Oscillating elastic defects: competition and frustration

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We consider a dynamical generalization of the Eshelby problem: the strain profile due to an inclusion or “defect” in an isotropic elastic medium. We show that the higher the oscillation frequency of the defect, the more localized is the strain field around the defect. We then demonstrate that the qualitative nature of the interaction between two defects is strongly dependent on separation, frequency and direction, changing from “ferromagnetic” to “antiferromagnetic” like behavior. We generalize to a finite density of defects and show that the interactions in assemblies of defects can be mapped to XY spin-like models, and describe implications for frustration and frequency-driven pattern transitions.

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In his seminal 1957 paper \cite{Eshelby1957}, Eshelby derived the strain fields created by an inhomogeneous ellipsoidal inclusion in an isotropic elastic medium. This result is a cornerstone of the theory of inhomogeneous elastic media, now routinely used in the physical and engineering sciences. The result is a statement of how a distortion is accommodated in the host material and implies that a local perturbation induces long range strain fields, slowly decaying as $1/r^d$ in $d$ dimensions ($d \geq 2$). Eshelby’s work considers static inhomogeneities or strain “defects” only. However, for many applications in physics and materials science, we are interested in the cooperative behavior of inhomogeneities in which the strain is varying or oscillating in time with a given frequency. We find that this situation is, as a function of the defect density and oscillation frequency, inherently frustrated, resulting in self-organization of the patterns, competing ground states, and sensitivity to internal and external perturbations. Such “dynamic” defects arise as small polarons in directionally-bonded transition metal oxides, including high-temperature superconductors, colossal magnetoresistance materials and ferroelectrics \cite{Hwang2004}. The collective behavior of these polarons in a crystal undergoing distortions, with their coupling to charge, spin or polarization, is believed to determine the overall macroscopic response. Our work also has ramifications for the non-destructive evaluation of elastic media. Methods in this field are typically based on the vibrational response from a defect-free crystal. Here we characterize the behavior of oscillating defects (external oscillatory fields inducing specific defect patterns and responses) extending the conventional analysis to describe the response of elastic media in the presence of such defects.

The dynamical generalization of the Eshelby problem has been investigated in the context of engineering sciences for spherical inclusions \cite{Curtis2003}, and very recently for inclusions of various shapes \cite{Naka2018}. However, such studies have focused on evaluating displacement fields as solutions to numerical boundary value problems. Our objective here is to understand the effect of dynamics on the nature of the elastic interaction itself and its influence on the collective behavior of assemblies of defects, using the formalism developed in Ref. \cite{Curtis2003}, which allows for tractable analytic calculations. We consider the dynamical Eshelby problem for localized oscillating defects in two dimensions for simplicity, and show that, although the strain fields still decay as $1/r^2$ far from the defect, the frequency fundamentally affects the nature of deformation. As expected, the higher the frequency, the more localized is the deformation. This renders the interaction between two defects strongly frequency (and direction) dependent, but the very nature of the interaction changes from “ferromagnetic” to “antiferromagnetic” like behavior as a function of separation and frequency. We subsequently generalize our results to a finite density of defects. This allows us to demonstrate the implications for frequency-driven patterning transitions and phase locking in assemblies of defects by mapping the elastic interaction energy between defects into XY spin-like models with competing interactions.

We use a strain only representation \cite{Curtis2003}. The state of strain is defined by three fields $e_i$, related to the displacement along the $x$-axis ($u$) and the $y$-axis ($v$) as follows: $e_1 = (u_x + v_y)/\sqrt{2}$, $e_2 = (u_y - v_x)/\sqrt{2}$, $e_3 = (u_x - v_y)/\sqrt{2}$ (the subscripts $x$ and $y$ indicate differentiation). We write an elastic energy which includes gradient terms:

\begin{equation}
E = \int \left[ \frac{A_1}{2} e_1^2 + \frac{A_2}{2} (e_2^2 + e_3^2) \right] d\mathbf{r} + \frac{g}{2} \int \left[ (\nabla e_1)^2 + (\nabla e_2)^2 + (\nabla e_3)^2 \right] d\mathbf{r},
\end{equation}

where $A_1$ and $A_2$ are the bulk and shear moduli of the isotropic elastic material, respectively, and $g$ is a strain gradient coefficient. Assuming first an overdamped dynamics (we comment later on the underdamped case), the equations to be solved read, in real space:

\begin{align}
e_1' &= -(A_1 + g\nabla^2)e_1 - \nabla^2 \lambda, \quad (2) \\
e_2' &= -(A_2 + g\nabla^2)e_2 + 2\partial x \partial y e_1 - 2\partial y \partial x e_2 - 2\partial x \partial y \lambda, \quad (3) \\
e_3' &= -(A_1 + g\nabla^2)e_3 + (\partial x^2 - \partial y^2)\lambda, \\
0 &= \nabla^2 e_1 - 2\partial x \partial y e_2 + (\partial x^2 - \partial y^2)e_3. \quad (5)
\end{align}
The last equation is the compatibility condition, reflecting the fact that the three strain fields are not independent; $\lambda$ is a Lagrange multiplier enforcing this constraint. The boundary conditions are taken to be periodic in space. We now add $n$ oscillating defects localized around the positions $(\vec{r}_i)_{i=1,\ldots,n}$. We assume for specificity that the oscillation is in $e_3$. Considering strictly point defects, that is $e_j(\vec{r}^2, t) = e_0 \delta(\vec{r} - \vec{r}_i) \sin(\omega_0 t + \varphi_i)$, with $\omega_0$ and $\varphi_i$ denoting oscillation frequency and phase, would lead to unphysical logarithmic divergences of the Green functions for the system of equations. Thus, we enforce the regularization: 
$$\int e_1(\vec{r}, t) g_1(\vec{r}) \, d\vec{r} = \int e_2(\vec{r}, t) g_2(\vec{r}) \, d\vec{r} = \int e_3(\vec{r}, t) g_3(\vec{r}) \, d\vec{r} = e_0 \sin(\omega_0 t + \varphi_i),$$
where $g_i(\vec{r}) = \exp(-r^2/2\sigma)/(2\pi\sigma)$, and $\sigma$ is chosen small enough that the defect is physically localized.

We have checked that our results, which apply to the far field created by the defects, do not qualitatively depend on the regularization.

We start with the case of one defect. As the problem is linear, we can construct the solution as a superposition of $\phi_{\pm}^{(ij)}$, the elementary solutions of the problem, defined as follows:

$$
\phi_{\pm}^{(11)} = -(A_1 + g\nabla^2)\phi_{\pm}^{(11)} - \nabla^2 \lambda + g_\sigma(\vec{r}) e^{\pm i\omega_0 t}, \quad (6)
$$
$$
\phi_{\pm}^{(12)} = -(A + g\nabla^2)\phi_{\pm}^{(12)} + 2\partial x \partial y \lambda, \quad (7)
$$
$$
\phi_{\pm}^{(13)} = -(A + g\nabla^2)\phi_{\pm}^{(13)} + (\partial^2 x - \partial^2 y) \lambda, \quad (8)
$$
$$
0 = \nabla^2 \phi_{\pm}^{(11)} - 2\partial x \partial y \phi_{\pm}^{(12)} + (\partial^2 x - \partial^2 y) \phi_{\pm}^{(13)}. \quad (9)
$$

The $\phi_{\pm}^{(2)}$ and $\phi_{\pm}^{(3)}$ are solutions of the same set of equations with the oscillatory excitation in the second and third equations, respectively. The $\phi_{\pm}^{(ij)}$ can be analytically calculated in Fourier space. Writing the $e_i$ as linear combinations of the $\phi_{\pm}^{(ij)}$, and finding the coefficients by enforcing the regularized oscillating defect conditions, we obtain the expressions for the fields. We give here explicitly the expression for $\phi_{\pm}^{(12)}$ (the other $\phi_{\pm}^{(ij)}$ have similar characteristics):

$$
\phi_{\pm}^{(12)} = \frac{2k_x k_y}{k^2} \frac{g_\sigma(\vec{k}) e^{i\omega_0 t}}{A + A_1 + 2g^2 k^2 + 2i\omega_0}. \quad (10)
$$

Two important results can be deduced from this expression. First, due to the compatibility condition, $\phi_{\pm}^{(12)}$ is not continuous around $\vec{k} = 0$. This creates the same $1/r^2$ tails as in the static case. The Eshelby result thus extends to oscillations. Second, from Eq. (10) we see that the larger $\omega_0$, the more spread out is $\phi_{\pm}^{(12)}(\vec{k})$. In real space this implies that the larger $\omega_0$, the more localized is the deformation created by the defect. This will be of primary importance for the interactions between defects, as detailed below.

These results are illustrated in Figs. 1 and 2 showing strain profiles for different $\omega_0$. A comment on the underdamped case is in order: an underdamped dynamics would not remove the discontinuity at $\vec{k} = 0$ created by the compatibility equation; thus, the $1/r^2$ decay is also valid in this case. The qualitative effect of increasing $\omega_0$ would not be modified either, although there would be some quantitative differences from the overdamped case. Finally, we have focused here on defects created by a locally oscillating $e_3$ strain; the solutions for locally oscillating $e_1$, $e_2$ strains, or combinations of the three strain components, can also be obtained, and are qualitatively similar. There is one exception to this statement: the functions $\phi_{\pm}^{(11)}(\vec{k})$ are continuous around $\vec{k} = 0$ and even infinitely differentiable. Their tail in real space is thus exponential instead of power law. This implies that the $e_1$ strain field created by a local $e_1$ defect in an isotropic elastic medium decays exponentially away from the defect with rate $\rho_0$; if the defect is oscillating, the exponential decay rate $\rho(\omega_0)$ grows with $\omega_0$ as $\omega_0^{1/2}$. To our
knowledge, this particular case has not been emphasized in the literature; it would be interesting to realize its experimental signatures.

We now consider two defects oscillating with the same frequency \( \omega_0 \), with the goal of studying the interactions between them. Let the two defects be centered at \( \vec{r} = 0 \), with phase \( \varphi_1 = 0 \), and \( \vec{r} = \vec{r}_0 \), with phase \( \varphi_2 = \varphi \). We express the fields as linear combinations of \( \phi_{ij}(\vec{r}) \) and \( \phi_{ij}(\vec{r} - \vec{r}_0) \). As above, the twelve complex coefficients are found by enforcing the regularized oscillating defects conditions. For each strain configuration, it is easy to calculate the elastic energy stored in the system from Eq. (1). Averaging this energy over one oscillation period, we obtain the interaction energy of the two defects \( U(\varphi, \vec{r}_0, \omega_0) \). Similar calculations in the static case were performed, for instance, by Eshelby in Ref. [3].

We consider first that the two defects are pinned, and study the function \( U(\varphi) \) at fixed \( \vec{r}_0 \) and \( \omega_0 \). It turns out that the energy can be approximated by an XY spin interaction term, \( U(\varphi, \vec{r}_0, \omega_0) = -J(\vec{r}_0, \omega_0) \cos \varphi \). A positive \( J \) then corresponds to a “ferromagnetic”, phase-locking interaction, and a negative \( J \) to an “antiferromagnetic” one. As expected, \( J \) decreases to zero at large distances; from the previous one-defect calculations, it can be anticipated that at fixed distance, \( J \) also approaches zero in the large \( \omega_0 \) limit. These effects are seen in Fig. 3 which shows the energy as a function of \( \varphi \) for two defects along the x-axis. This figure also emphasizes a striking effect: \( J \) may also change sign with varying \( \vec{r}_0 \) or \( \omega_0 \). For small enough \( \omega_0 \) and small enough distance, the interaction is ferromagnetic, and the defects tend to phase-lock; for larger distances and \( \omega_0 \), the interaction is antiferromagnetic, and the energy is minimized for a maximum phase difference \( \varphi = \pi \). Since the fields are anisotropic, the picture is different for defects situated along the diagonal; in this case, the interaction is always ferromagnetic, see Fig. 4.

This qualitative change in the interactions between defects from varying the frequency or the distance has important consequences when considering the collective properties of assemblies of defects, as shown below. We have focused here on oscillating \( e_3 \) strain fields for specificity; for oscillating \( e_1 \) or \( e_2 \) strain fields, the results are quantitatively different, but the main feature remains: changes in the frequency or the distance have dramatic effects on defect interactions.

Using a superposition of the elementary solutions \( \phi_{ij}(\vec{r}) \), it is possible to construct the strain profiles asso-
associated with an assembly of $N$ defects. The regularized oscillating conditions have now to be enforced for each defect, which yields the $6N$ coefficients of the linear combination. Calculating the energy (averaged over one period) as a function of all the phases, we are now in a position to study the collective behavior of the assembly of defects. For the sake of specificity, we focus again on oscillating $e_3$ strains. As a working example, we consider chains of equally spaced defects, along the $x$-axis or the diagonal, with different spacings and frequencies, and study the ground state of the system as a function of the phases of all defects.

To obtain a qualitative understanding of the patterning, it is useful to infer the behavior of $N$ defects from the pairwise interactions studied above. Note however that summing pairwise interactions is an approximation, neglecting three-body effects and beyond. These effects are included in the full numerical calculations. When defects are aligned along a diagonal, the pairwise interactions are always phase-locking, see Fig. 4 there is no frustration and the ground state should be a perfectly phase-locked, or “ferromagnetic” state, for all lattice spacings and frequencies. This is indeed observed in our full calculations. The case of defects aligned along the $x$-axis is richer, see Fig. 3. As “antiferromagnetic” interactions come into play, frustration and competition between different types of interactions, such as long-period patterns found in ANNNI spin systems, are likely to develop. However, at large enough spacing along the chain and/or large enough frequency, the interaction between nearest neighbors is dominant, and “antiferromagnetic”; the ground state is then expected to show neighboring defects with a phase difference of $\pi$. At small lattice spacing and frequency, the interaction between nearest neighbors is “ferromagnetic”; the interaction between next nearest neighbors however is “antiferromagnetic”. Frustration will then develop, and a non-trivial ground state may be expected. At intermediate lattice spacing and frequency, all interactions are “antiferromagnetic”, but the nearest neighbor interactions do not dominate; in this case also, a complicated ground state should be expected. Although this picture based on two-body interactions is approximate, it provides qualitatively correct results, see Fig. 5. Figure 6 also shows the numerically determined boundary between “antiferromagnetic” ground states (where nearest neighbor interactions dominate) and more complicated ones, as expected from the two-defect calculations. The boundary (dashed line) between ferromagnetic and antiferromagnetic nearest neighbor interactions is also sketched. We have performed our calculations here for special arrangements of defects, but these results demonstrate the existence of collective behavior, controlled by the frequency or interparticle distance.

In conclusion, we have generalized the well known Eshelby study of static elastic inhomogeneities to dynamical oscillating defects, focusing on the qualitative properties of the resulting strain fields. Our main results for a single defect are: a $1/r^2$ decay of the strain fields far from the defect, and that the higher the frequency, the more localized is the strain perturbation. These results have important consequences for the interaction between oscillating defects, which slowly decays at large distances, and is suppressed by increasing $\omega_0$. A more detailed study of the two oscillating defects situation shows a more dramatic effect: varying the frequency, or the distance, can result in a qualitative change in the interaction, from “ferromagnetic” (phase-locking) to “antiferromagnetic” (anti-phase-locking). Our work raises the possibility of controlling collective patterning of defects by the frequency or the defect density; we have explicitly demonstrated such effects by performing N-defect calculations.

Applications of our work include non-destructive evaluation of elastic media with internal oscillating defects, and the collective behavior of small-polaron dopant sites in directionally bonded electronic materials. There are natural extensions of our results to the dynamics of multiple defects. Thus, phase-locking among defects can be studied if specific phase dynamics controlling the relaxation pathways is added. Again, if the center-of-mass of the defects is given dynamics, we can expect self-assembly of defect patterns driven by the induced elastic fields; since the interaction range is reduced for higher frequency defect oscillations, this will reduce the domain of defect ordering. When there are competing ground states due to ferromagnetic and antiferromagnetic interactions, we also expect multiscale “glassy” dynamics. These extensions of our results will be reported elsewhere.

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