EFFECT OF COUPLING CONSTANT ON SPECTRAL FUNCTION: GREEN'S FUNCTION ANSATZ

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ABSTRACT

The Green's function ansatz is used to describe the effect of coupling constant both for weak and strong limit on the spectral function at zero temperature. Results of the spectral function for the various coupling constant give good insight on the Density of state (DOS) of particles.

Keywords: Green's function, coupling constant, spectral function, and density of state.

INTRODUCTION

Studies on the nature and behaviour of polarons in a tight binding system have drawn considerable attention in the last few years following indications of polaron charge carriers in high – T_C super conductor [1]. Intermediate or strong electron-phonon interaction gives rise to the existence of polaronic carriers in a number of interesting materials[2,3,4]. In temperature below 1K, the interaction between electrons and phonons in metals weakens to the point that the two systems can be out of thermal equilibrium with one another. Such weakened couping may be undesirable e.g., in dc superconducting quantum interference device (SQUIDs) where the noise may be limited by hot electron effects in the normal-metal shunt [5]. We look at a Hamiltonian which describes a fixed particle of energy ε_c interacting with a set of phonons with frequencies ω_q [6]. The interaction occurs only when the state is occupied and $\boldsymbol{c^\dagger c = 1}$. The phonons are the independent bosons.

The Hamiltonian we have considered is given as

$$H = C^\dagger C\left[\varepsilon_c + \sum_q \left(a_q + a_q^\dagger\right)\right] + \sum_q w_q a_q^\dagger a_q \tag{1}$$

Where $c^\dagger$and C are the creation and destruction operator of electrons and $a^\dagger(a)$ is the creation (annihilation) operator for the phonons. ω_q is the phonon frequency.

The Hamiltonian is solved first by canonical transformation and then by Green's function technique. In this work we look at the spectral function as the coupling constant varies from the weak limit to the strong limit for zero temperature regime, which has known the Einstein model.

The spectral function is defined as

$$A\ (r, r^1, E) = i\ [G^r(r, r'; E] - G^a(r, r^{'}; E)]$$

The A(w) provides information about the nature of the allowed electronic state, regardless whether they are occupied or not, and can be considered as a generalized density of states. The diagonal elements of the spectral function give the local density of states.

METHODOLOGY

We start with the particle Green's function that describes the interaction of electron with phonons for t > 0. The Green's function is given as,

$$G_{(t)} = -ie^{-it(\varepsilon_C - \Delta)} e^{-\phi_{(t)}} \left(1 - n_f\right), \qquad (1)$$

where $\phi_{(t)} = \sum_q \left(\frac{m_q}{w_q}\right)^2 \left[N_q\left(1 - e^{iw_q t}\right) + \left(N_q + 1\right)\left(1 - e^{-iw_q t}\right)\right]$, (2)

where N_q is the phonon-occupation number. The physics is best understood by examining a simple application of the model. All the phonons are taken to have the same energy w_0; which is called Einstein model. The case of zero temperature will be discussed. For zero temperature; all the phonon occupation factors are zero.

$N_q = N_0 = 0$

So equation (2) becomes

$$\phi_{(t)} = \sum_q \left(\frac{m_q}{w_q}\right)^2 \left(1 - e^{-iw_q t}\right),$$

where $g = \sum_q \left(\frac{m_q}{w_q}\right)^2$

which is the coupling constant

$$\therefore \phi_{(t)} = g(1 - e^{-iw_q t})$$

The particle Green's function will be evaluated for the case of a single particle, so set $n_f = 0$.

$$\therefore G_{(t)} - i\Theta(t)\exp\left[-it\varepsilon_C - g(1 - iw_o t - e^{-iw_o t)}\right] \quad (7)$$

The spectral function is the imaginary part of the retarded Green's function of frequency:

i.e $$A(w) = -2\,\mathrm{Im}\left\{-i\int_0^\infty dte^{iwt}\exp\left(-it\varepsilon_C - g(1 - iw_o t - e^{-iw_0 t}))\right)\right\} \quad (8)$$

$$\therefore A_{(w)} = 2\,\mathrm{Re}\left\{\int_0^\infty dte^{iwt}\exp\left[-it\varepsilon_c - g\left(1 - iw_0 t - e^{-1w_0 t}\right)\right]\right\} \quad (9)$$

Next expanding eqn (9) gives:

$$\therefore A_{(w)} = 2\,\mathrm{Re}\left\{\int_0^\infty dte^{iwt}e\left[-it\varepsilon_c - g + g^{iw_0 t} + g^{e-iw_0 t}\right]\right\}$$

$$= 2\left[\int_0^\infty dte^{iwt}e^{-it\varepsilon_c}e^{-g}e^{giw_o t}e^{ge^{-iw_o t}}\right] \quad (11)$$

Evaluating the time integral of the ge$^{-i\,w_o\,t}$ part of the exponent in a power series:

We know that

$$e^x = 1 + \frac{x^1}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots \equiv e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!} \quad (12)$$

Likewise

$$exp\ (ge^{-w_o t}) = e^{ge^{-iw_o t}}$$

By expansion similar to (12) $x = ge^{-iw_o t}$

$$\therefore e^{g^{e-w_o t}} = \sum_{l=0}^{\infty}\frac{\left(ge^{-w_0 t}\right)^l}{l!} \quad (13)$$

$$= \sum_{l=0}^{\infty}\frac{g^l e^{-w_0 tl}}{l!}$$

(14)

$$= \sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-iw_0 tl} \tag{15}$$

$\therefore$ Substitute $e^{ge-iw_0 t} = \sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-iw_0 tl}$

Into equation (11) then it becomes becomes;

$$A_{(w)} = 2\left\{ \int_0^{\infty} dt e^{iwt} e^{-it\varepsilon_c} e^{-g} e^{giw_o t} \left[\sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-iw_0 tl} \right] \right\} \tag{16}$$

$$= \int_0^{\infty} 2dt e^{iwt} \sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-iw_0 tl} e^{-g} e^{giw_0 t} e^{-it\varepsilon_c} \tag{17}$$

$$\therefore A_{(w)} = \int_0^{\infty} 2dt \sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-g} e^{iwt} e^{-it\varepsilon_c} e^{giw_o t} e^{-iw_0 tl} \tag{18}$$

$$= \int_0^{\infty} 2dt \sum_{l!}^{\infty} \frac{g^l}{l!} e^{-g} e^{it(w-\varepsilon_c+gw_0-w_0 l)} \tag{19}$$

$$= 2\sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-g} \int_0^{\infty} e^{it(w-\varepsilon_c+gw_0-w_0 l)} dt \tag{20}$$

Put $\Delta = gw_0$ into eqn (20)

$$A_{(w)} = 2\sum_{l=0}^{\infty} \frac{g^l}{l!} e^{-g} \int_0^{\infty} e^{it(w-\varepsilon_c+\Delta-w_0 l)} dt \tag{21}$$

$$\therefore \int_0^{\infty} \exp it(w-\varepsilon_c+\Delta-w_0 l) dt = \frac{i}{w-\varepsilon_c+\Delta-w_0 l+i\delta} \tag{22}$$

The factor $i\delta$ is added to force the convergence of the oscillating integrand at large values of time. Then take the limit $\delta \to 0$ and obtain.

$$\frac{i}{w-\varepsilon_c+\Delta-w_0 l+i\delta} = P\frac{i}{w-\varepsilon_c+\Delta-w_0 l} + \pi\delta(w-\varepsilon_c+\Delta w_0 l) \tag{23}$$

The above result is gotten by using the formula for the real and imaginary parts of the singular function.

$$(x+in)^{-1} = \frac{1}{x+in} = p\frac{1}{x} - i\pi\delta(x)$$

where P denotes the principal part. The spectral function is the real part of this time integral, which has just the delta function. i.e eqn (21)

i.e $$A_{(w)} = 2\sum_{l=0}^{\infty}\frac{g^l}{l!}e^{-g}\,\frac{P \quad i}{w-\varepsilon_c+\Delta w_0 t} + \pi\delta(w-\varepsilon_c+\Delta-w_o l) \qquad (24)$$

$$= 2e^{-g}\sum_{l=0}^{\infty}\frac{g^l}{l!}\pi\delta(w-\varepsilon_c+\Delta-wol) \qquad (25)$$

$$= 2\pi e^{-g}\sum_{l=0}^{\infty}\frac{g^l}{l!}\delta(w-\varepsilon_c+\Delta-w_o l) \qquad (26)$$

DISCUSSION AND RESULT

We have considered the Einstein model which assumed that at zero temperature, the phonon occupation number is zero.

The spectral function is a series of Delta function spaced exactly ω_o apart.

The spectra function is the probability that the particle has frequency w. if there were no interactions, the particle would always have energy ε_c and there would be a single delta function at $\omega = \varepsilon_c$, the different value of ω_l obviously correspond to the particle being coupled to some phonons which is certainly to be expected in this system. In the ground state of the coupled system of particle and phonon, some probability exists that the system will have the different sets of frequencies $\omega_l \equiv \in_c - \Delta + l\omega_o$. The different values of ω_l obviously correspond to the particle being coupled to some phonons, which is certainly to be expected in this system. In the ground state, the particle energy fluctuates among these different values of ω_l.

The spectral function is shown in Fig. 1 for the various values of the coupling constant ranging from the weak limit g = 0.5 to the strong coupling limit g = 5.5.

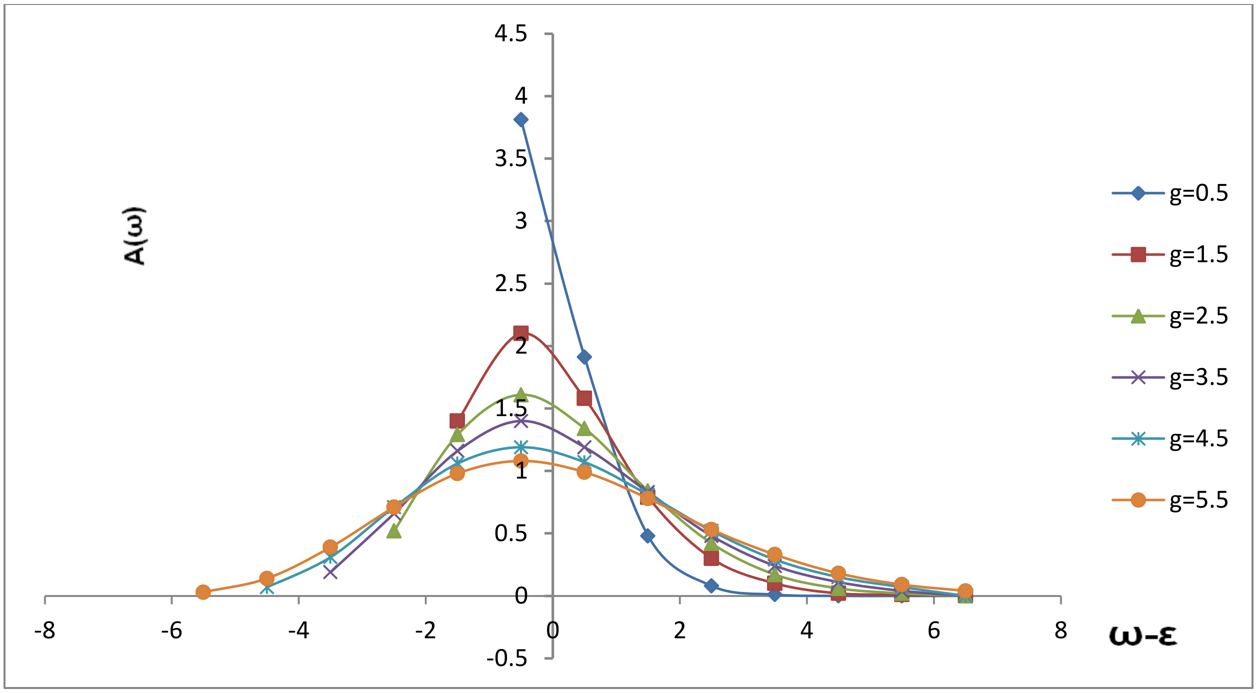

Fig. 1 The spectral function of the independent boson model, shown for an Einstein model and six values of coupling constant for g=0.5, 1.5, 2.5, 3.5, 4.5, and 5.5.

Conclusion

From Fig 1 it is observed that as the coupling constant increases from the weak limit to the strong limit, the shape of the graph gradually becomes Gaussian (i.e. at $w>\varepsilon$ or $w<\varepsilon$ non-bound state exist and there are fast phonon fluctuation) which when compared with other work [7] was in good agreement. The delta function peaks have an intensity envelope which does appear to have maximum near $\omega \approx \varepsilon_c$. As one increases the coupling g, the self energy $\Delta = g\omega_o$ becomes larger in magnitude so that the lowest energy peak shifts down ward in energy. But its intensity lowers also because of the factor e^{-g}.

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