Calculation of Elastic Green's Functions for Lattices with Cavities

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In this Brief Report, we present an algorithm for calculating the elastic Lattice Greens Function of a regular lattice, in which defects are created by removing lattice points. The method is computationally efficient, since the required matrix operations are on matrices that scale with the size of the defect subspace, and not with the size of the full lattice. This method allows the treatment of force fields with multi-atom interactions.

Lattice Green's function methods provide a very computationally efficient way of handling the long-ranged stress fields around defects in materials. The purpose of this Report is to generalize the lattice Green's function method of Thomson *et al.*[1] to problems in which a set of lattice points has been completely removed from the problem. Such problems may be the modeling of the elastic fields in crystalline systems in which cavities are created. An example of such systems that have been modeled in this way are blunt cracks[2,3]. This opens for the application of Green's function techniques to a new class of problems: The previously published method[1,4] has been used to study lattice defects where *connections* between lattice points have been altered[1,5–9] (for example leading broken to introduce cracks). The present extension of the method permits the study of problems where *lattice points* (atoms) have been removed from the system. The methodology was used in the calculations of Refs. 2 and 3, but the derivation has not been presented in the literature yet.

In the lattice Green's function method, one begins with a force constant matrix Φ_{ij}^{ab} defined by

$$E = \frac{1}{2} u_i^a \Phi_{ij}^{ab} u_j^b \tag{1}$$

where E is the total energy, u_i^a is the displacement in the i direction of atom a and summation over repeated indices is implied. Φ_{ij}^{ab} is thus the negative of the force in the i direction on atom a when atom b is displaced a unit distance in the direction j:

$$F_i^a = -\Phi_{ij}^{ab} u_j^b \tag{2}$$

For a simple pair potential with radial forces between atoms, Φ_{ij}^{ab} is given by

$$\Phi_{ij}^{ab} = -\frac{r_i^{ab}}{|\mathbf{r}^{ab}|} \lim_{u_i^b \to 0} \frac{f\left(\left|\mathbf{r}^{ab} + \mathbf{e}_j u_j^b\right|\right)}{u_j^b}, \qquad a \neq b \tag{3a}$$

$$\Phi_{ij}^{aa} = -\sum_b \frac{r_i^{ab}}{|\mathbf{r}^{ab}|} \lim_{u_i^a \to 0} \frac{f\left(\left|\mathbf{r}^{ab} - \mathbf{e}_j u_j^a\right|\right)}{u_j^a}. \tag{3b}$$

where $f(r)$ is the force between the two atoms, $\mathbf{r}^{ab}$ is the vector between the equilibrium positions of atoms a and b and $\mathbf{e}_i$ is a unit vector in the i direction. The $r_i^{ab}/\left|\mathbf{r}^{ab}\right|$ are a projection operators.

The Greens function gives the formal solution of equation (2) for u:

$$u_i^a = G_{ij}^{ab} F_j^b, \tag{4}$$

$$\mathbf{G} = \mathbf{\Phi}^{-1} \tag{5}$$

It is inconvenient to label the degrees of freedom by two indices (the atom and the component of the displacement). Therefore, we introduce a single labeling of all degrees of freedom, leading naturally to a matrix notation where a component of $\mathbf{G}$, G_{ij}, is the response by the degree of freedom i to a force acting on the degree of freedom j.

Thomson *et al.* demonstrate[1] how the Greens function of a regular lattice can be calculated in Fourier space in a time that scales linearly with the number of lattice points (N_{lat}). The Fourier-space approach breaks down when defects are present, breaking translational symmetry. Thomson *et al.* showed that defects can be treated without a complete "brute-force" inversion of equation (5), by the use of multiple-scattering theory. If the values of only a small number of "bonds" (i.e. elements in the Φ matrix) are changed, the new Greens function $\mathbf{G}$ can be calculated from the perfect-lattice Greens function $\mathbf{G}^0$ using a Dyson equation:

$$\mathbf{G} = \mathbf{G}^0 \left(\mathbf{1} - \delta\mathbf{\Phi}\mathbf{G}^0\right)^{-1} \tag{6}$$

where $\delta\mathbf{\Phi}$ is the change in the force constant matrix. This calculation scales as N_{def}^3, where $N_{def} \ll N_{lattice}$ is the number of rows or columns in $\delta\mathbf{\Phi}$ containing non-zero elements, i.e. the number of degrees of freedom of atoms where one or more bonds are modified, and $N_{lattice}$ is the total number of degrees of freedom in the lattice.

When atoms are removed from the system (see figure 1), it is important to be able to calculate the Green's function as efficiently as when only bonds are changed, i.e. the Greens function should be calculated starting

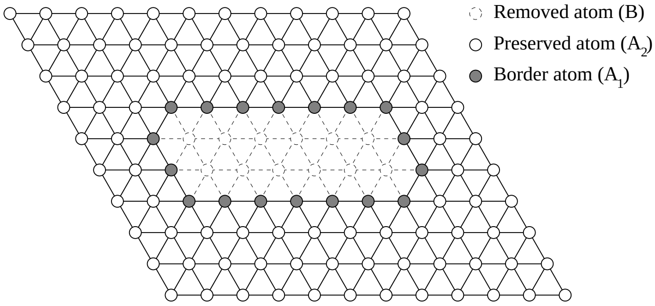

FIG. 1. A hexagonal lattice, where 12 atoms have been removed. The removed atoms and their bonds are shown with dashed lines. Border atoms that have lost one or more neighbors are shaded. The corresponding diagonal elements of $\delta\mathbf{\Phi}$ are non-zero, since the on-site force constant has changed: when such an atom is displaced it "feels" a different force since there is no force from the missing neighbors. In the text the following classification scheme is used: The removed atoms are in class B, the remaining atoms are in class A. Class A is further subdivided into two classes: the grey atoms, having lost one or more neighbors, are in class A_1, and the white atoms are in class A_2.

from the perfect-lattice Greens function $\mathbf{G}^0$, and not directly from equation (5). Let us divide the degrees of freedom in two classes: A are the degrees of freedom of atoms that are "kept", and B are those that are removed from the system. $\mathbf{M}_{AA}$ is then the sub-matrix of $\mathbf{M}$ obtained by keeping only columns and rows corresponding to degrees of freedom in class A. In a similar ways the other sub-matrices $\mathbf{M}_{BB}$, $\mathbf{M}_{AB}$, and $\mathbf{M}_{BA}$ are defined. Further, let $\mathbf{G}^*$ be the Green's function of the new system. $\mathbf{G}^*$ cannot be calculated by breaking all bonds to the atoms to be removed, and then applying the Dyson equation (6), since the resulting Greens function is singular[10].

The force-constant matrix entering $\mathbf{G}^*$ is perturbed relative to the full force-constant matrix in two ways. First, it has smaller dimension in the sense that it only contains atoms in the A-region. Second, the on-site force constants (corresponding to the force on an atom resulting from its own motion) of the A-region border atoms near the cavity are changed, since these are determined by the neighboring atoms (terms in the sum in equation (3b) are missing). For example, if an atom has no neighbors, then it has a vanishing on-site force constant. Then $\mathbf{G}^*$ is given by

$$\mathbf{G}^* = \left(\mathbf{\Phi}_{AA} + \delta\mathbf{\Phi}_{AA}\right)^{-1}, \tag{7}$$

where $\delta\mathbf{\Phi}_{AA}$ corresponds to the change in the on-site force constants of the border atoms. For clarity, we define the auxiliary Green's functions $\mathbf{G}^0 = \mathbf{\Phi}^{-1}$ for the perfect crystal, and $\mathbf{G}' = (\mathbf{\Phi}_{AA})^{-1}$ for the crystal with atoms removed but no changes in the force constants of the remaining atoms. (Note that $\mathbf{G}' = (\mathbf{\Phi}_{AA})^{-1} \neq (\mathbf{\Phi}^{-1})_{AA} = \mathbf{G}^0_{AA}$). The calculation of $\mathbf{G}^*$ then goes in two steps. We first calculate $\mathbf{G}'$, as an intermediate step:

$$\begin{aligned} \mathbf{G}' = (\mathbf{\Phi}_{AA})^{-1} &= \left(\left(\left(\mathbf{G}^0\right)^{-1}\right)_{AA}\right)^{-1} \\ &= \mathbf{G}^0_{AA} - \mathbf{G}^0_{AB}\left(\mathbf{G}^0_{BB}\right)^{-1}\mathbf{G}^0_{BA} \end{aligned} \tag{8}$$

(The last equality is proven in the appendix). We then calculate $\mathbf{G}^*$ with a Dyson equation:

$$\mathbf{G}^*\left(\mathbf{\Phi}_{AA} + \delta\mathbf{\Phi}_{AA}\right) = \mathbf{1} \tag{9}$$

which gives

$$\mathbf{G}^* = \mathbf{G}'\left(\mathbf{1} - \mathbf{G}'\delta\mathbf{\Phi}_{\mathbf{AA}}\right)^{-1}. \tag{10}$$

Equations (8) and (10) are the central results of this Report. We note that they can be used to describe systems with many-atom interactions such as the Embedded Atom Method[11], the Effective Medium Theory[12], the glue model[13] etc. In these methods, the force constants between different atoms in the A region also change because the effective interatomic potentials are environmentally dependent. This effect can be included straightforwardly by modification of the $\delta\mathbf{\Phi}_{AA}$ term.

Finally, let us show that this method is computationally feasible. Let the degrees of freedom that are kept be separated into two classes, A_1 and A_2, where A_1 is the set of degrees of freedom of atoms where the corresponding elements of $\delta\mathbf{\Phi}$ is non-zero, or where we are going to need the Greens function; the latter would include atoms on which nonlinear forces or loading forces will eventually be placed. Let $n(S)$ be the number of degrees of freedom of the atoms in set S. Typically, $n(A_1)$ will be a few hundreds or less, whereas A_2 contains millions of degrees of freedom[2,3]. $n(B)$ is also typically a few hundreds. Equation (8) then consists of the inversion of a $n(B)\times n(B)$ matrix, and two $n(A_1)\times n(B)$ matrix multiplication. Since $\delta\mathbf{\Phi}_{A_2A_2} = \mathbf{0}$ equation (10) consists of a $n(A_1)\times n(A_1)$ matrix inversion and a similar multiplication. With the relatively small sizes of A_1 and B, this is clearly computationally practical, whereas the direct matrix inversion in equation (7) is not. See also the discussion of the computational burden of equation (10) in Thomson *et al.*[1] if there are many atoms in A_1 where $\delta\mathbf{\Phi}$ is zero.

In conclusion, we have shown how to generate Lattice Green's functions for lattices where the defects are not limited to perturbations of a small number of bonds, but where lattice points have been removed. The Green's function is generated in a computationally efficient way, and has already been used to simulate the elastic fields near a blunted crack[3]. The method is not limited to elastic fields in crystal lattices, but to all problems where a lattice Green's function may be useful, and where a small number of lattice points are removed from the problem.

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APPENDIX

We here prove that

$$\left((\mathbf{M}^{-1})_{AA}\right)^{-1} = \mathbf{M}_{AA} - \mathbf{M}_{AB}\left(\mathbf{M}_{BB}\right)^{-1}\mathbf{M}_{BA} \quad (11)$$

Proof: Let $\mathbf{N} = \mathbf{M}^{-1}$. We then have $\mathbf{MN} = \mathbf{1}$, which can be split into four parts:

$$\mathbf{M}_{AA}\mathbf{N}_{AA} + \mathbf{M}_{AB}\mathbf{N}_{BA} = \mathbf{1}, \quad (12a)$$
$$\mathbf{M}_{AA}\mathbf{N}_{AB} + \mathbf{M}_{AB}\mathbf{N}_{BB} = \mathbf{0}, \quad (12b)$$
$$\mathbf{M}_{BA}\mathbf{N}_{AA} + \mathbf{M}_{BB}\mathbf{N}_{BA} = \mathbf{0}, \quad (12c)$$
$$\mathbf{M}_{BB}\mathbf{N}_{BB} + \mathbf{M}_{BB}\mathbf{N}_{BB} = \mathbf{1}. \quad (12d)$$

From (12c) we get

$$\mathbf{N}_{BA} = -\left(\mathbf{M}_{BB}\right)^{-1}\mathbf{M}_{BA}\mathbf{N}_{AA}. \quad (13)$$

When inserting in equation (12a) and multiplying from the right with $(\mathbf{N}_{AA})$, we get

$$\mathbf{M}_{AA} - \mathbf{M}_{AB}\left(\mathbf{M}_{BB}\right)^{-1}\mathbf{M}_{BA} = \left(\mathbf{N}_{AA}\right)^{-1}, \quad (14)$$

and since $(\mathbf{N}_{AA})^{-1} = ((\mathbf{M}^{-1})_{AA})^{-1}$, equation (11) has been proven.

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10 This is most easily seen by considering the center of mass of the removed atoms. Moving the center of mass does not result in any net force on the remaining atoms. Therefore a force acting on the center of mass of the removed atoms will result in an infinite displacement, and the corresponding element of $\mathbf{G}^*$ (transformed to the right coordinates) will be divergent. The corresponding divergence in $\mathbf{G}^0$ arising from the lack of a restoring force to the rigid displacement of the entire lattice can be eliminated, as discussed by Thomson *et al.*[1].

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