A-Exam Question #2

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1. *Identify the unique strains that exist in cubic, tetragonal, and orthorhombic lattices.*

   If a system has symmetry which is described by the group G, then its free energy F must be invariant under the action of any element $g \in G$, or $g \cdot F = F$. Let R^{Sp} be the space representation of G. If A is an n-tensor,

   $$[g \cdot A]_{i_1 \cdots i_n} = [R_g^{\mathrm{Sp}}]_{i_1 j_1} \cdots [R_g^{\mathrm{Sp}}]_{i_n j_n} A_{j_1 \cdots j_n}$$

   In the course of this question, we will also work with non-tensor objects which transform under different representations of G.

   The free energy due to strain ϵ is, to quadratic order,

   $$F_{\mathrm{e}} = \tfrac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl}$$

   where C is the elastic modulus tensor [6]. Since the strain tensor is symmetric, the elastic modulus tensor can be defined with symmetry under exchange of its first or last two indices without loss of generality. Since multiplication is commutative, it can be defined with symmetry under exchange of the first two indices and the last two indices. This leaves twenty-one free parameters.

   The form of C is further constrained by symmetry of the lattice. If G is the point group of the lattice, then for any $g \in G$,

   $$\begin{aligned} F_{\mathrm{e}} = g \cdot F_{\mathrm{e}} &= \tfrac{1}{2} C_{ijkl} (g \cdot \epsilon)_{ij} (g \cdot \epsilon)_{kl} \\ &= \tfrac{1}{2} C_{ijkl} [R_g^{\mathrm{Sp}}]_{im} [R_g^{\mathrm{Sp}}]_{jn} [R_g^{\mathrm{Sp}}]_{ko} [R_g^{\mathrm{Sp}}]_{lp} \epsilon_{mn} \epsilon_{op} \end{aligned}$$

   Consider a tetrahedral lattice with the point group $C_{4\mathrm{v}}$. The elements of this group and their representations are shown in Table 1 [9]. Since $(\sigma_{i\mathrm{v}} \cdot \epsilon)_{ij} = -\epsilon_{ij}$ for any $j \neq i$, all elements C_{ijkl} with an odd number of indices 1 or 2 must be zero. Likewise, since $(c_4 \cdot \epsilon)_{13} = -\epsilon_{23}$ and $(c_4 \cdot \epsilon)_{11} = \epsilon_{22}$, we must have

   $$C_{1111} = C_{2222} \qquad C_{1133} = C_{2233} \qquad C_{1313} = C_{2323}$$

g	description	R_g^{Sp}	g	description	R_g^{Sp}
e	identity	$\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}$	$\sigma_{1\mathrm{v}}$	reflection	$\begin{bmatrix}1&0&0\\0&-1&0\\0&0&1\end{bmatrix}$
c_4	$\frac{\pi}{2}$ rotation	$\begin{bmatrix}0&-1&0\\1&0&0\\0&0&1\end{bmatrix}$	$\sigma_{2\mathrm{v}}$	reflection	$\begin{bmatrix}-1&0&0\\0&1&0\\0&0&1\end{bmatrix}$
c_4^{-1}	$\frac{\pi}{2}$ rotation	$\begin{bmatrix}0&1&0\\-1&0&0\\0&0&1\end{bmatrix}$	$\sigma_{1\mathrm{d}}$	reflection	$\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}$
c_2	π rotation	$\begin{bmatrix}-1&0&0\\0&-1&0\\0&0&1\end{bmatrix}$	$\sigma_{2\mathrm{d}}$	reflection	$\begin{bmatrix}0&-1&0\\-1&0&0\\0&0&1\end{bmatrix}$

Table 1: Elements of the group $C_{4\mathrm{v}}$ and their space representations.

No other element provides further restriction. The most general tetrahedral free energy is thus

$$\begin{aligned} F_{\mathrm{e}} =& \tfrac{1}{2}C_{1111}(\epsilon_{11}^2+\epsilon_{22}^2)+\tfrac{1}{2}C_{3333}\epsilon_{33}^2+C_{1133}(\epsilon_{11}\epsilon_{33}+\epsilon_{22}\epsilon_{33}) \\ &+C_{1122}\epsilon_{11}\epsilon_{22}+2C_{1212}\epsilon_{12}^2+2C_{1313}(\epsilon_{13}^2+\epsilon_{23}^2) \end{aligned}$$

As you can tell from this procedure, doing this for many groups is tedious. I wrote software in *Mathematica* to automatically provide such reductions.[1] The results for the square lattice (with point group O) are

$$F_{\mathrm{e}} = \sum_i \left(\tfrac{1}{2}C_{1111}\epsilon_{ii}^2 + C_{1122}\epsilon_{ii}\epsilon_{(i+1)(i+1)} + 2C_{1212}\epsilon_{i(i+1)}^2\right)$$

and the results for the orthorhombic lattice (with point group $C_{2\mathrm{v}}$) are

$$F_{\mathrm{e}} = \sum_i \left(\tfrac{1}{2}C_{iiii}\epsilon_{ii}^2 + C_{ii(i+1)(i+1)}\epsilon_{ii}\epsilon_{(i+1)(i+1)} + 2C_{i(i+1)i(i+1)}\epsilon_{i(i+1)}^2\right)$$

where we assume the indices are defined cyclically: $\epsilon_{1(3+1)} = \epsilon_{11}$.

2. *Write down a Landau-type elastic free energy for a system with this nematic order parameter.*

   Nematic order can be thought of as the order of alignment. If a system is composed of microscopic elements with some aligning direction n_i, then the canonical nematic order parameter is given by the tensor

   $$Q_{ij} = \langle n_i n_j - \tfrac{1}{3}\delta_{ij}\rangle$$

   Generically, a nematic order parameter Q is a symmetric traceless tensor. We will guarantee tracelessness by writing $Q_{11} \to -\frac{1}{2}(Q_3+Q_1)$, $Q_{22} \to -\frac{1}{2}(Q_3-Q_1)$. Q thus has five free parameters. Since, as a tensor, Q is acted upon by a point group via the space representation, the permitted free energy for a nematic field in a tetragonal lattice is given exactly as it was for the strain tensor (to second order) with the substitution above made, or

   $$\begin{aligned} F_{\mathrm{n}} =& \tfrac{1}{4}D_{1,1,1,1}(Q_1^2+3Q_3^2)+\tfrac{1}{4}(D_{2222}-2D_{1122})(Q_1^2-Q_3^3) \\ &+(D_{3333}-2D_{1133})Q_3^2+4D_{1212}Q_{12}^2+4D_{1313}(Q_{13}^2+Q_{23}^2) \end{aligned}$$

[1] The notebook should be supplied with this writeup.

Rep	e	$c_4^{(-1)}$	c_2	$\sigma_{i\text{v}}$	$\sigma_{i\text{d}}$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Table 2: Character table for the irreducible representations and five conjugacy classes of $C_{4\text{v}}$.

$$\begin{aligned} F_{\text{e-n}} = &-\tfrac{1}{2}\Lambda_{1111}\big(Q_1(\epsilon_{11}-\epsilon_{22})+Q_3(\epsilon_{11}+\epsilon_{22})\big) \\ &+\tfrac{1}{2}\Lambda_{1122}\big(Q_1(\epsilon_{11}-\epsilon_{22})-Q_3(\epsilon_{11}+\epsilon_{22})\big) \\ &+\Lambda_{1133}Q_3(\epsilon_{11}+\epsilon_{22})+(\Lambda_{3333}-\Lambda_{3311})Q_3\epsilon_{33} \\ &+4\Lambda_{1212}Q_{12}\epsilon_{12}+4\Lambda_{1313}(Q_{13}\epsilon_{13}+Q_{23}\epsilon_{23}) \end{aligned}$$

I can (and have) used my software to explicitly write out the most general form of F_n to fourth order—which is required to see our phase transition—but that exercise wouldn't be useful. Encoded in such an expansion is the description of many phase transitions, the properties of which fill rich papers [5]. We are interested in a transition characterized by a scalar parameter that is acted on by elements of C_{4v} with the irreducible representation B_1, i.e., one that "transforms like x^2-y^2." Notice that Q_1, in our redefined tensor

$$Q=\begin{bmatrix} -\frac{1}{2}(Q_3+Q_1) & Q_{12} & Q_{13} \\ Q_{12} & -\frac{1}{2}(Q_3-Q_1) & Q_{23} \\ Q_{13} & Q_{23} & Q_3 \end{bmatrix}$$

is such a parameter—when Q is transformed by the space representation of $C_{4\text{v}}$, Q_1 behaves as if it is being transformed by B_1. Therefore, we will reduce our free energies to only depend on Q_1. We have

$$\begin{aligned} F_\text{n} &= \tfrac{1}{2}D_2Q_1^2+\tfrac{1}{4!}D_4Q_1^4 \\ F_{\text{e-n}} &= \tfrac{1}{2}\Lambda Q_1(\epsilon_{11}-\epsilon_{22}) \end{aligned}$$

On its own, the nematic parameter undergoes a standard ϕ^4 transition at $D_2=0$, with $Q_1=0$ for $D_2>0$ and $Q_1\neq 0$ otherwise. We therefore identify $D_2=\alpha t$, where $t=(T-T_c)/T_c$.

3. *Use this free energy to compute the temperature dependence of the elastic moduli immediately below and above T_n.*

   At equilibrium,

$$0=\frac{\partial F}{\partial Q_1}=\alpha t Q_1+\tfrac{1}{3!}D_4Q_1^3+\tfrac{1}{2}\Lambda_1(\epsilon_{11}-\epsilon_{22})$$

This can be solved for Q_1, yielding

$$Q_1^{(m)} = \frac{e^{2\pi i m/3}\left(\sqrt{32D_4^3\alpha^3t^3 + 9D_4^4\Lambda^2(\epsilon_{11}-\epsilon_{22})^2} - 3D_4^2\Lambda(\epsilon_{11}-\epsilon_{22})\right)^{2/3} - 2^{5/3}e^{-2\pi i m/3}D_4\alpha t}{2^{2/3}D_t\left(\sqrt{32D_4^3\alpha^3t^3 + 9D_4^4\Lambda^2(\epsilon_{11}-\epsilon_{22})^2} - 3D_4^2\Lambda(\epsilon_{11}-\epsilon_{22})\right)^{1/3}}$$

for $m = 1, 2, 3$. Whether these solutions are real and stable depends on the value of t. In particular, we find that

$$0 < \left.\frac{\partial^2 F}{\partial Q_1^2}\right|_{Q_1=Q_1^{(3)},\epsilon=0,t>0} \qquad 0 < \left.\frac{\partial^2 F}{\partial Q_1^2}\right|_{Q_1=Q_1^{(1)},\epsilon=0,t<0} \qquad 0 < \left.\frac{\partial^2 F}{\partial Q_1^2}\right|_{Q_1=Q_1^{(3)},\epsilon=0,t<0}$$

Since the solution $Q_1^{(3)}$ is stable at all temperatures, we shall use it in our analysis.

In the unperturbed case, one can consider as a definition of the elastic moduli tensor evaluating the expression

$$C_{ijkl} = \left.\frac{\partial^2 F}{\partial\epsilon_{ij}\partial\epsilon_{kl}}\right|_{\epsilon=0}$$

Now, assuming that the nematic degree of freedom always remains at equilibrium, we can apply the same reasoning here, defining $F' = F|_{Q_1=Q_1^{(3)}}$ and writing

$$C'_{ijkl} = \left.\frac{\partial^2 F'}{\partial\epsilon_{ij}\partial\epsilon_{kl}}\right|_{\epsilon=0}$$

Defining $\Delta C_{ijkl} = C'_{ijkl} - C_{ijkl}$, we find that $\Delta C_{ijkl} = 0$ expect for

$$\Delta C_{1111} = \begin{cases} -\frac{\Lambda^2}{4\alpha|t|} & t > 0 \\ -\frac{\Lambda^2}{8\alpha|t|} & t < 0 \end{cases} \qquad \Delta C_{1122} = \begin{cases} \frac{\Lambda^2}{4\alpha|t|} & t > 0 \\ \frac{\Lambda^2}{8\alpha|t|} & t < 0 \end{cases}$$

The change in two elastic constants diverges with a power law at the transition, one becoming smaller and the other larger. The amplitude of the power law on the high-temperature side of the transition is twice that of the low-temperature side. All other elastic constants remain unchanged.

4. *How is the case of a d-wave superconductor different than the nematic order above—what couplings are prohibited in the free energy? Can you give a physical explanation for why this makes sense? Think about what are the physical observables for a superconductor.*

   A d-wave superconductor is a system whose singlet ground state is characterized complex scalar order parameter that is acted on by $C_{4\mathrm{v}}$ via its B_1 representation [1, 11]. The principle difference between this case and that previous is that the order parameter is complex, not real. Along with the requirement that the free energy be invariant under the action of $C_{4\mathrm{v}}$, the free energy must also be invariant under conjugation, i.e., it must be real, or $F = F^*$. With these requirements, the most general free energy without gradient terms to fourth order is

$$F_{\text{d}} = \tfrac{1}{2}\alpha t|\eta|^2 + \tfrac{1}{4}\beta|\eta|^4$$

Using the same methods as above, we find the most general low-order coupling to strain is

$$F_{\text{e-d}} = \gamma_1|\eta|^2(\epsilon_{11} + \epsilon_{22}) + \gamma_3|\eta|^2\epsilon_{33}$$

5. *Do a literature search on the thermodynamics of the two-fluid model of a superconductor, incorporate this into the elastic free energy, and find the evolution of the moduli below T_c. Is the sign of the evolution general, or does it depend on the specific material?*

   While methods involving two fluids can also be used to solve this problem, they are unnecessary and two-fluid free energy contributions affect only high-order terms in the elastic constants [12, 2, 4].

   The free energy in this case is $F = F_{\text{d}} + F_{\text{e}} + F_{\text{e-d}}$. Writing $\eta = re^{i\phi}$, we have

$$F_{\text{d}} + F_{\text{e-d}} = \tfrac{1}{2}\alpha t r^2 + \tfrac{1}{4}\beta r^4 + \gamma_1 r^2(\epsilon_{11} + \epsilon_{22}) + \gamma_3 r^2\epsilon_{33}$$

   and the system is unsurprisingly independent of the phase ϕ. The Goldstone mode resulting from the symmetry broken by any choice of ϕ for nonzero r is unimportant to our analysis, so we will ignore it. Minimizing the free energy with respect to the field r, we find stables solutions of

$$r = \begin{cases} 0 & t > 0 \\ \pm\beta^{-\frac{1}{2}}\sqrt{\alpha|t| - 2\big[\gamma_1(\epsilon_{11} + \epsilon_{22}) + 2\gamma_3\epsilon_{33}\big]} & t < 0 \end{cases}$$

   when the strain is infinitesimal.[2] Upon substitution back into the free energy and evaluation of the elastic constants as before, we find that for $t > 0$, $\Delta C_{ijkl} = 0$ for all i, j, k, l, while for $t < 0$, $\Delta C_{ijkl} = 0$ except for

$$\Delta C_{1111} = -\tfrac{2\gamma_1^2}{\beta} \qquad \Delta C_{3333} = -\tfrac{2\gamma_3^2}{\beta}$$

$$\Delta C_{1122} = -\tfrac{2\gamma_1^2}{\beta} \qquad \Delta C_{1133} = -\tfrac{2\gamma_1\gamma_3}{\beta}$$

   Four of the elastic constants experience a discontinuity at the transition. The sign of three of these is independent of the particular coupling, but the sign of the fourth depends on the sign of the product $\gamma_1\gamma_3$, which in principle depends on the material at hand.

[2] Obviously the stability of these solutions, and therefore the transition temperature, shifts for nonzero strain, but we only need derivatives of the solution evaluated at zero strain, so this will suffice.

6. *Find the point-group symmetry of the p-wave superconducting order parameter of Sr_2RuO_4 (tetragonal lattice). Similar to question three, compute the response of the elastic moduli above and below T_c. How could you use ultrasound to discriminate between d- and p-wave superconductivity?*

   $\mathrm{Sr_2RuO_4}$ exhibits p-wave pairing with gap structure $(0,0,1)(x+iy)$ [10, 8, 3, 7]. This requires a triplet state which transforms as the representation E of $C_{4\mathrm{v}}$ [1, 11]. Since E is a two-dimensional representation, we must consider a six-component order parameter $\eta_{i\nu}$ where $\nu = 1,2$ are the indices acted upon by the group representation E and $i = 1,2,3$ are acted upon by the space representation, or

$$[g \cdot \eta]_{i\nu} = [R_g^{\mathrm{Sp}}]_{ij}[R_g^{\mathrm{E}}]_{\nu\mu}\eta_{j\mu}$$

   For such an order parameter, the ground state with the desired gap structure is [1]

$$\eta^0 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & i \end{bmatrix}$$

   To investigate the desired transition, we will restrict our order parameter to two nonzero components, η_{31} and η_{32}. The most general free energy in these parameters is

$$\begin{aligned} F_{\mathrm{p}} = {} & \alpha t(|\eta_{31}|^2 + |\eta_{32}|^2) + 4\beta_1|\eta_{31}|^2|\eta_{32}|^2 + \beta_2(|\eta_{31}|^4 + |\eta_{32}|^4) \\ & + \beta_3(\eta_{31}^{*2}\eta_{32}^2 + \eta_{32}^{*2}\eta_{31}^2) \end{aligned}$$

   and the most general interaction energy is

$$\begin{aligned} F_{\text{e-p}} = {} & \gamma_1(|\eta_{31}|^2\epsilon_{11} + |\eta_{32}|^2\epsilon_{22}) + \gamma_2(|\eta_{31}|^2 + |\eta_{32}|^2)\epsilon_{33} \\ & + \gamma_3(|\eta_{31}|^2\epsilon_{22} + |\eta_{32}|^2\epsilon_{11}) + 2\gamma_4(\eta_{31}^*\eta_{32} + \eta_{32}^*\eta_{31})\epsilon_{12} \end{aligned}$$

   The full free energy is $F = F_{\mathrm{e}} + F_{\mathrm{p}} + F_{\text{e-p}}$. Defining $\eta_{31} = re^{i\phi}$ and $\eta_{32} = (r+\delta r)e^{i(\phi+\frac{\pi}{2}+\delta\phi)}$, we have

$$F_{\mathrm{p}} = \alpha t\left[r^2 + (r+\delta r)^2\right] + 4\beta_1 r^2(r+\delta r)^2 - 2\beta_3 r^2(r+\delta r)^2\cos(2\,\delta\phi)$$

   and

$$\begin{aligned} F_{\text{e-p}} = {} & \gamma_1\left[r^2\epsilon_{11} + (r+\delta r)^2\epsilon_{22}\right] + \gamma_2\left[r^2 + (r+\delta r)^2\right]\epsilon_{33} \\ & + \gamma_3\left[r^2\epsilon_{22} + (r+\delta r)^2\epsilon_{11}\right] - 4\gamma_4 r(r+\delta r)\sin(\delta\phi)\epsilon_{12} \end{aligned}$$

   Note that the pure ground state corresponds to $\delta r = \delta\phi = 0$. If we set them to this value, we have the same free energy and coupling as in the d-wave case. However, the equilibrium behavior of these fields under strain will affect our effective elastic constants in a nontrivial way. Again, we ignore the Goldstone mode.

Solution	$F\|_{\epsilon=0}$	$\mathrm{Tr}\,\mathbf{H}(F)\|_{\epsilon=0}$
1	0	$6\alpha t$
2/3	$-\alpha^2 t^2/4\beta_2$	$-2\alpha(B+3)t$
4/5	$-\alpha^2 t^2/4\beta_2$	$-4\alpha B t$

Table 3: The energy at zero strain and stability at zero strain of the field extrema.

While we cannot simultaneously solve

$$0 = \frac{\partial F}{\partial r} = \frac{\partial F}{\partial\,\delta r} = \frac{\partial F}{\partial\,\delta\phi}$$

for the equilibrium fields r, δr, and $\delta\phi$, we can solve this simultaneous equation when F is expanded to first order in $\delta\phi$. The five solutions are $r^{(1)} = 0$, $\delta r^{(1)} = 0$, and

$$r^{(2/3)} = \delta\phi^{(2/3)} = 0 \quad \delta r^{(2/3)} = \pm\frac{1}{(2\beta_2)^{\frac{1}{2}}}\sqrt{-\alpha t - \gamma_1\epsilon_{22} - \gamma_2\epsilon_{33} - \gamma_3\epsilon_{11}}$$

$$\delta r^{(4/5)} = \delta\phi^{(4/5)} = 0 \quad r^{(4/5)} = \pm\frac{1}{(2\beta_2)^{\frac{1}{2}}}\sqrt{-\alpha t - \gamma_1\epsilon_{22} - \gamma_2\epsilon_{33} - \gamma_3\epsilon_{11}}$$

The stability and energy of these solutions is shown in Table 3, where $B = (2\beta_1 - \beta_3)/\beta_2$. The first solution is stable in the high temperature phase, while the other solutions are stable in the low temperature phase, given that $\beta_2 > 0$ and $B > -3$. For $-3 < B < 0$, only solutions two and three are stable.

We evaluate the effect on the elastic moduli the same way as before. In the high temperature phase, nothing is changed. In the low temperature phase the affected moduli for the 2/3 solution are

$$\Delta C_{1111} = -\frac{\gamma_3^2}{2\beta_2} \qquad \Delta C_{2222} = -\frac{\gamma_1^2}{2\beta_2} \qquad \Delta C_{3333} = -\frac{\gamma_2^2}{2\beta_2}$$
$$\Delta C_{1122} = -\frac{\gamma_1\gamma_3}{2\beta_2} \qquad \Delta C_{1133} = -\frac{\gamma_2\gamma_3}{2\beta_2} \qquad \Delta C_{2233} = -\frac{\gamma_1\gamma_2}{2\beta_2}$$

and those for the 4/5 solution are

$$\Delta C_{1111} = -\frac{\gamma_1^2}{2\beta_2} \qquad \Delta C_{2222} = -\frac{\gamma_3^2}{2\beta_2} \qquad \Delta C_{3333} = -\frac{\gamma_2^2}{2\beta_2}$$
$$\Delta C_{1122} = -\frac{\gamma_1\gamma_3}{2\beta_2} \qquad \Delta C_{1133} = -\frac{\gamma_1\gamma_2}{2\beta_2} \qquad \Delta C_{2233} = -\frac{\gamma_2\gamma_3}{2\beta_2}$$

Again there are discontinuities, but this time something very interesting happens. Without an interaction, due to the symmetry of the lattice, $C_{1111} = C_{2222}$ and $C_{1133} = C_{2233}$. However, the low-temperature state results in a spontaneous breaking of the symmetry of the elastic moduli tensor, and in that phase $C'_{1111} \neq C'_{2222}$. This symmetry breaking in the effective elastic moduli is a way that an experimentalist could differentiate p-wave superconductivity from d-wave superconductivity.

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