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Specific heat of doped armchair and zigzag carbon nanotubes

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HIGHLIGHTS

- Theoretical calculation of specific heat of zigzag carbon nanotubes in the context of the Holstein model.
- The investigation of specific heat versus electron–phonon interaction.
- The investigation of specific heat versus diameters and electronic concentration.

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ABSTRACT

We study the temperature behavior of electronic specific heat of metallic carbon nanotubes in the context of Holstein model Hamiltonian. Green's function approach has been implemented in order to calculate the electronic contribution to the specific heat of the compound. Second order perturbation theory has been used to obtain interacting Green's function of model Hamiltonian. The results show a monotonic increasing behavior for specific heat with temperature for both armchair and zigzag carbon nanotubes. Furthermore, the effect of various electronic concentrations and the electron–phonon coupling strengths on the specific heat has been investigated.

1. Introduction

Carbon nanotubes made of a single graphite layer rolled up into a hollow cylinder are a one-dimensional allotrope of carbon [1–3]. The investigation of the electronic properties of carbon *nanotubes* [3] has been of research interests for theorists for more than 50 years. Among these topics, one can point to the sensitive dependence of electronic structure on the diameter and chirality of the tubule. It has been shown that CNTs can be either metallic or semiconducting with a band gap varying from zero to a few tenths of an eV, depending on their diameter and chirality. Also the thermal properties of the compounds are not well characterized experimentally, however, they are important from the viewpoint of basic research and possible application. It has been predicted that the diameter of tubes affects the temperature dependence of specific heat and might be shown to be a sign of dimensional crossover as the temperature is varied [4]. The unusual linear wave vector dependence of the electronic structure of a single graphene sheet on fermi energy indicates that specific heat has a quadratic dependence on temperature in contrast to typical metals. The specific heat of the out-of- and in-plane phonon modes gets the higher values compared to the electronic contribution at low temperatures. At low temperature, only the acoustic bands will be populated and a linear temperature dependence for the phononic contribution to the specific heat has been evaluated analytically [4]. Also the electronic specific heat for a quasi-one-dimensional metallic CNT has a linear behavior for temperature dependence [4]. It has been seen that phonons have dominant contribution to the specific heat at all the temperatures. The electronic specific heat of a semiconducting tube should vanish roughly exponentially as $T \longrightarrow 0$ and reduces to lower amounts compared to the metallic one [5]. Using phononic density of states theoretically, the phonon specific heat of graphite has lower values below those of graphene and isolated (10,10) single-walled CNT [6]. A strikingly linear behavior for temperature dependence of a multi-walled CNT over the entire temperature range (10–300 K) has been found using experimental measurements [7].

The effect of lattice vibration of atoms is an important factor to study electronic properties of single-walled CNT [3]. It should be noticed that some aspects of electronic properties of nanotubes such as charge density wave and superconductivity instabilities can be understood by considering the coupling of electrons with phonons [8,9]. Local density of states of zigzag graphene ribbons and zigzag CNTs has been investigated due to electron–phonon coupling [10,11]. Among all the lattice vibrational modes, we concentrate on the out-of-plane vibrations along the radius of CNT. The symmetric

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property of this displacement with respect to their neighboring atoms leads to coupling between electronic density and this mode of phonons [12]. The out-of-plane vibrations are dispersionless and couple with electrons in the context of Holstein model Hamiltonian [13]. The behavior of optical spectrum of graphene and CNT has been studied in the context of the Holstein model using second order perturbation theory for self-energy [14]. Temperature dependence of transport properties such as electrical and thermal conductivities have been investigated based on the Holstein model [15–17].

The aim of this work is to study the temperature dependence of specific heat of doped metallic zigzag and armchair CNT in the context of Holstein model Hamiltonian. Using the equation of motion of Green's function, one can calculate the electronic contribution to specific heat. Interacting Green's function has been obtained under second order perturbation theory for self-energy. Afterwards, specific heat of the CNT can be found using corrected electronic Green's function and the effect of electron–phonon coupling strength on the specific heat can be found.

2. The effect of electron–phonon interaction on the excitation spectrum

The effect of interaction between itinerant electrons and local dispersionless phonon modes on the electronic properties of CNTs can be investigated in the context of the following Holstein model Hamiltonian [13]:

$$H=-t\sum_{\delta j}(a^{\dagger}_{j+\delta,\sigma}b_{j,\sigma}+h.c.)+g\sum_{i,\sigma}(a^{\dagger}_{i,\sigma}a_{i,\sigma}+b^{\dagger}_{i,\sigma}b_{i,\sigma})(c_i+c^{\dagger}_i)+\omega_0 c^{\dagger}_i c_i, \quad (1)$$

where t implies the hopping amplitude of moving electrons between nearest neighbor atoms belonging to sublattices A and B. Also, $a_{i,\sigma}(b_{i,\sigma})$ denotes the on-site annihilation operator for electrons in the sublattice A (B) with spin σ. $c_i(c^{\dagger}_i)$ denotes the annihilation (creation) operator for local modes of phonons. ω_0 and g are the phonon frequency and the electron–phonon coupling constant respectively. According to Fig. 1, the primitive unit cell vectors have been shown as the following vectors:

$$a_1=a\mathbf{i}, \quad a_2=\frac{a}{2}(-\mathbf{i}+\sqrt{3}\mathbf{j}), \quad (2)$$

where a is the length of the lattice translational vector. We consider unit vector $\mathbf{j}$ along the zigzag direction. The matrix element of noninteracting electronic Green's function has been introduced as $G^{(0)}_{AA}(R_{ij},\tau)=-\langle T(a_{i,\sigma}(\tau)a^{\dagger}_{j,\sigma}(0))\rangle$, where R_{ij} denotes the vector connecting nearest neighbor unit cells. After rewriting the Hamiltonian in terms of the Fourier transformation of operators, the elements of noninteracting electronic Green's function get the following forms [18]:

$$G^{(0)}_{AA}(\mathbf{k},i\omega_n)=G^{(0)}_{BB}(\mathbf{k},i\omega_n)=\sum_{j=\pm}\frac{1}{2}\frac{1}{i\omega_n-E_j(\mathbf{k})},$$

$$G^{(0)}_{AB}(\mathbf{k},i\omega_n)=\sum_{j=\pm}\frac{1}{2}\frac{\phi^*(\mathbf{k})}{E_+(\mathbf{k})}\left(\frac{j}{i\omega_n-E_j(\mathbf{k})}\right),$$

$$G^{(0)}_{BA}(\mathbf{k},i\omega_n)=\sum_{j=\pm}\frac{1}{2}\frac{\phi(\mathbf{k})}{E_+(\mathbf{k})}\left(\frac{j}{i\omega_n-E_j(\mathbf{k})}\right),$$

$$E_j(\mathbf{k})=tj|\phi(\mathbf{k})|, \quad \phi(\mathbf{k})=1+\cos(k_x/2)\exp(-ik_y\sqrt{3}/2), \quad (3)$$

where $\omega_n=(2n+1)\pi/\beta$ is Fermionic Matsubara's frequency and $\mathbf{k}$ is the electron wave vector belonging to the first Brillouin zone of honeycomb lattice. Moreover, noninteracting phononic Green's function is given by

$$D^{(0)}(\mathbf{p},ip_m)=\frac{2\omega_0}{(ip_m)^2-\omega_0^2}. \quad (4)$$

Based on the Migdal theorem [19], vertex correction in the construction of electronic self-energy is negligible. Also this theorem permits us to consider self-energy at lowest order perturbation theory and to neglect higher orders of electronic self-energy in honeycomb lattice. Using the Feynman rules [20], matrix elements of self-energy ($\Sigma_{\alpha\beta}(\mathbf{k},i\omega_n)$) at second order perturbation theory are given as

$$\Sigma_{\alpha\beta}(\mathbf{k},i\omega_n)=-\frac{1}{\beta}\sum_{p,m}g^2D^{(0)}(\mathbf{p},ip_m)G^{(0)}_{\alpha\beta}(\mathbf{k}-\mathbf{p},i\omega_n-ip_m), \quad (5)$$

where $G^{(0)}_{\alpha\beta}$ have been introduced in Eq. (3). Within the Dirac cone approximation that is valid in the energy range of 1 eV one can neglect the off-diagonal elements of the self-energy matrix and diagonal elements are independent of the wave vector. In other words we have $\Sigma_{\alpha\beta}(\mathbf{k},i\omega_n)=\delta_{\alpha\beta}\Sigma(i\omega_n)$. Substituting Eqs. (3) and (4) into Eq. (5) and summing over internal Matsubara's frequency according to the Feynman rules, the non-zero element of self-energy matrix gets the following form:

$$\Sigma(i\omega_n)=\frac{g^2}{2N}\sum_{k,j}\left(\frac{n_B(\omega_0)+n_F(tj|\phi(k)|)}{i\omega_n-jt|\phi(k)|+\omega_0}+\frac{n_B(\omega_0)+1-n_F(tj|\phi(k)|)}{i\omega_n-jt|\phi(k)|-\omega_0}\right), \quad (6)$$

where $n_F(E)=1/(e^{\beta E}+1)$ and $n_B(\omega_0)=1/(e^{\beta\omega_0}-1)$ are the Fermi and Bosonic distribution functions, respectively. N denotes the number of unit cells and summation in Eq. (6) is performed over $\mathbf{k}$ points belonging to the first Brillouin zone of graphene. The perturbative expansion for interacting Green's function in Matsubara's notation is given by [20]

$$\mathbf{G}^{-1}(\mathbf{k},i\omega_n)=\mathbf{G}^{(0)\,-1}(\mathbf{k},i\omega_n)-\Sigma(\mathbf{k},i\omega_n). \quad (7)$$

The self-energy and noninteracting Green's function matrices are given by

$$\mathbf{G}(\mathbf{k},i\omega_n)=\begin{pmatrix}G^{(0)}_{AA}(\mathbf{k},i\omega_n) & G^{(0)}_{AB}(\mathbf{k},i\omega_n)\\ G^{(0)}_{BA}(\mathbf{k},i\omega_n) & G^{(0)}_{BB}(\mathbf{k},i\omega_n)\end{pmatrix},$$

$$\Sigma(i\omega_n)=\begin{pmatrix}\Sigma(i\omega_n) & 0\\ 0 & \Sigma(i\omega_n)\end{pmatrix}, \quad (8)$$

in which the diagonal matrix elements of self-energy have been presented in Eq. (6). In analogy to noninteracting Green's function matrix presented in Eq. (8), there is a matrix form for the interacting one. After substituting the elements of noninteracting Green's function into Eq. (8) and applying Dyson's equation that has been indicated in Eq. (7), the elements of interacting Green's function are obtained as follows:

$$G_{AA}(\mathbf{k},i\omega_n)=G_{BB}(\mathbf{k},i\omega_n)=\sum_{j=\pm}\frac{1}{2}\frac{1}{i\omega_n-E_j(\mathbf{k})-\Sigma(i\omega_n)},$$

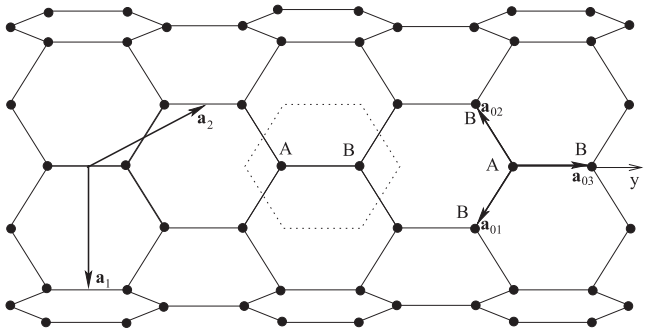

Fig. 1. A zigzag CNT whose axes is along the y axes. The light dashed lines denote the Bravais lattice unit cell. Each cell includes two nonequivalent sites, which are indicated by A and B. $\mathbf{a}_1$ and $\mathbf{a}_2$ are the primitive vectors of unit cell. $\mathbf{a}_{01}$, $\mathbf{a}_{02}$ and $\mathbf{a}_{03}$ are three vectors that connect nearest neighbor sites.