PHYSCIS

DoubleTime Green Function and the Electron Phonon Interaction in Superlattics

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ABSTRACT

The electron phonon interaction in a superlattices has been considered using double time Green function. This approach provides an easy method of obtaining the Absorption coefficient both for electrons and phonons and also calculating the shift in the ground state energy of electrons in superlattices due to the interaction.

INTRODUCTION

Solid state structures which have, in addition to the periodic potential of the crystal lattice, a one dimensional periodic potential whose period is much longer than the lattice constant are customarily called superlattices(SL).

Superlattices are a new type of semiconductor which is characterized by the presence of a larger number of bands, exhibiting very strong anisotropy. Such systems were first studied by L.V. Keldysh in 1962[1].

The rapid growth in theoretical and experimental interests in superlattices is associated with the recent development in the epitaxial crystal growth technique such as the molecular beam epitaxy (MBE) and the metal-organic chemical vapour deposition (MOCVD) [2-7] and also the number of interesting properties observed in SL which ordinary semiconductors do not posses.

It is known that the electron energy spectrum of a superlattice (SL) leads to a modification of the electron-proton interaction and consequently that of the phonon spectrum[8].

The purpose of this paper is to investigate the electron phonon interaction in SL. Using the double time Green function we obtain expressions for both the electrons and phonons absorption coefficient and calculate the shift in the ground state energy of electrons in SL due to the interaction.

This paper is organized as follows: In sec. II the double time Green functions is introduced and the Hamiltonian for the electron phonon interaction in SL is obtained. The dispersion equation is established in sec. III; we discuss the results in sec. IV and conclude in sec. V.

II. DOUBLE TIME GREEN FUNCTION AND THE ELECTRON-PHONON INTERACTION.

We shall confine ourselves to the retarded Green function.This is defined as

$$Gr(t,t') = \ll A(t);B(t') \gg_r = \quad (1)$$

$$-i\theta(t-t')\langle [A(t),B(t')] \rangle$$

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} \quad (2)$$

Where <...> means averaging over a grand canonical ensemble.

$$\langle \ldots \rangle = Q^{-1} Sp[\exp(-H/KT)], Q = Sp[\exp(-H/KT)],$$

Q is the partition function for the grand ensemble. The operator H includes a term with the chemical potential μ and is thus given by

$$H = H - \eta N \quad (3)$$

H is the time-independent Hamiltonian operator and N the operator of the total number of particles; A(t) and B(t) are the Heisenberg representations of the operators A and B, expressed in terms of a product of quantized field functions (or of particle creation and annihilation operations).

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Differentiating Eq (1) with respect to time we obtain

$$\frac{idG}{dt} = \delta(t-t') \tag{4}$$

$$< [A(t)b(t')] > = < \frac{idA(t)}{dt}; B(t') >$$

The Hamiltonian for an electron phonon interaction in the second quantization formalism written as

$$H = H_e + H_{ew} \tag{5}$$

$$H_e = \sum_{p,s} \epsilon_p^{(s)} a_p^{(s)+} a_p^{(s)} + \sum_q w_q b_q^+ b_q$$

$$H_{ew} = \sum_{p,q,s,s'} \langle sp|V(r)|s'p'\rangle a_p^{(s)+} a_p^{(s)} (bq^+ + b_q^+)$$

$$\text{where } \epsilon_p^{(s)} = \frac{P_z^2}{2m} + \epsilon_s - \Delta s \cos P_z d$$

$$s = 1,2,\ldots$$

ϵ_s and Δs are determined by SL potential parameters[8]. P_x, P_z are the component of crystal momentum across and the SL axis, d is the SL period $a_p^{(s)+}$ $a_p^{(s)}$ are the operators (creation and annihilation) of the s-th miniband ωq phonon frequency with wave vector q, b_q^+ b_q are the operators of phonon creation and annihilation. The matrix element presented in the equation is given in [9] as

$$\langle sp|V(r)|s'p'\rangle = \int \psi_p^{(s)}(r) V(r) \psi_{p'}^{(s')+}(r) dr \tag{6}$$

where

$$\psi(r) = \frac{1}{L}\exp[i(P_x X + P_y Y)]$$

$$\frac{1}{\sqrt{N}} \sum_{f=1}^{N} \exp(ip_z fd) \tag{7}$$

$$\psi s(Z - fd)$$

L-Normalized length; N-number of periods in SL. $\psi_s(z)$ is the wave function in the s-th state in one of the one-dimensional potential wells which composes the SL potential.

For a scattering potential V(r) in particular, the matrix element is given as

$$\langle SP|V(r)|S'P'\rangle = \sum_{n=-\infty}^{\infty} C_q M_{ss'}(q_z) \tag{8}$$

$$(\delta q_x, P_x - P_{x'}', \delta q_y, P_y - P_y', \delta q_z, P_z - P_z' + ng)$$

where g = (0,0,2π/d) the reciprocal SL vector.

Cq is fourier component of V(r)

$$M_{ss'}(qz) = \int \psi^*(z)\psi(z)\exp(iq_z Z)dz \tag{9}$$

Substituting Eq(9) into H_{ew} in Eq (5) we obtain

$$H_{ew} = \sum_{p,q,s,s'} C_q M_{ss'}(q_z) a_p^{(s)+} a_{p-q-nq}^{(s')} (b_q + b_{-q}^+) \tag{10}$$

III THE DISPERSION EQUATION

In order to obtain the dispersion relation for electrons and phonons we write the equation of motion for $a_p^{(s)+}$, $a_p^{(s)}$, b_q^+ and b_q. They are

$$\frac{idd_p}{dt} = \epsilon_p^{(s)} a_p^{(s)} + \sum_{q',s'} C_q M_{ss'}(q_z) a_{p-q-nq}^{(s')} (b_q + b_{-q}^+) \tag{11}$$

$$\frac{-idd_p^+}{dt} = \epsilon_p^{(s)} a_p^{(s)+} + \sum_{q',s'} C_q M_{ss'}(q_z) a_{p-q-nq}^{(s')+} (b_q + b_{-q}^+) \tag{12}$$

$$\frac{idb_q}{dt} = \omega_q b_q + \sum_{p',s',s'} C_q M_{ss'}(-q_z) a_{p-q-nq}^{(s)+} a_p^{(s')} \tag{13}$$

$$\frac{idb_q^+}{dt} = \omega_q b_q q^+ + \sum_{p',s',s'} C_q M_{ss'}(-q_z) a_{p-q-nq}^{(s)+} a_p^{(s')} \tag{14}$$

We introduce the single-particle Green functions of phonon type $G_q(t - t')$ which is defined as

$$G_q(t-t') = \langle b_q(t) b_q(t') \rangle \tag{15}$$

and we construct their equation of motion

$$\frac{idG_q(t-t')}{dt} = \delta(t-t') + \omega_q G_q + \sum_{p,s,s'} C_q M_{ss'}(-q_z) G_{p-q-nq,p,q}^{(ss')}(t-t') \tag{16}$$

Here we have introduced a mixed type Green functions, containing both Fermi and Bose operators.

$$G_{p-q-nq,p,q}^{(ss')}(t-t') = \langle\langle a_{p-q-nq}^{(s)+} a_p^{(s')}(t') b_q^+(t') \rangle\rangle \tag{17}$$

We get the exact equation for the Green function

$$\frac{id}{dt} G_{p-q-nq,p,q}(t-t') = (\epsilon_p^{(s')} - \epsilon_{p-q-nq}^{(ss)}) - \sum_{q,s,j} C_q I M_{ss'}(q_z) \langle\langle a_{p-q-nq}^{(s)+} a_{p-q-nq}(t) | b_q(t) - b_q^+(t), b_q^+(t') \rangle\rangle \tag{18}$$

We carry out decoupling of the higher Green functions occurring in Eq (18)

$$\left\langle\left\langle a_{p-q-nq}^{(\sigma)}(t)\left(b_{q_1}(t)+b_{-q_1}^{+}(t)\right)a_{p'}^{+(\sigma')}(t');b_q^{+}(t')\right\rangle\right\rangle =$$

$$\delta s'l;\delta n-n_1'\delta_{q,q_1}f_p^{(\sigma)}G_q(t-t') \qquad (19a)$$

$$\left\langle\left\langle a_{p-q-nq}^{(\sigma)}(t)a_{p-q-nq}^{+(\sigma)}(t)\left(b_q(t)+b_{-q}^{+}(t)\right);b_q^{+}(t')\right\rangle\right\rangle =$$

$$\delta_{\sigma\sigma'}\delta_{n-n'}\delta_{q,q'}f_{p-q-nq}^{(\sigma)}G_q(t-t') \qquad (19b)$$

where $\langle a_p^{+\sigma}, a_p^{(\sigma)}\rangle = f_p^{(\sigma)}$ is the electron distribution function. It is worth noting that since

$$\varepsilon_{p-q-nq} = \varepsilon_{p-q}$$

then

$$f_{p-q+nq} = f_{p-q} \quad .$$

Thus Eq (18) becomes

$$\frac{id}{dt}G_{p-q,p,q}^{(\sigma\sigma')}(t-t')=\left(\varepsilon_p^{(\sigma')}-\varepsilon_{p-q}^{(\sigma)}\right)G_{p-q,p,q}^{(\sigma\sigma')}(t-t')+$$

$$C_q M_{\sigma\sigma'}(q_z)\left(f_{p-q}^{\sigma}-f_p^{\sigma'}\right)G_q(t-t') \qquad (20)$$

Changing over to the fourier components of the Green functions in Eq (20) using the following formulae

$$G_q(t) = \int_{-\infty}^{\infty} G_q(E)e^{-iEt}dt$$

$$G_{p-q,p,q}^{(\sigma\sigma')} = \int_{-\infty}^{\infty} G_{p-q,p,q}(E)e^{-iEt}dt \qquad (21)$$

$$\delta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iEt}dt$$

We obtain

$$(E-\omega_q)G_p(E)=\frac{1}{2\pi}+$$

$$\sum_{p\sigma'} C_q M_{\sigma\sigma'}(q_z)G_{p-q,p,q}^{(\sigma\sigma')}(E) \qquad (22)$$

where $G_{p-q,p,q}^{(\sigma\sigma')}(E)$ is given as

$$G_{p-q,p,q}^{(\sigma\sigma')}(E)=\frac{C_q M_{\sigma\sigma'}(q_z)\left(f_{p-q}^{\sigma}-f_p^{\sigma'}\right)G_q(E)}{E-\varepsilon_p^{\sigma'}+\varepsilon_{p-q}^{\sigma}}$$

Taking into consideration that

$$M_{\sigma\sigma'}(-q_z)M_{\sigma\sigma'}(q_z) = |M_{\sigma\sigma'}(q_z)|^2$$

Then from Eq (22) we obtain the dispersion equation.

$$\left\{E-\omega_q-Cq^2\sum_{p\sigma'}\frac{|M_{\sigma\sigma'}(q_z)|^2 f_{p-q}^{(\sigma)}-f_p^{(\sigma')}}{E-\varepsilon_p^{(\sigma')}-\varepsilon_{p-q}^{(\sigma)}}\right\}G_q(E)=\frac{1}{2\pi} \qquad (23)$$

We introduce the $\pi q(E)$ which by analogy with the quantum field theory can be called polarization operator:

$$\Pi_q(E)=\sum_{\sigma\sigma' p}\frac{|Ass'(\bar{q}q_z)|^2 f_{p-q}^{(\sigma)}-f_p^{(\sigma')}}{E-\varepsilon_p^{(\sigma')}-\varepsilon_{p-q}^{(\sigma)}} \qquad (24)$$

Where $A_{\sigma\sigma'}(qq_z) = C_q M_{\sigma\sigma'}(q_z)$

We obtain

$$G_p(E) = \frac{1}{2\pi}\frac{1}{E-\omega_q-\Pi_q(E)} \qquad (25)$$

The electron dispersion is obtained analogically as the phonon one, that is we introduce the electron Green function.

$$G_p^{\sigma\sigma'}(t-t') = \left\langle\left\langle a_p^{(\sigma)}(t);a_p^{+(\sigma')}(t')\right\rangle\right\rangle \qquad (26)$$

Then going through the same process as for the phonon we obtain for the Fourier component

$M_p(E)$ is the Mass operator and is given as

$$G_p(E) = \frac{1}{E-\varepsilon_p-M_p(E)} \qquad (27)$$

$$M_p(E) = \sum_q |A(q,q_z)|^2$$

$$\left\{\frac{N_q+1-f_{p-q}}{E-\varepsilon_{p-q}-\omega_q}-\frac{f_{p-q}+N}{E-\varepsilon_{p-q}+\omega_q}\right\} \qquad (28)$$

$N_q = \langle b_q^{+} b_q\rangle$ phonon distribution function.

Using the Green functions we can also find the correlation functions.

$$\left\langle a_p^{+}(t')a_p(t)\right\rangle=\int_{-\infty}^{\infty}J_p(\omega)e^{-i\omega(t-t')}d\omega$$

$$\left\langle b_p^{+}(t')b_q(t)\right\rangle=\int_{-\infty}^{\infty}J_q(\omega)e^{-i\omega(t-t')}d\omega \qquad (29)$$

Where J_p and J_q are the spectral intensities

$$G_p(\omega+i\varepsilon)-G_p(\omega-i\varepsilon)=iJ_p(\omega)/e^{\beta\omega}+1)$$

$$G_q(\omega+i\varepsilon)-G_q(\omega-i\varepsilon)=iJ_q(\omega)/e^{\beta\omega}-1) \qquad (30)$$

Using Eq (25) and Eq (27) to write Eq (30) down in detail, we get

$$\Pi_q(\omega\pm i\varepsilon)=\Pi_q(\omega)\mp i\delta_q(\omega) \qquad (31)$$

$$M_p(\omega \pm i\varepsilon) = M_p(\omega) \mp i\delta_p(\omega) \quad (32)$$

Where

$$\Pi_q(\omega) = |A(qq_z)|^2 P\sum_p \frac{f_{p-q} - f_p}{\omega - \varepsilon_p + \varepsilon_{p-q}} \quad (33)$$

$$\gamma_q(\omega) = \pi |A(qq_z)|^2 \sum_p (f_{p-q} - f_p)\delta(\omega - \varepsilon_p + \varepsilon_{p-q}) \quad (34)$$

$$M_p(\omega) = P\sum_q |A(qq_z)|^2 \left\{ \frac{(N_q + 1 - f_{p-q})}{\omega - \varepsilon_{p-q} - \omega_q} + \frac{(f_{p-q} + N_q)}{\omega - \varepsilon_{p-q} + \omega_q} \right\} \quad (35)$$

$$\gamma_p(\omega) = \pi \sum_q |A(qq_z)|^2 [(N_q + 1 - f_{p-q}) \gamma(\omega - \varepsilon_{p-q} - \omega_q) + (f_{p-q} + N_q)\delta(\omega - \varepsilon_{p-q} - \omega_q)] \quad (36)$$

(p means the principal value)

IV DISCUSSIONS

We have obtained the expression for the coefficient of absorption both for the phonon and electron as indicated in Eq (34) and Eq (36) respectively. The functions $\gamma_q(\omega)$ and $\gamma_p(\omega)$ which are also temperature dependent play the role of damping.

As $q \to 0$; $\gamma_q \to 0$

Consider the propagation of a hypersound in a SL. When $q1 >> 1$ the problem is formulated as an electron phonon interaction. The sound wave is then taken as a monochromatic phonon (of frequency ωq) so with the help of Eq (34) the absorption coefficient can easily be calculated. Taking a concrete situation where the wave vector q is constant and directed along the axis of the SL; q = (o,o, q_z) and also $\omega << \varepsilon_+ - \varepsilon_-$.

In the potential deformation approximation, $C_q^m = i\Lambda q(2\rho\omega_q)^{-\frac{1}{2}}$
where Λ is the constant of deformation potential; ρ is the density of the sample (SL). For a non degenerate electron gas

$$\gamma_q = \frac{|\Lambda^2 q^2|\,|M(q_z)|^2}{\rho\,\omega_q} \frac{\theta(4\Delta^2 Sin^2 qd/2 - \omega_q^2)}{\sqrt{4\Delta^2 Sin^2 qd/2 - \omega_q^2}} \quad (37)$$

This result has been obtained [10]. It can be observed that when
$q \to O$, $\gamma_q \to O$ and that absorption is possible if and only if $\omega_q < 2\Delta Sin\ qd/2$ when $\omega_q > 2\Delta Sin\ qd/2$; $\gamma_q = 0$. This is a consequence of the law of conservation. In this case the SL sample is behaving as a filter permitting certain frequencies. This has been confirmed in [11].

The shift in the ground stage energy $\Delta\varepsilon_p$ was calculated by expressing the mass operator $Mp(\omega)$ in a power seres in ω at $\omega = \tilde{\varepsilon}_p$ and taking into account that $\gamma_p(\omega)$ a slowly varying function, $[\gamma_p(\omega) = \gamma_p(\tilde{\varepsilon}_p)]$. We get $\tilde{\varepsilon}_p - \varepsilon - M_p(\tilde{\varepsilon}_p) = 0$. Inserting the value of the value of the mass operator into it, i.e

$$\tilde{\varepsilon}_p - \varepsilon_p + P\sum |A(qq_z)|^2 \left\{ \frac{(N_q + 1 - f_{p-q})}{\varepsilon_p - \varepsilon_{p-q} - w_q} + \frac{f_{p-q} + N_q}{\varepsilon_p - \varepsilon_{p-q} + w_q} \right\} \quad (38)$$

and for

$$\tilde{\varepsilon}_p - \varepsilon_p = \Delta\varepsilon_p = 2\rho\sum_p \frac{C_p^2 |M(q_z)|^2 N_q}{\varepsilon_p - \varepsilon_{p-q}} \quad (39)$$

solving this expression yields

$$\Delta\varepsilon_p = \frac{\Lambda^2}{\pi^2} \frac{M^* K_I}{\rho V_s^2 d} \ln \left| \frac{q_{max}}{\sqrt{p_z^2 + P_y^2}} \right| \phi \quad (40)$$

where

$$\phi = \int_{-\pi/2}^{\pi/2} |m(x)|^2 dx$$

considering a simple situation where

$$M(x) = \sin\frac{x}{2};\ \phi = 2.43$$

Thus taking

$$\phi = 2.43; \Lambda \sim 16.7eV; m^* \sim 0.1 m_e; T \sim 3000^\circ k;$$
$$\rho = 5gm/cm^3; V_s = 5.10^5 cm/sec; \quad (41)$$
$$q_m \sim 10cm^{-1}; P_1 \sim 10^{-17}/cm^{-1}; d \sim 10^{-4}cm;$$

than the shift in ground state energy $\Delta\varepsilon_p \approx 10^{-3}$ e.

CONCLUSION

The electron-phonon interaction in superlattices has been studies theoretically using the double time Green function. The absorption coefficients both for electrons and phonons have been calculated. The shift in the ground state energy of SL has also been calculated.

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