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Phonon Green's Function; a Quanta Approaches

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Abstract: *The present paper reviews the concepts of source and quantum action principle used to produce the phonon Green's function appropriate for an initial phonon vacuum state.*
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I. Introduction

An essential concept and tool of any field theory is that of Green's function –the response, at one space-time point to an excitation at another such point the purpose of this study is to develop Green's function with lattice phonons [1]. K.H. Michel, M.J. Van LeeUWen have calculated the solution of a set of two coupled kinetic equations for both the electron and the phonon distribution functions in which the phonon drag appears in a natural way and in this case of a static electrical field (ω = 0), the set of equations reduces to two linearised Boltzmann equations[2]. Peter F. Meier derived a transport equation for phonons in a dielectric anharmonic crystal and applied the approximations which reduce this generalized equation to the Peierls equation are exhibited with the discussion of the coupling between the phonon and the dilatation fields[3]. N. Mingo and Liu Yang presented an approach for the atomistic study of phonon transport in real dielectric nanowires via Green's functions and the formalism is applied to investigate the phonon flow through nanowires coated by an amorphous material[4]. In the present paper, we have discussed the concepts of source and quantum action principle used to produce the phonon Green's function appropriate for an initial phonon vacuum state.

II. Method

In the interests of notational simplicity, I adopt units such that $\hbar = 1$ and I suppress the indices on N-component objects (such as $r_{a,} P_a$) as they enter the Hamiltonian, as[5]

$$H = \frac{P^2}{2M} + \frac{M}{2}(r - r_0).\Omega^2(r - r_0) - \frac{3}{2}tr\Omega \qquad \text{.....(1)}$$

The symbol Ω denotes as $N \times N$ matrix, which in the Phonon Spectrum space, has the angular frequency eigen values ω_Φ so that,

$$t_r \Omega \sum_\Phi \omega_\Phi \equiv N < \omega >_L \qquad \text{.....(2)}$$

The latter identity illustrates a lattice spectral average.
The transformations between co-ordinate and spectral levels are characterized by

$$< a / \phi >= \frac{1}{N^{1/2}} e^{iraik\phi} \quad \text{and} < \phi / a >= \frac{1}{N^{1/2}} e^{-iraik\phi} \qquad \text{.....(3)}$$

Where, as in eqn(1) r_{oa} vectors are the equilibrium positions and $k\phi$ is the propagation vectors of phonon mode ϕ. Accordingly, the co-ordinate representation of Ω^2 is

$$(\Omega^2)_{ab} = \sum_\phi < a / \phi > \omega_\phi^2 (\phi / b)$$

$$= \frac{1}{N} \sum_\phi \omega_\phi^2 e^{i(r_a o - r_o b)K_o}$$

$$= < \omega^2 e^{i(r_a o - r_o b)K} >_L \qquad \text{.....(4)}$$

The mutuallyadjoint N-component objects Y and Y^+, defined by

$$\Omega^{1/2} Y = \left(\frac{M}{2}\right)^{1/2} \Omega(r - r_0) + i(2M)^{-1/2} P$$

$$Y^{+}\Omega^{1/2}=\left(\frac{M}{2}\right)^{1/2}(r-r_o)\Omega-i\left(2M\right)^{-1/2}P \qquad \text{……(5)}$$

are such that

$$\left[Y,Y^{+}\right]=1, H=Y^{+}.\Omega Y \qquad \text{……(6)}$$

Where the unit symbol includes that for vectoral indices.

The Hamilton of equation (6) will now be extended to include external driving or source terms:

$$H\rightarrow\left(Y^{+}.\Omega Y\right)+\left(J^{*}.Y\right)+Y^{+}.J \qquad \text{……(7)}$$

where the vector sources J are V-component, complex numerical objects. The equation of motion derived from this extended Hamilton are the mutually adjoint statements[6].

$$\left.\begin{aligned} &i\frac{d}{dt}Y=\Omega Y-J\\ &and,-i\frac{d}{dt}Y^{+}=Y^{+}\Omega-J^{*}\end{aligned}\right] \qquad \text{..……(8)}$$

$\left\langle ot_1/ot_2\right\rangle$ Symbolizes the probability amplitude for the persistence of the phonon vaccumstate (V_{Pa}). In the absence of sources, the zero energy assigned to the vaccum state at any time

$$\left\langle V/Y^{+}.\Omega Y/V\right\rangle=0 \qquad \text{……(9)}$$

$$\left\langle Y/V\right\rangle=0 \text{ and } \left\langle V/Y^{+}\right\rangle=0 \qquad \text{……(10)}$$

And the V_{pa}=1

Now let the source act within the time interval between t_1 and t_2. According to the quantum action principle (3), an infinitesimal variation of sources produces $(1,2\equiv t_1,t_2)$.

$$\delta\left(V_1/V_2\right)=-i\left\langle V_1\right|\int_2^1 dt\left(\delta_{J^*}.Y+Y^{+}\delta_J\right)\left|V_2\right\rangle \qquad \text{……(11)}$$

The appropriate solution of the equation of motion in equation (8) is

$$Y(t)=e^{-i\Omega(t-t_2)}Y(2)-i\int_2^1 dt' e^{-i\Omega(t-t')J(t')}$$

$$\equiv iG(t-t_2)Y(2)+\int_2^1 dt' G(t-t')J(t') \qquad \text{……(12)}$$

along with,

$$Y^{+}(t')=Y^{+}(1)iG(t_1-t')+\int_2^1 dtJ^{*}(t)G(t-t') \qquad \text{……(13)}$$

Here,

$$\left.\begin{aligned} &G(t-t')=\frac{1}{i}e^{-i\Omega(t-t')\eta(t-t')}\\ &\eta(t-t')=\begin{cases}t>t':1\\ t<t':0\end{cases}\end{aligned}\right] \qquad \text{……(14)}$$

which obeys,

$$\left(i\frac{d}{dt}-\Omega\right)G(t-t')=\delta(t-t') \qquad \text{……(15)}$$

isGreen's function, the spectral version requires no more then $\Omega\rightarrow\omega_{\Phi}$, the coordinate form is

$$G(t-t')_{ab}=\sum_{\Phi}\left\langle a/\Phi\right\rangle G_{\Phi}(t-t')\left\langle\Phi'/b\right\rangle$$

$$= \frac{1}{N}\sum_{\Phi} e^{ir_{oa}.K_{\Phi}} \frac{1}{i} e^{-i\omega_{\Phi}(t-t')\eta(t-t')} e^{-ir_{ob}.K_{\Phi}} \quad \text{.……..(16)}$$

$$= \frac{1}{i}\eta(t-t')\left\langle \exp\left\{ i\left[\left(r_{oa} - r_{ob}\right).K - \omega(t-t') \right] \right\} \right\rangle L$$

On combination of the characteristics of the vaccumeqn (10) with eqn(12) and (13). The variational structure of eqn(11) becomes

$$\delta \log < V_1 / V_2 > = -i\delta \left[\int_2^1 dtdt' J^*(t).G(t-t')J(t') \right] \quad \text{…..……..(17)}$$

Which yields V_{Pa} in the presence of sources J as

$$< V_1 / V_2 > = \exp\left[-i \int_2^1 dtdt' J^*(t).G(t-t')J(t') \right] \quad \text{……(18)}$$

By noting that

$$iG(t-t') + \left[iG(t'-t) \right]^* = e^{-i\Omega(t-t')} \quad \text{…….……..…(19)}$$

We find the vaccum persistence probability to be

$$\left| \left\langle V_1 / V_2 \right\rangle \right|^2 = e^{-V} \quad \text{…….(20)}$$

Where,

$$V = \left| \int_2^1 dt e^{i\Omega t} J(t) \right|^2 \quad \text{..…….. (21)}$$

is the above average number of phonons emitted by the source (4). The closely related average emitted energy E is

$$E = \left[\int_2^1 dt J^*(t) e^{-i\Omega t} \right] .\Omega \left[\int_2^1 dt e^{i\Omega t} J(t) \right] \quad \text{..……(22)}$$

Consider the impulsive source

$$J(t) = i\delta(t) \left(\frac{M}{2} \right)^{\frac{1}{2}} \Omega^{\frac{1}{2}} D \quad \text{…...…...……(23)}$$

For real D. according to eqn(8) there is , in passing through time O, an instantaneous change in Y

$$\Delta Y = \left(\frac{M}{2} \right)^{\frac{1}{2}} \Omega^{\frac{1}{2}} D \quad \text{……..…(24)}$$

Which eqn(5) tells us – means a displacement of Y equal to D. The resulting Hamiltonian at time t = + O is

$$H = \left[Y^+ + \left(\frac{M}{2} \right)^{\frac{1}{2}} D\Omega^{\frac{1}{2}} \right] .\Omega \left[Y + \left(\frac{M}{2} \right)^{\frac{1}{2}} \Omega^{\frac{1}{2}} D \right]$$

$$= Y^+ .\Omega Y + \left(\frac{M}{2} \right)^{\frac{1}{2}} \left(Y^+ .\Omega^{3/2} D + D.\Omega^{3/2} Y \right) + \frac{M}{2} D.\Omega^2 D \quad \text{……(25)}$$

The vaccum expectation value of this Hamiltonian the average energy of the system that was initially in the vaccum state, is just

$$E = \frac{1}{2} MD.\Omega^2 D \quad \text{…….(26)}$$

The same result expressed as the energy of emitted Phonons is produced by eqn (22) and (23). Either approach can be used to get the measure of energy dispersion.

$$\left(\delta E\right)^2 \equiv \left\langle \left(H - E^2 \right) \right\rangle_t = \frac{1}{2} MD.\Omega^2 D \quad \text{……..(27)}$$

And of course, the average number of phonons is

$$V = \frac{1}{2} MD.\Omega D \qquad \text{……(28)}$$

For the example of a displacement at a single lattice site on has

$$V = \frac{1}{2} MD^2 < \omega >_L$$

$$E = \frac{1}{2} MD^2 < \omega^2 >_L = \frac{< \omega^2 >_L}{< \omega >_L} .V \qquad \text{……..……..(29)}$$

$$\left(\delta E\right)^2 = \frac{1}{2} MD < \omega^3 >_L = \frac{< \omega^3 >_L}{< \omega^2 >_L} .E$$

The outcome for the E in terms of D gives a general interpretation to an earlier result (i.e. eqn (6)) that assumed a large value of D[7].

A variant of the impulsive source in eqn (23) is-

$$J(t) = -\delta(t)(2M\Omega)^{-1/2} \Delta P \qquad \text{……..…..(30)}$$

It produces the instantaneous change

$$\Delta\gamma = i(2M\Omega)^{-1/2} \Delta P \qquad \text{……(31)}$$

Where, indeed, ΔP is the resulting displacement of P .

The immediate consequences are

$$V = \frac{1}{2M} \Delta P.\Omega^{-1} \Delta P$$

$$E = \frac{1}{2M} \left(\Delta P\right)^2 \qquad \text{…….……(32)}$$

$$\left(\delta E\right)^2 = \frac{1}{2M} \Delta P.\Omega \Delta P$$

and the implication for ΔP at one lattice site are given by

$$E = \frac{1}{2M} \left(\Delta P\right)^2$$

$$V = \left\langle \omega^{-1} \right\rangle_L E \qquad \text{……..……...(33)}$$

$$\left(\delta E\right)^2 = \left\langle \omega \right\rangle_L E$$

If the momentum impulse ΔP is applied, not at one, but at all lattice sites so eqn (32) implies that

$$E = \sum_a \frac{1}{2M} \left(\Delta P\right)_a^2 = N \frac{1}{2M} \left(\Delta P\right)^2 \qquad \text{…….(34)}$$

Then, $V = \sum_{ab} \frac{1}{2M} \Delta P_a .\Omega_{ab}^{-1} \Delta P_a$

$$= \frac{1}{2M} \left(\Delta P\right)^2 \sum_{ab} \frac{1}{N} \sum_{\Phi} \omega_{\Phi}^{-1} e^{i(r_{oa} - r_{ob}).K\delta} \qquad \text{……..(35)}$$

Where the a summation, for example, pick out the mode for which $K_{\Phi} = 0, \omega_{\Phi} = \omega'$

$$\sum_{\Phi} \omega_{\Phi}^{-1} \frac{1}{N} \sum_a e^{i(r_{oa} - r_{ob}).K\Phi} = \underline{\omega}^{-1} \qquad \text{…….……(36)}$$

theoutcome is not surprisingly

$$V = N.\frac{1}{2M} (\Delta P)^2 \frac{1}{\underline{\omega}} = \frac{E}{\underline{\omega}} \qquad \text{……..……(37)}$$

and similarly $\left(\delta E\right)^2 = N\frac{1}{2M}(\Delta P)^2 \underline{W} = \underline{W} E = \frac{E^2}{V}$ ……..……(38)

The huge value of N, for a small macroscopic body usually produce such a large number for Y that a well – defined amount of energy is released in the lattice. To clearify its interpretation, write

$$E = \frac{\left(N\Delta P\right)^2}{2NM} \qquad \text{……(39)}$$

and recall that the lattice geometry is not absolute but relative to the position of the center of mass for the entire system. Thus eqn(39) can be read as the kinetic energy transferred to the lattice as a whole.

III. Result And Discussion:

In the present article, the essential concept and tool of any field theory of Green's function for one space-time point to an excitation at another such point is studied to develop Green's function with lattice phonons. The work has been started with the Hamiltonian given by the equation(1) in which symbol Ω denotes as $N \times N$ matrix, which in the Phonon Spectrum space, has the angular frequency eigen values ω_{Φ} so that the equation(2) is satisfied. The Hamilton of equation will now be extended to include external driving or source terms given by the equation(7), in which the vector sources J are V-component, complex numerical objects. The equation of motion derived from this extended Hamilton are the mutually adjoint statements. For the vaccum expectation value of the Hamiltonian, the average energy of the system is determined given by the equation(26). This equation is extended for the huge value of N and a small macroscopic body usually produce such a large number for Y that a well – defined amount of energy is released in the lattice in the form of equation(39). This work presents that the lattice geometry is not absolute but relative to the position of the center of mass for the entire system and thus the kinetic energy can be transferred into the lattice as a whole.

IV. Conclusion

The present work gives the average energy of the system , when the Hamiltonian equation is extended for the huge value of N and a small macroscopic body usually produce such a large number for Y that a well – defined amount of energy is released in the lattice in the form of equation(39).This work also presents that the lattice geometry is not absolute but relative to the position of the center of mass for the entire system and thus the kinetic energy can be transferred into the lattice as a whole.

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