Investigation of the soft mode behavior in superconducting Heusler $LiPd_2Ge$

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$LiPd_2Ge$ is a type-I superconductor with transition temperature $T_c = 1.96$ K. It belongs to the rich Heusler family of more than a thousand compounds which exhibit all kind of physical phenomena. $LiPd_2Ge$ was recently synthesized and characterized experimentally as well as with DFT calculations [1]. In this work we investigate observed phonon anomalies using *ab initio* computations. Acoustic phonons are strongly softened and become imaginary at Γ-K near vector $\boldsymbol{q}$=(1/3,1/3,0). It is worth noting that isoelectronic $LiPd_2Si$ and $LiPd_2Sn$ show similar behavior. $LiPd_2Ge$ has highest T_c and strongest softening, which suggests that the soft mode enhances superconductivity. Many other reported Heusler compounds show phonon anomalies, which is also observed experimentally. We examined whether distorted or modulated structures are favorable. Fermi surface nesting could be another explanation for phonon softening, especially considering the presence of Pd atoms for which the Kohn anomaly is well known. We calculated generalized susceptibility function to look for features indicating Fermi surface nesting. Then we probed potential energy surface by calculating energy of cells with distorted atoms along phonon eigenvectors. Resulting curve deviated from a parabola expected for a harmonic potential as it had a double well structure.

References:

[1] K. Górnicka et al., "Soft-mode enhanced type-I superconductivity in LiPd2Ge", PHYSICAL REVIEW B 102, 024507 (2020).

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