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Self-consistent RPA retarded polaron Green function for quantum kinetics

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Abstract. We compute numerically the time dependent retarded Green function of the polaron within the self-consistent RPA approximation. The results show an approximately Gaussian behaviour at $t = 0$ changing at later times its concavity to an exponential decay, as it has been predicted in the approximate form of an inverse hyperbolic cosine function. The result contrasts with the non-selfconsistent RPA, where the exponential decay is only a transitory behaviour and the asymptotics is rather oscillatory. Our conclusions are significant in the context of the quantum kinetics with LO-phonons, where the transition from an intitially coherent scattering kinetics to a Markov kinetics with energy conservation is controlled by the time behaviour of the retarded Green function.

PACS. 78 Optical properties, condensed-matter spectroscopy and other interactions of radiation and particles with condensed matter – 71.38.+i Polarons and electron-phonon interactions

In the quantum-kinetic theory of the population and polarization dynamics in semiconductors excited by ultrashort laser pulses (see Ref. [1] for a modern review) the memory kernel of the delayed scattering kinetics plays a central role.

For not too strong laser pulses this kernel is given by a product of retarded equilibrium one-particle Green functions. If the interaction of the electrons with the dispersionless LO-phonons provides the dominant scattering mechanism, the decay in time of these Green functions is the only mechanism, that ensures asymptotically an approximate locality in time and implicitely irreversibility, *i.e.*, the familiar Markov structure of the semiclassical kinetics. In order to improve the dissipative behaviour of the retarded Green function we limit ourselves like in our previous paper [2] to a one-band polaron problem.

Often the Wigner-Weisskopf approximation for the retarded Green functions is used, which consists of the free-particle Green function corrected with an exponential decay factor, which is determined by the golden rule [3]

$$G^r_{\mathbf{k}}(t) = \frac{1}{i\hbar}\theta(t)\mathrm{e}^{-i\frac{\epsilon_{\mathbf{k}}t}{\hbar}}\mathrm{e}^{-\gamma t}.$$

This approximation leads in the Markov regime to a Lorentzian broadening of the energy conservation, which is not acceptable, because wide wings of this resonance function lead to run-away effects in the long-time relaxation kinetics. Therefore it is crucial to improve the approximation through a better knowledge of the time-behaviour of the Green functions.

As it has been shown in reference [2], the short-time behaviour of the retarded Green functions plays the decisive role. This is a simple consequence of the correspondence of the short times to large energies after Fourier transformation. The fact that the short-time behaviour has nothing to do with the long-time exponential decay stays at the origin of the relatively sharp energy conservation in the Markov regime. By interpolating the short-time and long-time asymptotics, we derived a simple damping law, which replaces the exponential decay by $1/\cosh^{\alpha}(\omega_0 t)$, where ω_0 is the LO-phonon frequency and α is the dimensionless Fröhlich constant. This form of the damping has been shown to improve the energy conservation in the long time limit essentially [2]. In this work we solve numerically the Dyson equation to illustrate this behaviour.

Let us consider the electron-LO-phonon interaction

$$\mathrm{H}_{\mathrm{int}} = \sum_q g_q \mathrm{a}^+_k \mathrm{a}_{k-q}(\mathrm{b}_q + \mathrm{b}^+_{-q}) \tag{1}$$

with the Fröhlich coupling

$$g_q^2 = \alpha \frac{4\pi\hbar\left(\hbar\omega_0\right)^{3/2}}{\left(2m\right)^{1/2} q^2 V};$$
$$\alpha = \frac{\mathrm{e}^2}{\hbar}\left(\frac{m}{2\hbar\omega_0}\right)^{1/2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right). \tag{2}$$

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where ω_0 is the dispersionless LO-phonon energy, m is the electron effective mass and ϵ_0, ϵ_∞ are the static and high frequency dielectric constants respectively.

The Boltzmann form of the collision term of the electron population $f_k(t)$ due to emission or absorption of longitudinal optical phonons then has the structure

$$\left.\frac{\partial f_k(t)}{\partial t}\right|_{\rm coll}^{\rm Boltzmann} = = -\sum_{q,\pm} W_{k,q,\pm} f_k(t)(1-f_{k-q}(t))N_q^{\pm}(t)\cdots , \quad (3)$$

where $N_q^+(t) = N_q(t)+1, \quad N_q^-(t) = N_q(t)$ are the phonon population factors. For simplicity we assume that the phonons are in thermal equilibrium, *i.e.* $N_q \equiv N = 1/(\mathrm{e}^{\beta\hbar\omega_0}-1)$. ω_0 is the frequency of the LO-phonons. The energy conserving transition probability per unit time is given by

$$W_{k,q,\pm} = \frac{2\pi}{\hbar} g_q^2 \delta(e_k \mp \hbar\omega_0 - e_{k-q}) \, . \quad (4)$$

In the quantum-kinetic version of the theory, this Markov structure of the collision term has to be replaced by a memory integral

$$\left.\frac{\partial f_k(t)}{\partial t}\right|_{\rm coll}^{\rm QK} - \sum_{q,\pm} {\rm Re}\int_{-\infty}^{t} {\rm d}t' K_{k,q,\pm}(t-t') \times f_k(t')(1-f_{k-q}(t'))N_q^{\pm}(t')\cdots , \quad (5)$$

where the memory kernel is given by

$$K_{k,q,\pm}(t-t') = g_q^2 G_k^{\rm r}(t-t') G_{k-q}^{\rm a}(t'-t)\mathrm{e}^{\pm i\omega_0(t-t')}, \quad (6)$$

here $G^{\rm r,a}$ are the retarded and advanced electron Green functions, respectively.

The Dyson equation for the retarded Green function, *e.g.*, is

$$(i\hbar\frac{\partial}{\partial t} - \epsilon_{\mathbf{k}})G_{\mathbf{k}}^{\rm r}(t) - \int_0^t {\rm d}t' \Sigma^{\rm r}(t-t',\mathbf{k})G_{\mathbf{k}}^{\rm r}(t') = \delta(t). \quad (7)$$

After a simple transformation

$$G_{\mathbf{k}}^{\rm r}(t) = \frac{1}{i\hbar}\mathcal{G}_{\mathbf{k}}(t)\theta(t)\mathrm{e}^{-i\frac{\epsilon_{\mathbf{k}}t}{\hbar}} \quad (8)$$

we get

$$\frac{\partial}{\partial t}\mathcal{G}_{\mathbf{k}}(t) = \frac{1}{i\hbar}\int_0^t {\rm d}t' \mathrm{e}^{i\epsilon_{\mathbf{k}}\frac{(t-t')}{\hbar}}\Sigma^{\rm r}(t-t',\mathbf{k})\mathcal{G}_{\mathbf{k}}(t'); \quad \mathcal{G}_{\mathbf{k}}(0) = 1. \quad (9)$$

Since in the polaron theory (electron vacuum) no electronic loops are possible, the self-energy can be expressed again through the retarded Green function. Ignoring vertex corrections we have (with the Keldysh diagram technique) the following self-consistent expression for the self-energy:

$$\Sigma^{\rm r}(t,\mathbf{k}) = \frac{1}{i\hbar}\sum_{\mathbf{q}} g_q^2 \left[(N+1)\mathrm{e}^{-i\omega_0 t} + N\mathrm{e}^{i\omega_0 t}\right] \times \mathrm{e}^{-i\frac{\epsilon_{\mathbf{k}-\mathbf{q}}t}{\hbar}}\mathcal{G}_{\mathbf{k}-\mathbf{q}}(t)\theta(t) \quad (10)$$

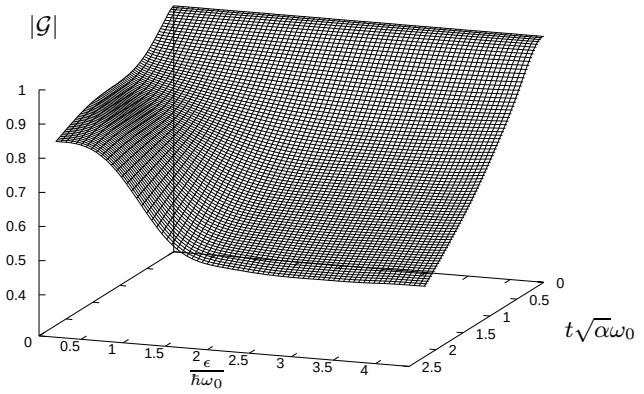

Fig. 1. Absolute value of the s.c. retarded Green-function for $\alpha = 0.1$

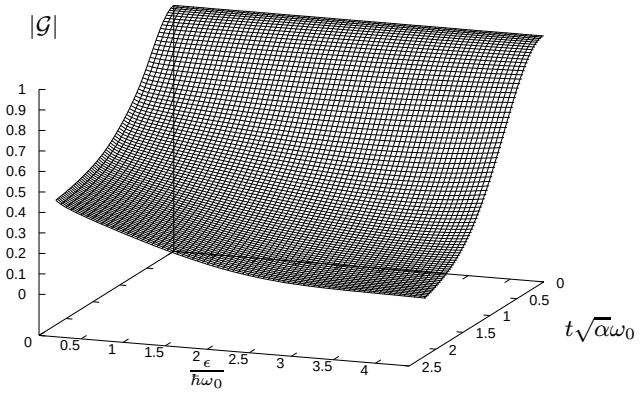

Fig. 2. Absolute value of the s.c. retarded Green-function for $\alpha = 1$

with

$$\mathcal{G}_{\mathbf{k}}(0) = 1. \quad (11)$$

If the self-energy $\Sigma^{\rm r}$ vanishes sufficiently rapidly as $t \to \infty$, then

$$\frac{\partial}{\partial t}\mathcal{G}_{\mathbf{k}}(t) \approx \mathcal{G}_{\mathbf{k}}(t)\frac{1}{i\hbar}\int_0^t {\rm d}t' \mathrm{e}^{i\frac{\epsilon_{\mathbf{k}}(t-t')}{\hbar}}\Sigma^{\rm r}(t-t',\mathbf{k}) \approx \mathcal{G}_{\mathbf{k}}(t)\frac{1}{i\hbar}\tilde{\Sigma}^{\rm r}(\epsilon_{\mathbf{k}}), \quad (12)$$

where

$$\tilde{\Sigma}^{\rm r}(\epsilon_{\mathbf{k}}) = \int_0^\infty {\rm d}t \; \mathrm{e}^{i\frac{\epsilon_{\mathbf{k}}t}{\hbar}}\Sigma^{\rm r}(t). \quad (13)$$

Consequently one gets an asymptotic behaviour

$$\mathcal{G}_{\mathbf{k}}(t) \sim \exp(it\frac{\delta\epsilon_{\mathbf{k}} + i\hbar\gamma_{\mathbf{k}}}{\hbar}). \quad (14)$$

To lowest order in the coupling constant

$$\gamma_{\mathbf{k}} = \frac{\pi}{\hbar}\sum_{\zeta=\pm1}\sum_q g_q^2 N_\xi \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}} - \xi\hbar\omega_0) \quad (15)$$

which corresponds to the "golden rule".

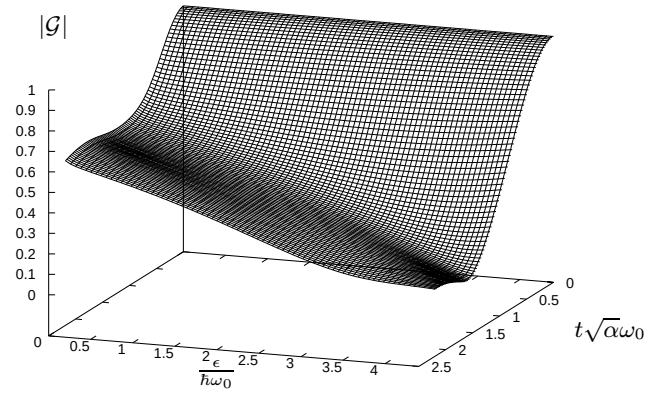

Fig. 3. Absolute value of the non-s.c. retarded Green-function for $\alpha = 1$

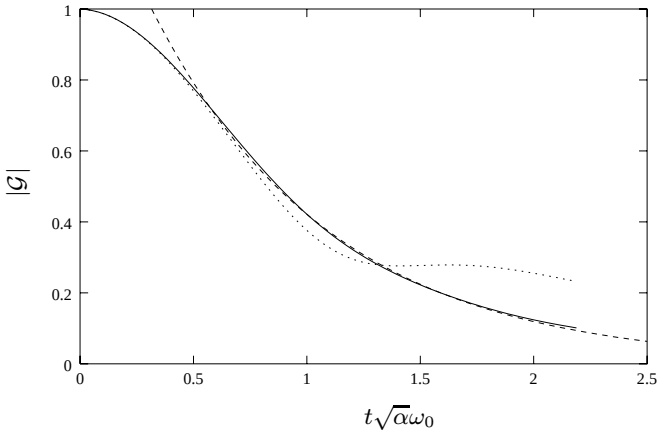

Fig. 4. Different large-time behaviours of the s.c. (full line) and non s.c. retarded (dotted line). Green-functions for $\alpha = 1$ and $E = 3\hbar\omega_0$ The dashed line represent an asymptotical fit with 1.49 $\mathrm{e}^{-1.26\alpha\omega_0 t}$.

On the other hand, one sees from the Dyson equation, that for $t \to 0$

$$\frac{\partial}{\partial t}\mathcal{G}_{\mathbf{k}}(t) \to 0. \tag{16}$$

Therefore we have two rather different behaviours at $t \to 0$ and $t \to \infty$.

In what follows we shall study this transition between the two asymptotic regimes through the numerical solution of the Dyson equation (9) for different coupling strengths both in the self-consistent (s.c.) as well as non self-consistent (n.s.c.) versions. Our numerical solutions were obtained with phonons characterized by $\hbar\omega_0 =$ 36 meV at room temperature ($k_{\mathrm{B}}T = 26$ meV) and an electron energy cut-off of $6\hbar\omega_0$.

The approximation method we used to solve the non-linear and non-local system of equations (9) is its discretization in time and energy. Of course we took advantage of the isotropy of the problem, which ensures, that the Green functions depend actually only on $|\mathbf{k}|$ and therefore on the energy. The mesh was refined until a good convergence has been achieved.

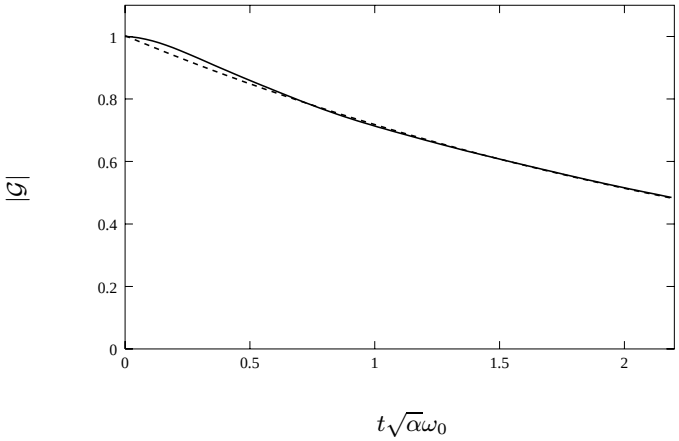

Fig. 5. Absolute value of the s.c. retarded Green-function for $\alpha = 0.1$ and $E = 3\hbar\omega_0$ and an asymptotical fit with $1.01\exp(-1.056\alpha\omega_0 t)$ (dashed line)

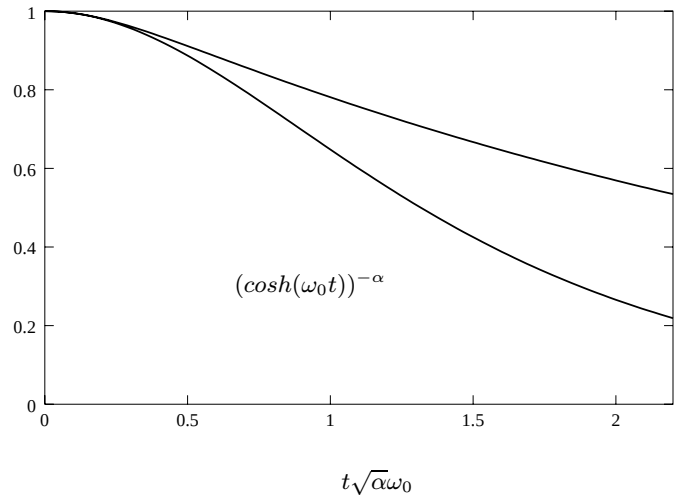

Fig. 6. A simple analytic approximation for the absolute value of the retarded Green functions for $\alpha = 1$ (lower curve) and $\alpha = 0.1$ (upper curve)

For a weak coupling $\alpha = 0.1$ the absolute value of the s.c. retarded Green function is shown in Figure 1. A rescaled time variable $t\sqrt{\alpha}\omega_0$ is used in order to represent results for different couplings on the same time-scale. One sees the flat start at $t = 0$ and also the asymptotic exponential decay, which is well described by the "golden rule". Below the one-LO-phonon threshold the decay is very slow, but otherwise almost constant. The self-consistency brings only very small corrections.

At an intermediate coupling of $\alpha = 1$ (see Fig. 2), one has a specific Gaussian-like shape *i.e.* the function first drops strongly and is concave and only later enters the exponential decay regime. Here, and even more so at still larger values of the coupling strength, the Gaussian decay dominates and leads to the typical Gaussian strong-coupling line-shape [4]. For the $\alpha = 1$ coupling strength, one sees already a significant deviation compared

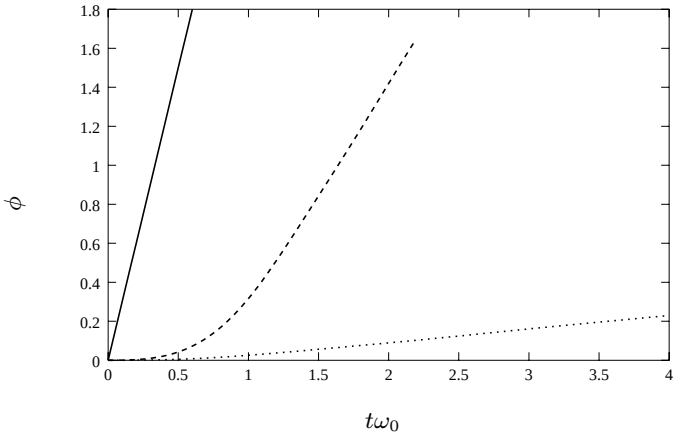

Fig. 7. Unperturbed phase (full line) and phase correctures of the s.c. retarded Green function for $\alpha = 1$ (dashed line) and for $\alpha = 0.1$ (dotted line) at $E = 3\hbar\omega_0$

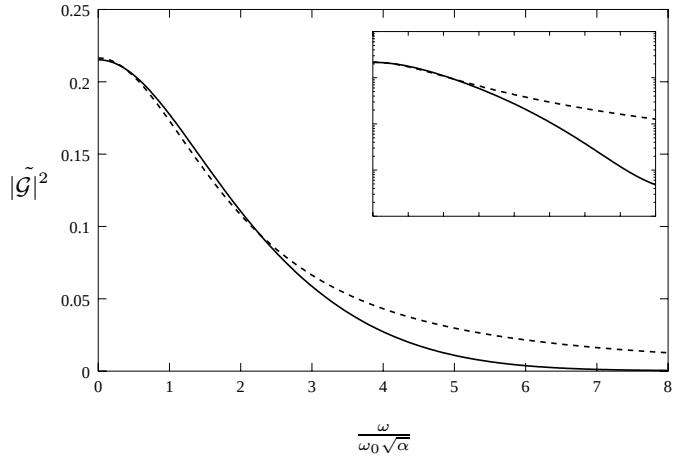

Fig. 8. Laplace-Fourier transform of the squared absolute value of the s.c. Green function for $\alpha = 1$ (solid line) and Lorentzian behaviour (dashed line). The insert represents the same curves on a logarithmic scale.

to the n.s.c. calculation (see Fig. 3). First at all, one sees a smearing out of the LO-phonon threshold, which anyway could have been expected. On the other hand, a much more important difference is seen particularly above the LO-phonon threshold: The n.s.c. Green function drops like the s.c. one up to the time $\sqrt{(\alpha)}t\omega_0 = 1.5$, but increases again for later times.

We conclude, that in the n.s.c. version the self-energy Σ^{r} does not vanishes sufficiently rapidly for $t \to \infty$, as it has been assumed in the derivation of the asymptotic exponential decay law! On the contrary, the s.c. self-energy seems to satisfy the criterion very well. The important difference between the large-time behaviour of the s.c. and non-s.c. Green functions can be better seen at a fixed energy ($3\hbar\omega_0$) at $\alpha = 1$ shown in Figure 4.

In the same figure one sees, that the asymptotic behaviour of the s.c. Green function is nearly exponential. At this energy with phonons at room temperature ($k_{\mathrm{B}}T = 26$ meV) one would expect from the "golden rule" a behaviour like $\exp(-1.1\ t\alpha\omega_0)$ whereas the asymptotic behaviour of the s.c. solution at $\alpha = 1$ shows a slightly more rapid decay like $\exp(-1.26\ \alpha\omega_0 t)$. For the weak coupling $\alpha = 0.1$ the s.c. Green function (see Fig. 5) also decays exponentially, but (within numerical accuracy) exactly according the "golden rule".

The calculated time dependence of the retarded Green function is roughly speaking the same as it has been predicted within a simple inverse hyperbolic cosine approximation approximation in our previous paper [2]. Indeed as it might be seen from Figure 6, the curves of the s.c. Green functions of Figures 4, 5 are well described as $1/\cosh^{\alpha}(\omega_0 t)$. Naturally this qualitative analytic approximation has no momentum dispersion, but connects the two asymptotic regimes very much like the numerical s.c. solutions. In a way the time evolution from a Gaussian short-time regime to an exponential long-time regime reminds one of the Toyozawa's concept of motional narrowing [4] in frequency space, which is obtained if the average kinetic energy increases in comparison with the average potential energy.

The relatively small time-dependent corrections to the phase ϕ of the Green function (defined as $\mathcal{G} = |\mathcal{G}|\mathrm{e}^{i\phi}$) for the two coupling values are shown in Figure 7. In the same figure also the unperturbed phase $\frac{\epsilon_{\mathbf{k}}t}{\hbar}$ is shown by the full curve.

In the frame of the quantum kinetics the Laplace-Fourier transform

$$\Re \int_0^{\infty} \mathrm{d}t G^{\mathrm{r}}_{\mathbf{k}}(t)\, G^{\mathrm{r}}_{\mathbf{k}'}(t)^*\, \mathrm{e}^{i\omega_0 t} \tag{17}$$

is of special interest, since in the Markov limit it defines the energy conservation.

Because the phase correction of the Green function is relatively small and the $\mathbf{k}$-dependence of the absolute value of the Green function again is very weak, we shall represent in Figures 8, 9 only

$$\Re \int_0^{\infty} \mathrm{d}t |G^{\mathrm{r}}_{\mathbf{k}}(t)|^2 \mathrm{e}^{i\omega t} \tag{18}$$

for the energy $E = 3\hbar\omega_0$. One sees from the numerical curves, that indeed the Fourier transform of the squared modulus of the retarded Green function decays in energy much faster than a Lorentzian corresponding to the purely exponential decay of the Wigner-Weisskopf approximation. Even if in the weak coupling case this difference is seen only on a logarithmic scale it is of major importance, since in the collision term it intervenes under an integral and its asymptotic behaviour is very crucial.

To conclude, we have shown through numerical calculations, that the time-dependent retarded polaron Green function has both an exponential decay at infinity as well as a Gaussian behaviour around the origin. The first property is not shared by the simple RPA approximation. On the other hand, both these properties are essential in order to get an acceptable Markov behaviour in the slow asymptotic regime.

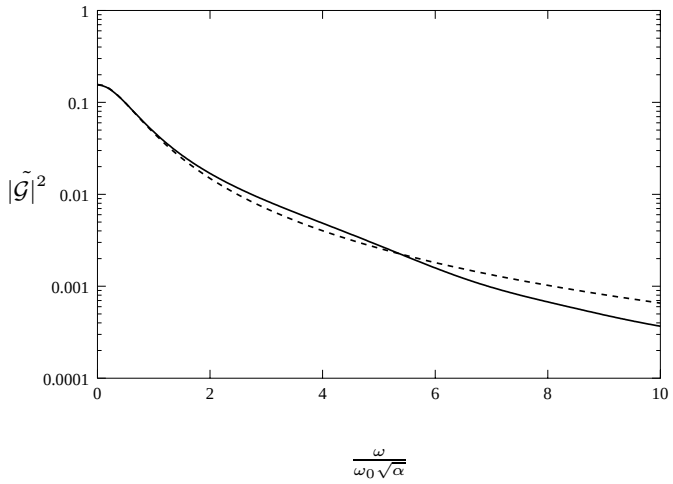

Fig. 9. Laplace-Fourier transform of the squared absolute value of the s.c. Green function for $\alpha = 0.1$ (solid line) and Lorentzian behaviour (dashed line) on logarithmic scale

It is interesting to remark, that in an exactly solvable one-dimensional (1D) electron model coupled to LO-phonons qualitatively similar results have been obtained [5]. This model emerges after a linearization of an 1D electron spectrum around the Fermi level ($\epsilon_{\mathbf{k}} = v_{\mathrm{F}}k$). The resulting Green function at $T = 0$ is

$$G_{\mathbf{k}}(t) = \mathrm{e}^{i\epsilon_{\mathbf{k}}t - F(t)}.$$

For a LO-phonon coupling with a momentum cut-off q_{c}

$$g_{\mathrm{q}} = g v_{\mathrm{F}} q_{\mathrm{c}} / \sqrt{q^2 + (v_{\mathrm{F}} q_{\mathrm{c}})^2},$$

one finds (for $t > 0$)

$$F(t) = g^2 \pi q_{\mathrm{c}} \frac{1 + i(i v_{\mathrm{F}} q_{\mathrm{c}} - \omega_0)t - \mathrm{e}^{-(i\omega_0 + v_{\mathrm{F}} q_{\mathrm{c}})t}}{(i v_{\mathrm{F}} q_{\mathrm{c}} - \omega_0)^2}.$$

For any finite cut-off q_{c}, the absolute value of this Green function behaves as a Gaussian around $t = 0$, while at $t \to \infty$ it decays exponentially.

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