic shape of the sample (an essential feature in Coulomb problems) was incorporated using the well-known depolarizing factors for an ellipsoidal dielectric.⁵ The work in I was the first calculation to show, unequivocally,

significant LO-TO effects in a disordered solid. In this paper, which should be read in conjunction with I, we show how these same results can be obtained through a simplified approach that is helpful conceptually and is computationally faster.

The requirement of any implementation of Coulomb forces is that the effects of *all* the ions in the system on a particular ion are included. This can be done using the Ewald method, but this method requires large computational resources, typically supercomputers, for samples large enough to yield reliable results. In I, we used this approach to obtain results on a periodic random network containing 1536 ions. In the simplified approach presented here, we approximate the bulk of the material as a continuous polarizable medium. Only in the local environment of a given ion do its neighbors need to be treated as discrete particles. This means that the forces become effectively short ranged, so long as the shape-dependent terms are included in the proper way. This approximate numerical technique gives accurate results for most quantities of interest, in particular the dielectric response, $\epsilon(\omega)$, and the vibrational density of states (DOS) $\rho(\omega)$. The method involves truncating the Coulomb forces in real space and restricting them to lie within a sphere of radius R_c around each ion. We adopt an empirical approach by choosing R_c to be from 3 to 8 bond lengths, and testing for convergence by making R_c slightly larger. For almost all quantities, this approach has been found to

work well. An exception, where the technique is not effective, is the calculation of $\epsilon(\mathbf{k}, \omega)$ for small $\mathbf{k}$, where special care must be taken because of the long-ranged coherence involved in the associated eigenstates.

In the next section we briefly review the technique of numerical simulations of random materials, describing both the Ewald and truncated approaches. In Secs. III and IV, we describe the physical models used for illustration. One of these models has an underlying crystalline lattice and one does not. In Sec. III, we reexamine the silica model used in I, and in Sec. IV we look at a diluted simple cubic array of point dipoles in which the interactions are exclusively long ranged. Results are presented for the DOS and the dielectric response.

II. IMPLEMENTATION OF COULOMB FORCES

In numerical simulations as in I, random systems are represented as periodic structures with very large unit cells called supercells, typically containing from hundreds to a few thousand particles. Within each supercell, the ions are arranged in the desired disordered structure but with the constraint of periodic boundary conditions. For crystalline alloys, this is easily done and methods are now available for building random networks with periodic boundary conditions.⁶ Deviations from some given static structure for a solid in equilibrium are described by the harmonic Hamiltonian

$$H = \sum_{i,\alpha} \frac{p_\alpha^2(i)}{2m_i} + \frac{1}{2} \sum_{i,j,\alpha,\beta} v_{ij}^{\alpha\beta} u_\alpha(i) u_\beta(j). \quad (1)$$

Here the first term is the kinetic energy, which involves the mass m_i of the ion i and the α component of its momentum $p_\alpha(i)$. The potential energy involves the displacements $u_\alpha(i)$, and includes both short-ranged terms and the long-ranged Coulomb interactions. We will describe the form of the short-ranged part used for the silica model in greater detail in the next section. In this section we discuss only the long-range Coulomb terms.

We consider a cubic supercell of linear dimension L containing N ions of charge q_i ($i=1, 2, \dots, N$) with instantaneous positions $\mathbf{r}_i$. Electrical neutrality is necessary. These supercells form a simple cubic lattice described by translation vectors $\mathbf{n}=(n_x, n_y, n_z)L$. The electrostatic energy of ion i with all other charges in the system is given by

$$V_i = \frac{q_i}{\epsilon_\infty} \sum_{\mathbf{n}}' \sum_{j=1}^N \frac{q_j}{|\mathbf{r}_{ij} + \mathbf{n}|}. \quad (2)$$

The sum is over all translation vectors $\mathbf{n}$, and over all the ions in the supercell. The prime on the summation symbol indicates that the term $i=j$, $\mathbf{n}=0$ is excluded. Within the rigid-ion model, the electronic screening is instantaneous and implemented through the high-frequency dielectric constant ϵ_∞ . The sum (2) is only conditionally convergent, reflecting the need to specify the macroscopic shape of the sample. Our technique is to employ an ellipsoidal convergence factor, which includes the sphere and slab as special cases. The interested reader is referred to I and references contained therein

for details. The Ewald method allows us to reexpress Eq. (2) as a real-space term (Gaussian damped Coulomb potential), a reciprocal-space term (Gaussian damped structure factor), and a shape term involving the appropriate shape-dependent depolarization factor. Because of the role it plays in the truncated method, it is important to better understand physically this latter term. To do so, we calculate the resulting force $\mathbf{F}_{i,\text{shape}}$ exerted on the i th ion from the shape-dependent part of the potential V_{shape} that can be extracted from (1),

$$\mathbf{F}_{i,\text{shape}} = -\nabla_i V_{\text{shape}} = -\frac{4\pi}{\epsilon_\infty} q_i \sum_{\alpha=1}^3 B_\alpha \mathbf{P}_\alpha, \quad (3)$$

where the polarization is given by

$$\mathbf{P}_\alpha = \frac{1}{\Omega} \sum_{j=1}^N q_j \mathbf{r}_j = \frac{1}{\Omega} \left[\sum_{j=1}^N q_j \mathbf{R}_j + \sum_{j=1}^N q_j \mathbf{u}_j \right], \quad (4)$$

with the volume $\Omega=L^3$ and $\mathbf{r}_j=\mathbf{R}_j+\mathbf{u}_j$. Hence we see that the shape term gives the potential energy due to the polarization surface charge for a uniformly polarized continuous medium. The macroscopic shape is ellipsoidal with the usual depolarization factors B_α . The materials we are considering have no permanent dipole moment, and therefore the first term in Eq. (4) is zero and we are only concerned with the dynamic polarization.

For any given ion, the probability of finding another particle a distance r from a given particle increases as r^2 as r becomes large. That is, the discrete nature of the solid becomes less important at large r . We now assume that we can neglect the discrete nature of the solid at large r , replacing the system with an "effective" solid shown schematically in Fig. 1. Thus each ion is surrounded by a sphere of radius R_c . Inside this sphere, the interactions between the particles are treated exactly, whereas outside the sphere the material is replaced by a homogeneous polarizable continuum. This discontinuity does not cause any problems if R_c is sufficiently large that the Coulomb interactions have decayed to a small value and have opposing signs that lead to significant cancellation.

FIG. 1. This sketch shows a spherical region of the solid of radius R_c surrounded by a homogeneous polarizable continuum. The outer ellipsoidal boundary corresponds to the macroscopic sample.

We derive the electrostatic potential term for a given ion for this hybrid system. First consider the continuous region. As the charges in the medium oscillate, a uniform, time-dependent polarization (defined operationally as the polarization of the supercell) is produced. There are two surfaces: the actual outer (ellipsoidal) surface and the fictitious inner spherical one. From Eq. (3) we find that the macroscopic electric field E_{pol} is obtained as the sum of these two surface terms. Using (3), we find

$$\mathbf{E}_{\text{pol}} = \frac{4\pi}{\epsilon_{\infty}} \sum_{\alpha=1}^3 \left(\frac{1}{3} - B_{\alpha} \right) \mathbf{P}_{\alpha}. \quad (5)$$

The first term in parentheses is due to the internal spherical surface. Note that the radius of this sphere does not appear. Within the sphere we treat the ions as discrete particles and have

$$V_{\text{near}} = q_i \sum_j' \frac{q_j}{|\mathbf{R}_{ij} + \mathbf{u}_{ij}|}, \quad (6)$$

which upon expansion leads to

$$V_{\text{near}} = -q_i \sum_j' \frac{q_j}{2} \left[\frac{u_{ij}^2}{R_{ij}^3} - \frac{3(\mathbf{u}_{ij} \cdot \mathbf{R}_{ij})^2}{R_{ij}^5} \right] + O(u^3),$$

where $\mathbf{u}_{ij} = \mathbf{u}_i - \mathbf{u}_j$ and $R_{ij} = |\mathbf{R}_{ij}|$. This gives the needed harmonic form. Because the equilibrium positions are chosen so that there is no net static force on any of the ions, there is no resultant linear term. Therefore, the effective force $\mathbf{F}_i$ on the i th ion due to the electrostatic interaction in our model is given by

$$\mathbf{F}_i = q_i \left[\sum_j' q_j \left[\frac{\mathbf{u}_{ij}}{R_{ij}^3} - \frac{3(\mathbf{u}_{ij} \cdot \mathbf{R}_{ij})\mathbf{R}_{ij}}{R_{ij}^5} \right] + \frac{4\pi}{\epsilon_{\infty}} \sum_{\alpha=1}^3 \left(\frac{1}{3} - B_{\alpha} \right) \mathbf{P}_{\alpha} \right]. \quad (7)$$

In practice, the extent of the first sum is determined by choosing larger truncation radii R_c until the simulation results stabilize.

For a spherical sample, the second term in Eq. (7) due to the continuous medium (the long-range part) vanishes. We can therefore consider the problem for a spherical sample to be effectively short ranged. From relations in I, we can relate the transverse and longitudinal responses to the spherical response, although in practice it is sometimes more convenient and more accurate to compute them directly. When calculating the DOS, the ions are given random initial displacements, a procedure which is described in full in I. Therefore, the macroscopic polarization $\mathbf{P}$ vanishes and once again the problem becomes effectively short ranged. Note that this result implies that surface effects are unimportant in the calculation of the DOS, which is reasonable, as only a few modes, the number of which is thermodynamically insignificant, are affected by the surface shape. A similar division and truncation has been employed for polar fluids by Neumann, Steinhäuser, and Pawley.⁷

We now discuss briefly the equation of motion technique³ used to calculate the DOS and dielectric response

of the system. The focus of this technique is the Green's function defined by

$$G_{\alpha\beta}(i, j; \omega) = \frac{1}{(m_i m_j)^{1/2}} \sum_n \frac{\xi_n(i, \alpha) \xi_n^*(j, \beta)}{\omega^2 - \lambda_n^2}, \quad (8)$$

where ξ and λ are the eigenvectors and eigenvalues of the dynamical matrix. Both the density of states and the dielectric response, or more precisely, the susceptibility χ , can be written in terms of this function. From Sec. II in I, we have

$$\rho(\omega) = -\frac{2\omega}{3\pi N} \sum_{i,\alpha} m_i \text{Im} G_{\alpha\alpha}(i, i; \omega), \quad (9)$$

$$\chi_{\alpha\beta}(\omega) = \frac{1}{\Omega} \sum_{i,j} q_i q_j G_{\alpha\beta}(i, j; \omega), \quad (10)$$

where there are N ions in the volume Ω . Equation (10) follows from linear response theory. Because we are interested primarily in the imaginary (absorptive) part of the susceptibility, we need only the imaginary part of the Green's function for both these quantities. The real part of $\epsilon(\omega)$ can be found using the Kramers-Kronig relation. It is shown in Sec. VI of I that this imaginary part can be computed numerically from

$$G(\omega) = \frac{2}{\pi} \int_0^T dt \cos(\omega t) e^{-\lambda(t/T)^2} \sum_{i,\alpha} A_{i\alpha} u_{i\alpha}(t), \quad (11)$$

where $\mathbf{u}_i(t)$ is the displacement from equilibrium of the i th particle. The smoothing factor, $\lambda=3$, lessens the ripples in the convolution function introduced by the finite T truncation. For the DOS, we let

$$A_{i\alpha} = u_{i\alpha}^0 = \sqrt{2} \cos(\theta_{i\alpha}),$$

where $\theta_{i\alpha}$ is a random angle uniformly distributed in the interval $0 \leq \theta_{i\alpha} \leq 2\pi$. If we average over many sets of random angles, then

FIG. 2. The density of states $\rho(\omega)$ for the 1536 atom model for SiO_2 . The solid curve is calculated using the Ewald method as described in I. The dashed curve is calculated using a cutoff radius $R_c = 8.64d$, where d is the equilibrium Si—O bond length. The dot-dashed curve is for $R_c = 3.45d$.

FIG. 3. The same as for Fig. 2, except for the dielectric function $\epsilon(\omega)$.

$$\langle G(\omega) \rangle_{av} \rightarrow \rho(\omega) .$$

If we let $A_{i\alpha} = \hat{\mathbf{E}}_{\alpha} q_i$ and $u_{i\alpha}^0 = \hat{\mathbf{E}}_{\alpha} q_i / m_i$, where $\hat{\mathbf{E}}$ is a unit vector in the direction of the electric field of the incident light, then we get, using slab geometry:

$$\text{Im}[\epsilon_t(\omega) - \epsilon_{\infty}] = \frac{2\pi^2}{\Omega\omega} G(\omega), \quad \hat{\mathbf{E}} \text{ parallel to slab}, \quad (12)$$

$$\text{Im}[\epsilon_l(\omega) - \epsilon_{\infty}] = \frac{2\pi^2}{\Omega\omega} G(\omega), \quad \hat{\mathbf{E}} \text{ perpendicular to slab}. \quad (13)$$

The spherical dielectric function $\epsilon_s(\omega)$ is computed from a relation identical to Eqs. (12) or (13), but with the depolarization factors B_{α} set equal to $\frac{1}{3}$ in Eq. (5). The quantity $\epsilon_s(\omega)$ is related to $\epsilon_l(\omega)$ through a Clausius-Mossotti type of relation [see Eq. (54) in I].

FIG. 4. The same as for Fig. 2, except for the dielectric function $\epsilon_s(\omega)$.

FIG. 5. The same as for Fig. 2, except for the dielectric function $\epsilon_l(\omega)$.

To calculate $\epsilon(\mathbf{k}, \omega)$ we modulate $u_{i\alpha}^0$ and $A_{i\alpha}$ with the factor $\exp(i\mathbf{k} \cdot \mathbf{r}_i)$ and its complex conjugate, respectively, with $\mathbf{k}$ parallel or perpendicular to the field direction as appropriate.

III. SILICA GLASS MODEL

As this model was described in detail in I, we will only summarize it here. The glass network, consisting of 512 silicon and 1024 oxygen atoms per supercell, was computer generated using a modified algorithm of Wooten and Weaire.⁶ In addition to the electrostatic potential described in the preceding section, there are also important short-ranged interactions between the ions. These are (see I)

FIG. 6. The same as for Fig. 2, except for the dielectric function $\epsilon(\mathbf{k}, \omega)$ for the smallest possible nonzero $\mathbf{k}$ allowed by the boundary conditions, $k = 2\pi/28.5 = 0.220 \text{ \AA}^{-1}$.

$$V_{CF} = \frac{3}{8} \frac{\alpha}{d^2} \sum_{\langle l, \Delta \rangle} [\mathbf{r}_l^2(\Delta) - d^2]^2, \quad (14)$$

$$V_K = \frac{3}{8} \frac{\beta}{d^2} \sum_{\langle l, \Delta, \Delta' \rangle} [\mathbf{r}_l(\Delta) \cdot \mathbf{r}_l(\Delta') - d^2 \cos \theta_l]^2, \quad (15)$$

$$V_r = \sum_{\langle l, m \rangle} A_{lm} \exp(-|\mathbf{r}_{lm}|/\rho), \quad (16)$$

where V_{CF} is the nearest-neighbor central force term describing bond stretching, V_K is the three-body Keating term describing angular bond bending, and V_r is a repulsive term which was found necessary for stability when the Coulomb interactions are included. In these equations, α and β are the force constants, and $\hat{\mathbf{r}}_l(\Delta)$ the vector from ion l to its nearest-neighbor Δ . The equilibrium bond length is d and the equilibrium bond angle is θ_l . In the repulsive term, A_{lm} reflects the strength of the repulsive and ρ its range. The initial glass structure was relaxed using the conjugate gradient method⁸ under the total potential (with the electrostatic term) to establish the equilibrium ion positions. The interaction terms were then expanded to second order in the displacements to give the harmonic potential used in the simulations. The reader is referred to Sec. VII in I for further details.

We present the results for the silica simulations in Figs. 2–6. The equations of motion were integrated numerically using Verlet's algorithm as in I, with a time step of 5 fs. The evolution of the initial state was followed for 600 steps for the $\mathbf{k}=0$ dielectric response and the density of states, and 300 steps otherwise. Since these results were discussed at length in I, we merely point out the essential equivalence of the Ewald and truncation results for all but the last set, $\epsilon_l(\mathbf{k}, \omega)$ for $\mathbf{k}=2\pi(0,0,1)/L$. In this case, the truncation method underestimates the peak frequency. Note also that in this case, the net polarization is nearly zero, and hence the surface and continuum terms vanish. Thus the net interactions are quite short ranged. This negative result tells us that correlations greater than 0.5 L are important for this mode and that the continuum approximation is least adequate for this case. From a computational point of view, it is important to note the improvement as the cutoff distance R_c increases, so that a converging scheme could be devised by successively increasing R_c until convergence is reached or the supercell size has to be increased.

IV. DILUTED POINT DIPOLE MODEL

In this model, point dipoles⁹ are placed on a simple cubic lattice sites with probability p . For the numerical simulations we choose a supercell of $6^3=216$ sites and populate them with probability $p=0.9$, giving 194 active dipoles. We chose this probability as the most severe test of the truncation technique because it leads to a relatively large number of low-symmetry local environments. For $p=1$, the sample is cubic and the contributions to the Coulomb sums vanish, shell by shell, going outward from the reference ion. For small values of p , the gaslike structure also leads to a similar cancellation, because of the average spherical symmetry. The small sample size used here is for demonstration purposes only. The equation of motion for the point dipoles¹⁰ is given by

$$d^2\boldsymbol{\mu}_i/dt^2 + \omega_0^2\boldsymbol{\mu}_i + \frac{\omega_p^2}{4\pi} \sum_{j \neq i} \left[\frac{\boldsymbol{\mu}_j}{R_{ij}^3} - \frac{3(\boldsymbol{\mu}_j \cdot \mathbf{R}_{ij})\mathbf{R}_{ij}}{R_{ij}^5} \right] = 0, \quad (17)$$

where ω_0 is the natural frequency of an isolated point dipole, $\omega_p = 4\pi pq^2/(md^3)$ is the plasma frequency, with m the reduced mass of the two charges that make up the dipole; R_{ij} is the equilibrium distance between dipoles i and j in units of the lattice parameter. Because of the long-range nature of the dipolar system, the sum is over all the other dipoles in the system. Note also that the dynamical variable is the dynamic dipole moment $\boldsymbol{\mu}$. This equation leads to a dynamical matrix whose eigenvalues are the normal mode frequencies of the problem. If we look for solutions of the form

$$\boldsymbol{\mu}(t) = \boldsymbol{\mu} \exp(i\omega t),$$

where

$$\boldsymbol{\mu} = (\mu_{1x}, \mu_{1y}, \mu_{1z}, \dots, \mu_{Nx}, \mu_{Ny}, \mu_{Nz}),$$

we obtain the secular determinant equation

$$\left| \left[\frac{\omega^2 - \omega_0^2}{\omega_p^2} \right] \delta_{ij}^{\alpha\beta} - D_{ij}^{\alpha\beta} \right| = 0, \quad (18)$$

where

$$D_{ij}^{\alpha\beta} = \frac{\delta_{\alpha\beta}}{R_{ij}^3} - \frac{3R_{ij}^\alpha R_{ij}^\beta}{R_{ij}^5}, \quad i \neq j. \quad (19)$$

From Eq. (18), we see that as ω_0 is varied, the spectrum is rigidly shifted. In simulations, it is desirable to minimize the maximum frequency of the system, and since ω_0 merely determines the frequency origin, we would like to

FIG. 7. The density of states $\rho(E)$ for the point dipole model on a simple cubic lattice containing 216 sites of which $p=0.9$ are randomly occupied. The solid curve is obtained using the full Ewald method as described in I. The dashed curve is calculated with a cutoff radius $R_c=3d$, where d is the nearest-neighbor distance. The dot-dashed curve is for $R_c=2.4d$. The box size is $6d \times 6d \times 6d$.

FIG. 8. The same as for Fig. 7, except for the dielectric function $\epsilon(E)$.

set it equal to zero. However, this would lead to some negative ω^2 , i.e., imaginary frequencies and unbounded exponential solutions, which cannot be simulated, and are unacceptable. To avoid this difficulty, we solve instead a first-order equation in time with solutions of the form

$$\mu(t) = \mu \exp(iEt) .$$

This leads to a secular equation identical to (18) but with an energy E substituted for ω^2 . In this case, a negative E causes no problems with numerical instabilities. The solution is still oscillatory and bounded. Thus we can set $E_0 = 0$, expressing our results in units of $E_p = \omega_p^2$. Equations analogous to (8)–(13) can be derived for this case. The dipole-dipole term can be rewritten using the Ewald method or, following the same argument in Sec. II of this paper, we can express it in truncated form as

FIG. 10. The same as for Fig. 7, except for the dielectric function $\epsilon_l(E)$.

$$i d\mu_i/dt = \frac{E_p}{4\pi} \left[\sum_j' \left[\frac{\mu_j}{R_{ij}^3} - \frac{3(\mu_j \cdot \mathbf{R}_{ij})\mathbf{R}_{ij}}{R_{ij}^5} \right] + 4\pi \sum_{\alpha=1}^3 \left(\frac{1}{3} - B_\alpha \right) \mathbf{P}_\alpha \right] , \quad (20)$$

where

$$\mathbf{P}_\alpha = \frac{1}{\Omega} \sum_{j=1}^N \mu_j . \quad (21)$$

The sum in Eq. (20) is over the dipoles within the truncation radius R_c of a given dipole. Simulations were run for ten cycles on one configuration with a time step of $2\pi/15$, i.e., one-fifteenth of a cycle of frequency E_p . For $\epsilon(\mathbf{k}, \omega)$, we used smaller time steps of $2\pi/20$ and $2\pi/25$ for the truncated and Ewald runs, respectively. For the runs using the truncated method, the truncation radius

FIG. 9. The same as for Fig. 7, except for the dielectric function $\epsilon_s(E)$.

FIG. 11. The same as for Fig. 7, except for the dielectric function $\epsilon(\mathbf{k}, E)$ for the smallest nonzero $\mathbf{k}$ allowed by the boundary conditions, $k = 2\pi/6d$.

was chosen to be 0.4 and 0.5 of the box length. These correspond to spheres of radius R_c containing 52 and 102 dipoles, respectively. The results are shown in Figs. 7–11. The time savings for this case, in contrast to that for the silica model, were quite dramatic. The truncated runs ran at least 50 times faster than the Ewald runs. This ratio might be slightly misleading, as the Ewald code was not fully optimized although it was partially vectorized. Once again, as in the case for silica, the truncated and Ewald results agree rather closely for all quantities except $\epsilon(\mathbf{k}, \omega)$. The density of states in Fig. 7 shows a broad peak; many of the features in this peak are due to the finite size of the model. It is the comparisons between the three results that is of interest to us here. The various dielectric functions shown in Figs. 8–10 are less sensitive to the sample size, and agreement between the three calculations is excellent. The same problems with convergence that were found for the dielectric function at finite wavelengths are also seen in the dipole model in Fig. 11.

V. CONCLUSIONS

We have shown that the Coulomb potential, previously incorporated into numerical simulations of random harmonic systems via the Ewald method, can alternatively be included using a simplified truncated approach based on the partition of the solid into a near region where interactions are treated exactly, and a far region considered as a polarizable continuum. We tested this approach on

both an ionic disordered solid representing silica, previously studied in I, and a depleted simple cubic lattice of point dipoles. In both cases, for the density of states $\rho(\omega)$ and the dielectric response $\epsilon(\omega)$, the agreement between the two techniques is excellent. Only for the finite wavevector dielectric response, $\epsilon(\mathbf{k}, \omega)$, is there some discrepancy at long wavelengths. This discrepancy disappears for infinite wavelengths as the coherency is taken care of properly by the macroscopic field. At short wavelengths, the coherency is only over short distances. However, our results indicate that the response $\epsilon(\mathbf{k}, \omega)$ converges to the correct result as the cutoff distance R_c increases. Thus one can devise a scheme in which R_c increases until convergence at the proper limit is reached. This truncated technique is conceptually simpler than the Ewald method and easier to implement in computer codes. For the case of the point dipoles, running on a mainframe computer, the decrease in running time is significant. It is hoped that the simplification achieved by this method will encourage greater use of this important but often neglected interaction in the numerical simulations of disordered materials.

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