



FIG. 2. Plot of the squared transverse optic mode frequency vs. pressure for different temperatures. Quantities are expressed in the reduced units of Fig. 1. The arrows indicate the pressure P_1 above which the static dielectric constant deviates from a linear dependence.

$(h\omega/k_B T) < 1$. It is clear that as the pressure is increased the density of these modes decreases and, hence, T_1 increases. Figure 2 illustrates the behavior of $\omega_{TO}^2(\Gamma)$ vs. pressure for fixed temperature. For pressures less than 0.006 (~ 8

kbar) it is clear that the dependence of $\omega_{TO}^2(\Gamma)$ on pressure is essentially linear at all temperatures, in agreement with the experimental measurements of Abel. However, we note that at high enough pressures deviations from a linear pressure dependence appear for pressures in excess of P_1 , with P_1 increasing with temperature. This dependence of $\omega_{TO}^2(\Gamma)$ on pressure at fixed temperature is what one would expect on physical grounds. If we fix the temperature, then an increase in pressure will induce a corresponding increase in $\omega_{TO}^2(\Gamma)$ arising from the decrease in atomic volume. For small enough pressures, this change will be linear in the pressure, with deviations from linearity occurring at high pressure.

In summary, we emphasize that although our calculations were carried out on a model crystal of the NaCl structure for simplicity, the qualitative features of the results are essentially model independent and mirror similar behavior in the perovskite KTaO_3 .

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Используя самосогласованную методику перенормировки при обработке спектра частот модельного параэлектрика, мы воспроизводим существенные характеристики зависимости статического диэлектрического константа зарождающегося ферроэлектрика KTaO_3 от давления.

Utilisant une procédure de renormalisation auto-consistante pour le traitement du spectre de fréquence d'un paraélectrique modèle, les caractéristiques essentielles de la fonction de pression de la constante diélectrique statique de KTaO_3 ferroélectrique naissant sont reproduits.