Short Visit Grant 2287

Grantee:
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Host:
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Final report

The purpose of this visit was to develop a collaborative project with Prof. A.O. Gogolin on the topic of phonon-phonon (ph-ph) interactions in single-wall carbon nanotubes. The main idea of the project was to provide an analytical treatment of ph-ph interactions by exploiting a formulation of the low-energy long-wavelength vibrational dynamics of nanotubes in terms of a continuum elastic model.

During the stay, a significant progress has been achieved, as described below, and we plan to submit soon a paper on this topic.

(1) The elastic formulation has been used to explicitly compute all the amplitudes for the three- and four-phonon scattering processes allowed by kinematics. Here, the crucial point has been to realize that one has to formulate the elastic theory in terms of the *nonlinear* strain tensor. As a consequence, one finds two kinds of nonlinearities: the first kind of terms comes from the *harmonic part* of the Hamiltonian due to the nonlinearity of the strain tensor. These terms, which have been dubbed *geometric* or *induced* nonlinearities, contain only two (known) parameters, the bulk and the shear moduli. The second kind of terms are the usual anharmonicities (cubic and quartic terms in the linear part of the strain tensor). These terms contain additional parameters (higher order elastic constants) which are in general not known.

We found the unexpected result that, with only one exception, the dominant term in the amplitudes is always given by the geometric nonlinearities, which will eventually allow for quite reliable estimates using just the known values of the bulk and shear moduli. Furthermore, we found, among other things, that the amplitude for the scattering between a twisting mode and two flexural modes has a q^5 dependence, at variance with the q^3 dependence expected on general grounds for acoustic modes (here q is momentum). This difference originates from the peculiar cylindrical geometry of the nanotube.

To summarize, the main result obtained in this first part of the project is a complete analytical theory for ph-ph interactions in nanotubes in the low-energy long-wavelength regime.

(2) The calculation of the amplitudes provides the necessary ingredients for the next step, the calculation of physical properties due to ph-ph interaction processes. Here we focussed, as planned, on lifetime and frequency shift of the vibrational normal modes. By means of Fermi's golden rule, we computed the decay rates at zero temperature, obtaining unusual dependencies on momentum for all the acoustic modes. These calculations should then be complemented by the finite temperature ones. In this case, following a standard approach, we reformulated the problem in the more convenient diagrammatic language, whereby lifetime and frequency shift can be expressed in terms of the imaginary and real parts of the appropriate self-energy. The corresponding calculations, which should be completed soon, will provide the temperature dependence of lifetimes and frequency shifts. These results will also be important for the planned calculation of the thermal expansion coefficient.

As mentioned at the beginning, we plan to submit soon a long publication on the results obtained during this stay, and to continue our collaboration with the host institution on various developments of this project.

The visit took place from 14/04/08 to 28/04/08 (please notice the change in the final date with respect to the originally planned one).