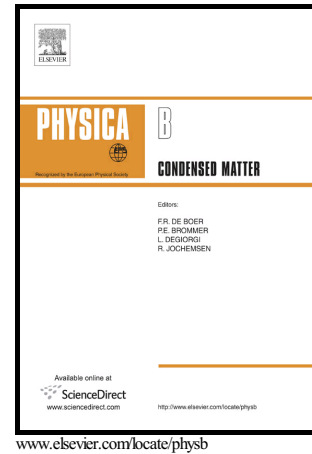


Author's Accepted Manuscript

The Effect of Thermal Fluctuations on Holstein Polaron Dynamics in Electric Field

Nikolaos K. Voulgarakis



PII: S0921-4526(17)30212-0
DOI: <http://dx.doi.org/10.1016/j.physb.2017.04.030>
Reference: PHYSB309921

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 21 March 2017
Revised date: 27 April 2017
Accepted date: 28 April 2017

Cite this article as: Nikolaos K. Voulgarakis, The Effect of Thermal Fluctuations on Holstein Polaron Dynamics in Electric Field, *Physica B: Physics of Condensed Matter*, <http://dx.doi.org/10.1016/j.physb.2017.04.030>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

The Effect of Thermal Fluctuations on Holstein Polaron Dynamics in Electric Field

Nikolaos K. Voulgarakis*

Department of Mathematics and Statistics, Washington State University, Pullman, 99164, United States

*Correspondence to: n.voulgarakis@wsu.edu

Abstract

In this work, we have studied the effects of thermal fluctuations on the stability of polaron motion under the influence of an external electric field. Zero temperature calculations have been reported previously showing the existence of critical electric field, E_{cr} , where the system transitions from a stable polaron motion to a Bloch-like oscillation. In this study, we further report that for intermediate polaron sizes the lifetime of such Bloch-like oscillations decay with time due to excessive phonon emission. Our numerical simulations show that the value of E_{cr} is finite for small temperatures. However, E_{cr} rapidly decreases with increasing T and becomes practically zero for $T > T_{cr}$. In this small but finite temperature window, we report how temperature affects (a) the electric current density, and (b) the Bloch-like frequencies.

Keywords: Holstein model, polaron mobility, thermal fluctuations, Bloch oscillation, Langevin dynamics.

1. Introduction

Charge transport in organic compounds has been an active research area for more than three decades, mainly because of their potential use in electronic devices. Experimental observations have reported high mobilities in rubrene and pentacene that are comparable to inorganic semiconductors [1-3]. This high mobility can, however, be altered by any type of disorder that induces localization of the charge carriers [1]. Understanding the influence of thermal fluctuations on the charge transport mechanism is, thus, crucial for improving the performance of organic-based electronic devices.

Download English Version:

<https://daneshyari.com/en/article/5491944>

Download Persian Version:

<https://daneshyari.com/article/5491944>

[Daneshyari.com](https://daneshyari.com)