

A New Equation for Period Vectors of Crystals under External Stress and Temperature in Statistical Physics

Mechanical Equilibrium Condition and Equation of State

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<https://doi.org/10.1140/epjp/s13360-020-01010-6>

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July, 2021

Outlines

- 1 Paper about it
- 2 Derivation of the equation
- 3 Net force on the right by the left in the example

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The screenshot shows a web browser window with three tabs: 'Mail - Gang Liu - Outlook', 'multiline.equation.by.beamer - C x', and 'A new equation for period vector - x +'. The address bar shows the URL link.springer.com/article/10.1140/epjp/s13360-020-01010-6. The page header includes the SpringerLink logo and a search bar. The article title is 'A new equation for period vectors of crystals under external stress and temperature in statistical physics: mechanical equilibrium condition and equation of state' by Gang Liu. It is a Regular Article, Open Access, published on 06 January 2021. The article is from 'The European Physical Journal Plus' 136, Article number: 48 (2021). It has 1950 accesses. The abstract starts with 'Starting with the rigorous derivation of the work done on the center cell by external forces, a new equation is derived for the period vectors (cell edge vectors) in crystals under external stress and temperature. Since the equation is based on the principles of statistical physics, it applies to both classical and quantum systems. The existing theory for crystals under external pressure is covered as a special case. The new equation turns out to be the mechanical equilibrium condition and the equation of state for crystals under external stress and temperature. It may be used to predict crystal structures and to study structural phase transitions and crystal expansions. For linear elastic crystals, it takes the microscopic and'. The right sidebar contains a 'Download PDF' button and a 'Sections' menu with items: Abstract, Introduction, Equation derivation for period vectors in a crystal u..., Existing statistical theory for external pressure as a ..., Internal stress and mechanical equilibrium condition, Equation of state and system expansion, Work and energy in quasi-equilibrium process, Discussion, A one-dimensional simplified model system, Summary, Data Availability Statement, Notes, References, and Acknowledgements.

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A new equation for period vectors of crystals under external stress and temperature in statistical physics: mechanical equilibrium condition and equation of state

Gang Liu

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Abstract

Starting with the rigorous derivation of the work done on the center cell by external forces, a new equation is derived for the period vectors (cell edge vectors) in crystals under external stress and temperature. Since the equation is based on the principles of statistical physics, it applies to both classical and quantum systems. The existing theory for crystals under external pressure is covered as a special case. The new equation turns out to be the mechanical equilibrium condition and the equation of state for crystals under external stress and temperature. It may be used to predict crystal structures and to study structural phase transitions and crystal expansions. For linear elastic crystals, it takes the microscopic and

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Abstract

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Section

Abstract

Introduction

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Existing

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Equation

Work

Discussion

A one-

Summary

Data A

Notes

Reference

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The European Physical Journal Plus 136, 48 (2021)
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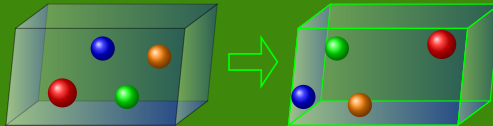
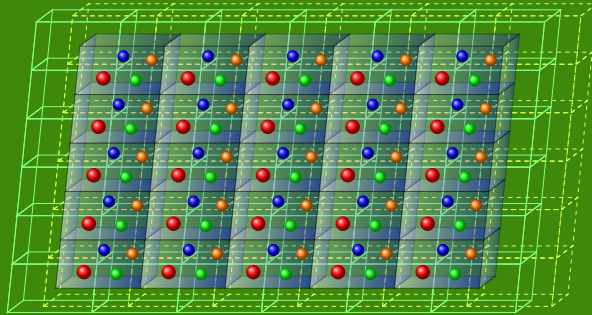
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The work done on the center cell by the external stress \mathbf{S}

$$dW = (\mathbf{S} \cdot \sigma_{\mathbf{a}}) \cdot d\mathbf{a} + (\mathbf{S} \cdot \sigma_{\mathbf{b}}) \cdot d\mathbf{b} + (\mathbf{S} \cdot \sigma_{\mathbf{c}}) \cdot d\mathbf{c} \quad (1)$$



Then based on the principles of statistical physics, the new equation determining the period vectors (**a**, **b**, **c**) for crystals under external stress **S** and temperature T :

$$\mathbf{S} \cdot \boldsymbol{\sigma}_{\mathbf{h}} = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \mathbf{h}} \quad (\mathbf{h} = \mathbf{a}, \mathbf{b}, \mathbf{c}), \quad (2)$$

where $\beta = 1/(kT)$, and k and Z are the Boltzmann constant and the system partition function. The cell surface vectors are $\sigma_{\mathbf{a}} = \mathbf{b} \times \mathbf{c}$, $\sigma_{\mathbf{b}} = \mathbf{c} \times \mathbf{a}$, and $\sigma_{\mathbf{c}} = \mathbf{a} \times \mathbf{b}$.

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The net force by the left half on the right half of the one-dimensional crystal

$$F_{L \rightarrow R}(a) = -\frac{d}{da} E_p^{(L-J)}(a) \quad (3)$$

The net force by the left half on the right half of the one-dimensional crystal

$$F_{L \rightarrow R}(a) = -\frac{d}{da} E_p^{(L-J)}(a) \quad (3)$$

$$= \frac{1}{2} \sum_{j=-\infty}^{\infty (j \neq 0)} j f^{(L-J)}(ja) \quad (4)$$

The net force by the left half on the right half of the one-dimensional crystal

$$F_{L \rightarrow R}(a) = -\frac{d}{da} E_p^{(L-J)}(a) \quad (3)$$

$$= \frac{1}{2} \sum_{j=-\infty}^{\infty (j \neq 0)} j f^{(L-J)}(ja) \quad (4)$$

$$= \sum_{j=1}^{\infty} \frac{4\epsilon}{a} \left[12 \left(\frac{\lambda}{ja} \right)^{12} - 6 \left(\frac{\lambda}{ja} \right)^6 \right] \quad (5)$$