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Flow equations for electron-phonon interactions: phonon damping*

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Abstract. A recently proposed method of a continuous sequence of unitary transformations will be used to investigate the dynamics of phonons, which are coupled to an electronic system. This transformation decouples the interaction between electrons and phonons. Damping of the phonons enters through the observation, that the phonon creation and annihilation operators decay under this transformation into a superposition of electronic particle-hole excitations with a pronounced peak, where these excitations are degenerate in energy with the renormalized phonon frequency. This procedure allows the determination of the phonon correlation function and the spectral function. The width of this function is proportional to the square of the electron-phonon coupling and agrees with the conventional result for electron-phonon damping. The function itself is non-Lorentzian, but apart from these scales independent of the electron-phonon coupling.

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1 Introduction

Since the discovery of polarons and the theoretical explanation of superconductivity the electron-phonon problem has been studied extensively. Essential for the theoretical description of the superconducting state was the interpretation of an effective interaction between the electrons of a many-particle system. The famous BCS-theory developed by Bardeen, Cooper and Schrieffer [2] is based on this idea. In 1952 Fröhlich gave a procedure to eliminate the electron-phonon interaction and to generate an effective electron-electron interaction by use of a unitary transformation [4]. This phonon-induced term appears in the Hamiltonian in addition to the Coulomb interaction.

Fröhlich's approach yields attractive and repulsive contributions to the interaction separated by a singularity. Using the flow equations [18] Lenz and one of the authors [16] obtained an interaction without such singularity, which is attractive for all electron momenta.

Mielke [5,6] calculated from this effective interaction as well as from the interaction obtained by Glazek's and Wilson's similarity renormalization approach [7] which is similar in spirit the critical temperature for superconductivity and compared the results with those obtained from the Eliashberg theory [8], in particular with those obtained by Allen and Dynes [9] and with the approximation by Mac Millan [10] and with experiment. He found that the results for T_c obtained with these methods agree within a few percent for various types of spectra (Einstein, lead, mercury). Only for stronger coupling the T_c by Mac Millan was distinctly smaller. This shows that this method works well for this static quantity.

The basic idea of this procedure is to perform a sequence of infinitesimal unitary transformations instead of transforming the Hamiltonian in one single step. Following this approach the transformed Hamiltonian and the infinitesimal generator of the unitary transformations η become functions of the so called flow parameter l, which has dimension $(\text{Energy})^{-2}$. It corresponds to the energy difference that is just being decoupled, that is, for small l large energy differences are decoupled first; smaller energy differences are dealt with later for larger values of l. In a differential formulation the transformation reads

$$\frac{dH}{dl} = [\eta(l), H(l)], \quad H(l=0) = H \tag{1}$$

with an anti-hermitian generator $\eta(l)$ related to the unitary transformation $U(l)$ by

$$\eta(l) = \frac{dU(l)}{dl} U^{\dagger}(l). \tag{2}$$

In order to remove off-diagonal contributions, the choice $\eta = [H^d, H^r]$ has been suggested in reference [18], where

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* Dedicated to Prof. Heinz Horner on the occasion of his 60th birthday.

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H^d is the diagonal, H^r the off-diagonal part. Considering the electron-phonon problem the phonon-number violating part will be eliminated in order to obtain a block-diagonal Hamiltonian which conserves the number of phonons. In order to develop the differential equations (1) some approximations will be necessary. By means of the unitary transformations new types of interactions mainly involving larger numbers of particles will be generated. They will be neglected after normal ordering.

At this point the question arises whether besides calculating renormalized energies one can also obtain some information about the dynamics of the electron-phonon problem. At first sight it is unclear how the transformed Hamiltonian, which does not contain any interaction between electrons and phonons can describe a phenomenon like damping of phonons. Usually such properties are determined by calculating dynamical correlation functions like $\langle [a_q(t), a_q^\dagger(0)] \rangle$, where $a^{(\dagger)}$ are phonon creation and annihilation operators, respectively. As we will see, dynamics enters through the following fact: if one performs a unitary transformation, all the observables have to be transformed as well. In other words, every unitary transformation causes a change of basis. Therefore the creation and annihilation operators also have to be transformed to the "new" basis. This requires to solve the flow equation

$$\frac{da_q(l)}{dl} = [\eta(l), a_q(l)]. \qquad (3)$$

As we will see these operators will "decay" completely under the unitary transformation, *i.e.* are completely transformed into terms which only contain electron operators. In this way we will see that the information on the dynamical properties of the solid is contained in the unitary transformation that has been used to block-diagonalize the Hamiltonian. This approach was used by Kehrein, Mielke and Neu for the spin-correlation in the spin-boson model [11–14]. A rather general examination of dissipation in the frame of flow equations is given by Kehrein and Mielke in [15].

Our paper is organized as follows. In the following section a short review of the transformation of the Hamiltonian will be given. Additionally we will be able to give an analytical expression for the q-dependence of the asymptotic solution for the phonon energies given in [16]. In Section 3 the flow equations describing the transformation of the phonon operators will be derived and a sum rule for these operators will be given. In the next section the coupled differential equations will be reduced to a nonlinear equations of the Volterra-type. In Section 4 the solutions of the equations in particular their asymptotic behavior will be given. An important role plays the asymptotic behavior of the phonon energies. In Section 5 we will be able to calculate the phonon-spectral function for the non-superconducting state and to give an analytical expression for the dependence of this function on the electron-phonon coupling. The last section contains a short summary.

2 Flow equations for the Hamiltonian

The Hamiltonian of the model will be written as

$$H = \sum_q \omega_q : a_q^\dagger a_q : + \sum_k \varepsilon_k : c_k^\dagger c_k : + E + \sum_{k,q} M_q (a_{-q}^\dagger + a_q) c_{k+q}^\dagger c_k \equiv H_0 + H_{e-p}. \qquad (4)$$

Here and in the following k stands for $k = \{\mathbf{k}, \sigma\}$, *i.e.* the spin is conserved by the electron-phonon interaction, thus no spin-subscript is needed. In the following all k and k' sums imply summation over the spin. As soon as we transfer to integrals we will no longer imply summation over spin (compare Eq. (19)). $a^{(\dagger)}$ are bosonic creation and annihilation operators, respectively. $c^{(\dagger)}$ denote the corresponding fermionic operators. : ... : denotes normal-ordering and E is a constant energy. Further M_q is the coupling between electrons and phonons. Following the approach of Bloch [3] or Nordheim [17] it is independent of the electron momentum. If there is need to specify ε_k or ω_q a quadratic dispersion for electrons and a linear dispersion for phonons will be assumed. Finally it should be emphasized that neither the Coulomb repulsion nor umklapp-processes will be taken into consideration.

To eliminate the electron-phonon interaction Fröhlich used unitary transformations as mentioned above. The transformed Hamiltonian contains a generated new interaction between the electrons, and the occurring energies are renormalized. But Fröhlich's approach leads to some problems. In certain regions of momentum space the effective electron-electron interaction exhibits singularities and the electron-phonon interaction is not transformed away at the singularity.

By applying one single unitary transformation to a Hamiltonian one treats all energy scales in one step. It seems to be more reasonable to diagonalize step by step between states with different energy differences. This will be achieved if a sequence of transformations is used for diagonalization. In an infinitesimal formulation of this continuous transformation the renormalization of the coupling constants is described by the flow equations. In 1996 Lenz and one of the authors where able to transform the Hamiltonian of the electron-phonon problem using flow equations. In the following sections we will often refer to this paper [16]. For convenience a short summary of their results will be given here. Additionally we will further examine the q-dependence of the asymptotic solution for $\omega_q(l)$. The notation and the approximations we will use are similar to [16].

In order to eliminate the electron-phonon coupling by flow equations one divides the Hamiltonian of the model

$$H = H^d + H^r, \qquad (5)$$

into the phonon-number conserving part

$$H^d = \sum_q \omega_q : a_q^\dagger a_q : + \sum_k \varepsilon_k : c_k^\dagger c_k : + \sum_{k,k',\delta} V_{k,k',\delta} : c_{k+\delta}^\dagger c_{k'-\delta}^\dagger c_{k'} c_k : + E \equiv H^{ph} + H^e + H^{e-e} + E$$

and the phonon-number violating part

$$H^r \equiv H^{e-p} = \sum_{k,q} (M_{k,q} a_{-q}^\dagger + M_{k+q,-q}^* a_q) c_{k+q}^\dagger c_k.$$

The initial conditions for the occurring coefficients are

$$M_{k,q}(l=0) = M_{k+q,-q}^*(l=0) = M_q(0) \equiv M_q$$
$$V_{k,k',\delta}(l=0) = 0.$$

If the electron-phonon coupling M_q is not real, then it can be made real by a simple gauge transformation. Therefore in the following we will assume, that it is real. Moreover we assume invariance under reflection, that is

$$M_{-q} = M_q, \quad \omega_{-q} = \omega_q, \quad \varepsilon_{-k} = \varepsilon_k. \tag{6}$$

The choice of the generator of the continuous unitary transformation follows the suggestion $\eta = [H_d, H_r]$ and takes into account the approximation to neglect terms of order $M_q(0)^3$ and higher. Therefore H^{e-e} will not be considered in the determination of η and one obtains

$$\eta := \sum_{k,q} M_{k,q} \alpha_{k,q} (a_{-q}^\dagger c_{k+q}^\dagger c_k - a_{-q} c_k^\dagger c_{k+q}), \tag{7}$$

where

$$\alpha_{k,q} = \varepsilon_{k+q} - \varepsilon_k + \omega_q. \tag{8}$$

The commutator $[\eta, H]$ contains newly generated interactions describing two-phonon processes and the interaction of a phonon with two electrons, which have been neglected. A further interaction representing the generation and annihilation of two phonons has been transformed away by adding the term

$$\eta^{(2)} = \sum_q \xi_q \left(a_q^\dagger a_{-q}^\dagger - a_q a_{-q} \right) \tag{9}$$

to the generator of the unitary transformation η, where

$$\xi_q = \frac{1}{2\omega_q} \sum_k n_k \big(M_{k,q} M_{k+q,-q} \alpha_{k+q,-q} - M_{k-q,q} M_{k,-q} \alpha_{k,-q} \big) \tag{10}$$

and n denotes the electron occupation number being 1 below the Fermi-edge and 0 above. The desired block-diagonal Hamiltonian becomes

$$H^d(\infty) = \sum_q \omega_q(\infty) : a_q^\dagger a_q : + \sum_k \varepsilon_k(\infty) : c_k^\dagger c_k : + \sum_{k,k',\delta} V_{k,k',\delta}(\infty) : c_{k+\delta}^\dagger c_{k'-\delta}^\dagger c_{k'} c_k : + E(\infty) + \text{irrelevant terms.} \tag{11}$$

In second order in M_q and taking into account the initial condition $V_{k,k',\delta}(0) = 0$ the renormalization of the coefficients is described by the flow equations

$$\frac{dM_{k,q}}{dl} = -\alpha_{k,q}^2 M_{k,q} \tag{12}$$

$$\frac{dV_{k,k',q}}{dl} = -M_{k,q} M_{k'-q,q} \alpha_{k'-q,q} - M_{k+q,-q} M_{k',-q} \alpha_{k',-q} \tag{13}$$

$$\frac{d\omega_q}{dl} = 2 \sum_k M_{k,q}^2 \alpha_{k,q} (n_{k+q} - n_k) \tag{14}$$

$$\frac{d\varepsilon_k}{dl} = 2 \sum_q \Big((\hat{n}_q + n_{k+q})\, M_{k+q,-q}^2 \alpha_{k+q,-q} - (\hat{n}_q + 1 - n_{k+q})\, M_{k,q}^2 \alpha_{k,q} \Big) \tag{15}$$

$$\frac{dE}{dl} = 2 \sum_{k,q} (\hat{n}_q n_{k+q} + n_k n_{k+q} - n_k - n_k \hat{n}_q) \times M_{k,q}^2 \alpha_{k,q}. \tag{16}$$

The phonon occupation number (which actually vanishes at zero temperature) is denoted by $\hat{n}$. In the following sections we will be mainly concerned with the dynamical properties of the phonons. That is why only equations (12, 14) will be of further interest. They can be solved exactly if again all terms of order M_q^3 and higher are neglected. For the renormalized value of the phonon energy one finds the same result as one obtains using Fröhlich transformation or perturbation theory. It is given by

$$\omega_q(\infty) = \omega_q(0) - \sum_k M_q^2 n_k \left(\frac{1}{\varepsilon_{k+q} - \varepsilon_k + \omega_q} + \frac{1}{\varepsilon_{k+q} - \varepsilon_k - \omega_q} \right). \tag{17}$$

For a variety of physical questions of interest it is necessary to solve the flow equations not only for the singular value $l = \infty$ but also to consider the approach to this value, which is described by the asymptotic behavior. This gives the opportunity to go beyond perturbation theory if one takes into account any order of M_q. The renormalization of the electron energies ε_k was neglected, assuming that the electron-phonon coupling is not strong enough to cause a significant change of ε_k. To derive the asymptotic behavior of $\omega_q(l)$ one integrates equation (12) to obtain

$$M_{k,q}(l) = M_q(0) e^{-\int_0^l dl' \left(\varepsilon_{k+q} - \varepsilon_k + \omega_q(l') \right)^2}. \tag{18}$$

As the authors mentioned in [16] the coupling $M_{k,q}$ decays exponentially as long as $\alpha_{k,q}$ does not lie in the vicinity of a resonance $\alpha_{k,q} \approx 0$. Thus the behavior of ω_q for large l is determined only by the contributions coming from small $\alpha_{k,q}$. We will now evaluate the sums in equation (14) specializing to three spatial dimensions and for the case of quadratic electron dispersion $\varepsilon_k = k^2/2m$. This can be written as a sum of the form $\sum_k n_k f(\mathbf{q} \cdot \mathbf{k})$. Performing the thermodynamic limit, introducing $\sigma = \mathbf{q} \cdot \mathbf{k}/q$ one obtains with the quantity $\Gamma := 4\pi\left(V/(2\pi)^3\right)$

$$\sum_k n_k f(\mathbf{q}\cdot\mathbf{k}) = \frac{\Gamma}{2}\int\limits_{-k_F}^{k_F} d\sigma(k_F^2-\sigma^2)f(\sigma q) \qquad (19)$$

with the Fermi-momentum k_F. It is useful to introduce the function

$$\alpha_q(\sigma,\omega) = \frac{\sigma q}{m} + \frac{q^2}{2m} + \omega_q. \qquad (20)$$

Then one obtains

$$\begin{aligned}\frac{d\omega_q}{dl} &= 2\sum_k n_k(M_{k-q,q}^2\alpha_{k-q,q} - M_{k,q}^2\alpha_{k,q})\\ &= -\Gamma M_q^2\int\limits_{-k_F}^{k_F} d\sigma(k_F^2-\sigma^2)\\ &\quad\times\alpha_q(\sigma,-\omega_q(l))e^{-2\int_0^l dl'\alpha_q^2(\sigma,-\omega_q(l'))}\\ &\quad-\Gamma M_q^2\int\limits_{-k_F}^{k_F} d\sigma(k_F^2-\sigma^2)\\ &\quad\times\alpha_q(\sigma,\omega_q(l))e^{-2\int_0^l dl'\alpha_q^2(\sigma,\omega_q(l'))}. \end{aligned} \qquad (21)$$

Extending the integrals over σ from $-\infty$ to $+\infty$ and neglecting the exponentially decaying tails which holds for sufficiently large l, if the sound velocity is smaller than the Fermi-velocity (which is the normal situation) and q is less than the Fermi-momentum, then one obtains

$$\begin{aligned}\frac{d\omega_q}{dl} &= -2\Gamma M_q(0)^2\\ &\quad\times\exp\left(-2\int\limits_0^l \omega_q^2(l')dl' + \frac{2}{l}\left(\int\limits_0^l \omega_q(l')dl'\right)^2\right)\\ &\quad\times\frac{m^2}{q}\sqrt{\frac{\pi}{2l}}\cdot\left[\overline{\omega}_q(\overline{\omega}_q-\omega_q)+\frac{1}{4l}\right]\cdot\end{aligned} \qquad (22)$$

with the average frequency

$$\overline{\omega}_q := \frac{1}{l}\int\limits_0^l dl'\omega_q(l'). \qquad (23)$$

Assuming an algebraic decay of ω_q a consistent solution to this equation for large l is

$$\omega_q(l) \approx \omega_q(\infty) + \frac{1}{2\sqrt{l}}\cdot \qquad (24)$$

This solution implies that the approach to the limit $l\to\infty$ is independent of q. One can show, however rescaling equation (22) that the value of the flow parameter l, for which the asymptotic behavior starts to be valid depends on q [16]. To get an analytical understanding of this statement one makes the following new ansatz:

$$\omega_q(l) = \omega_q(\infty) + \frac{1}{2\sqrt{l+l_0(q)}}\cdot \qquad (25)$$

Substituted in equation (22) this yields in leading order in l

$$l_0 = \frac{1}{(4\Gamma M_q^2\frac{m^2}{q}\omega_q(\infty)\sqrt{\frac{\pi}{2}}e^2)^2}\cdot \qquad (26)$$

Therefore we have found a solution for $\omega_q(l)$ which explicitly contains the domain of validity in dependence of q. Since for acoustic phonons $M_q^2 \propto q$ the dependence $l_0 \propto 1/q^2$ shows that for small q the asymptotic behavior is only reached for very large l. On the other hand it is obvious that for vanishing coupling no renormalization of the phonon energies takes place. Furthermore the solution is universal in the sense that different couplings yield in principle the same asymptotic behavior, they only differ in the value of l for which the asymptotic behavior starts to be valid.

3 Flow equations for the phonon operators

In this section we will describe the transformation of the bosonic creation and annihilation operators $a_q^{(\dagger)}$, respectively. We will derive the corresponding flow equations. Approximations which will be very similar to those performed in the preceding section will be necessary. Finally we will find a sum rule for the relevant coefficients. We use the following ansatz for $a_q(l)$

$$a_q(l) = \mu_q(l)a_q + \nu_q(l)a_{-q}^\dagger + \sum_k \gamma_{k,q}(l) : c_{k-q}^\dagger c_k : . \qquad (27)$$

The initial conditions for the coefficients are

$$\mu_q(l=0)=1; \quad \nu_q(l=0)=\gamma_{k,q}(l=0)=0. \qquad (28)$$

The generator of the unitary transformation is given in equations (7, 8). Then the flow equation for $a_q(l)$ yields

$$\begin{aligned}\frac{da_q}{dl} &= -\sum_k(M_{k-q,q}\alpha_{k-q,q}\nu_q + M_{k,-q}\alpha_{k,-q}\mu_q) : c_{k-q}^\dagger c_k :\\ &\quad+\sum_k \gamma_{k,q}(n_k-n_{k-q})(M_{k-q,q}\alpha_{k-q,q}a_{-q}^\dagger\\ &\quad-M_{k,-q}\alpha_{k,-q}a_q) - 2\xi_q(\mu_q a_{-q}^\dagger + \nu_q a_q)\\ &\quad+\sum_{k,q'}(M_{k,q'}\alpha_{k,q'}a_{-q'}^\dagger - M_{k+q',-q'}\alpha_{k+q',-q'}a_{q'})\\ &\quad\times(\gamma_{k+q,q} : c_{k+q'}^\dagger c_{k+q} : -\gamma_{k+q',q} : c_{k-q+q'}^\dagger c_k :).\end{aligned} \qquad (29)$$

The last line contains newly generated terms describing two-phonon processes. Similar to the transformation of the Hamiltonian we will neglect these interactions here. Furthermore the additional term $\eta^{(2)}$ in the generator of the unitary transformation will produce contributions to the commutator which decay exponentially as function of the flow parameter l. Therefore $\eta^{(2)}$ will not be of further interest in the following considerations. With these approximations in mind we obtain the following flow equations

$$\frac{d\mu_q}{dl} = -\sum_k \gamma_{k,q}(n_k - n_{k-q}) M_{k,-q}\alpha_{k,-q} \tag{30}$$

$$\frac{d\nu_q}{dl} = \sum_k \gamma_{k,q}(n_k - n_{k-q}) M_{k-q,q}\alpha_{k-q,q} \tag{31}$$

$$\frac{d\gamma_{k,q}}{dl} = -M_{k-q,q}\alpha_{k-q,q}\nu_q - M_{k,-q}\alpha_{k,-q}\mu_q. \tag{32}$$

As a first step in actually analyzing equations (30–32) one observes that

$$|\mu_q(l)|^2 - |\nu_q(l)|^2 + \sum_k |\gamma_{k,q}(l)|^2 (n_{k-q} - n_k) = 1 \tag{33}$$

is a constant. This sum rule reflects the fact that the commutator $[a_q(l), a_q^\dagger(l)]$ should be conserved under the unitary transformation. Within our approximation this holds for the constant after normal ordering. A similar relation holds also for the spin-boson problem [14]. From this sum rule Kehrein and Mielke obtained estimations about the convergency of the coefficients since only sums over positive numbers were involved. A similar procedure is not possible in our case due to the minus signs in equation (33).

Integration of equation (32) and insertion in (30, 31) gives

$$\begin{aligned}\frac{d\mu_q}{dl} &= \sum_k \Big[(n_k - n_{k-q}) M_{k,-q}(l)\alpha_{k,-q}(l) \\ &\quad \times \int_0^l dl' \big(M_{k-q,q}(l')\alpha_{k-q,q}(l')\nu_q(l') \\ &\quad + M_{k,-q}(l')\alpha_{k,-q}(l')\mu_q(l')\big)\Big]\end{aligned} \tag{34}$$

$$\begin{aligned}\frac{d\nu_q}{dl} &= -\sum_k \Big[(n_k - n_{k-q}) M_{k-q,q}(l)\alpha_{k-q,q}(l) \\ &\quad \times \int_0^l dl' \big(M_{k-q,q}(l')\alpha_{k-q,q}(l')\nu_q(l') \\ &\quad + M_{k,-q}(l')\alpha_{k,-q}(l')\mu_q(l')\big)\Big].\end{aligned} \tag{35}$$

Again we replace the sums by integrals, specialize to three spatial dimensions and the case of quadratic electron dispersion $\varepsilon_k = k^2/2m$, and obtain

$$\frac{d\mu_q}{dl} = \int_0^l dl' K_1(l,l')\mu_q(l') + \int_0^l dl' K_2(l,l')\nu_q(l'), \tag{36}$$

$$\frac{d\nu_q}{dl} = \int_0^l dl' K_2(l,l')\mu_q(l') + \int_0^l dl' K_1(l,l')\nu_q(l') \tag{37}$$

where

$$\begin{aligned}K_1(l,l') &= \sum_k n_k \big[\alpha_{k,-q}(l)M_{k,-q}(l)\alpha_{k,-q}(l')M_{k,-q}(l') \\ &\quad - \alpha_{k+q,-q}(l)M_{k+q,-q}(l)\alpha_{k+q,-q}(l')M_{k+q,-q}(l')\big] \\ &= \frac{\Gamma}{2}M_q^2 \int_{-k_F}^{k_F} d\sigma(k_F^2 - \sigma^2)\Big[\alpha_q\big(\sigma,\omega_q(l)\big)\alpha_q\big(\sigma,\omega_q(l')\big) \\ &\quad \times e^{-(\int_0^l dl'' + \int_0^{l'} dl'')\alpha_q^2[\sigma,\omega_q(l'')]} - \{\omega \to -\omega\}\Big]\end{aligned} \tag{38}$$

$$\begin{aligned}K_2(l,l') &= \sum_k n_k \big[\alpha_{k,-q}(l)M_{k,-q}(l)\alpha_{k-q,q}(l')M_{k-q,q}(l') \\ &\quad - \alpha_{k+q,-q}(l)M_{k+q,-q}(l)\alpha_{k,q}(l')M_{k,q}(l')\big] \\ &= -\frac{\Gamma}{2}M_q^2 \int_{-k_F}^{k_F} d\sigma(k_F^2 - \sigma^2)\Big[\alpha_q\big(\sigma,\omega_q(l)\big) \\ &\quad \times \alpha_q\big(\sigma,-\omega_q(l')\big) \\ &\quad \times e^{-\int_0^l dl''\alpha_q^2\left(\sigma,\omega_q(l'')\right) - \int_0^{l'} dl''\alpha_q^2\left(\sigma,-\omega_q(l'')\right)} \\ &\quad - \{\omega \to -\omega\}\Big].\end{aligned} \tag{39}$$

The solutions of these linear integro-differential equations of the Volterra-type will be discussed in the next section.

4 The asymptotic behavior

In this section we derive the behavior of $\mu_q(l)$ and $\nu_q(l)$ for large l. In a first approach we will neglect the flow of the phonon energies ω_q and of the electron energies ε_k; only the l-dependence of the couplings $M_{k,q}(l)$ and of the coefficients $\mu_q(l)$, $\nu_q(l)$, $\gamma_{k,q}(l)$ will be taken into consideration.

For sufficiently large l the integrand decays rapidly as a function of σ and we extend the integration from $-\infty$ to $+\infty$ as before. Then one has

$$K_1(l,l') = -\Gamma \frac{M_q^2 m^2 \omega_q \sqrt{\pi}}{2q} \frac{1}{(l+l')^{3/2}} \tag{40}$$

$$\begin{aligned}K_2(l,l') &= \Gamma \frac{M_q^2 m^2 \omega_q \sqrt{\pi}}{q} \frac{l-l'}{(l+l')^{5/2}} \\ &\quad \times \left(\frac{3}{2} - 4\omega_q^2 \frac{ll'}{l+l'}\right) \exp\left[-4\omega_q^2 \frac{ll'}{l+l'}\right].\end{aligned} \tag{41}$$

The equations (36, 37) can be added and subtracted, so that

$$\begin{aligned}\frac{d(\mu_q(l) + \nu_q(l))}{dl} &= \\ &\int_0^l dl' \big[K_1(l,l') + K_2(l,l')\big]\big(\mu_q(l') + \nu_q(l')\big)\end{aligned} \tag{42}$$

$$\frac{d(\mu_q(l)-\nu_q(l))}{dl} = \int_0^l dl' \big[K_1(l,l') - K_2(l,l')\big]\big(\mu_q(l')-\nu_q(l')\big). \quad (43)$$

The kernel $K_2(l,l')$ decays exponentially for large l and l', whereas $K_1(l,l')$ decays algebraically. From the initial conditions $\mu_q(0)=1$ and $\nu_q(0)=0$ and the property of the kernels $K_1(l'',l') \gg K_2(l'',l')$ it follows, that $\mu_q(l) \pm \nu_q(l)$ differ only weakly, which implies $\mu_q(l) \gg \nu_q(l)$. This argument is valid only if ν_q stays small until the exponential decay becomes important, which happens for $l > 1/(4\omega_q^2)$. Integration of equation (37) with equation (41) and $\mu_q(l')=1$, $\nu_q(l')=0$ yields $\nu_q = const\ \Gamma M_q^2 m^2/q$. Thus for small couplings M_q we find, that ν remains small since for acoustic phonons $M_q^2 \propto q$. This has to be expected, since excitations by $a_{-q}^\dagger$ and a_q differ by an energy $2\omega_q$ and should only mix for strong interactions.

Although significant simplifications have been obtained for the coupled equations no analytical solution seems to be possible yet. A numerical solution yields an oscillating slowly decaying behavior. To get a better understanding of the behavior in the asymptotic regime we will take into account the l-dependence of ω.

When transforming the Hamiltonian, one has learned that it is possible to go beyond perturbation theory, if one takes into account the flow of the phonon energies ω_q. We will see that the flow of ω_q significantly alters the convergency of the coefficients. Since the coupling $M_{k,q}$ decays exponentially as long as $\alpha_{k,q}$ does not lie in the vicinity of a resonance $\alpha_{k,q} \approx 0$ the behavior of the coefficients for large l is determined only by the contributions coming from small $\alpha_{k,q}$. Again we start from equations (38, 39) and perform first the l'' integrals

$$\int_0^l dl'' \alpha_q^2(\sigma,\omega_q(l'')) = l\alpha_q^2(\sigma,\overline{\omega}_q(l)) + \int_0^l dl''(\omega_q(l'') - \overline{\omega}_q(l))^2 = l\alpha_q^2(\sigma,\overline{\omega}_q(l)) + \frac{1}{4}\ln\frac{l+l_0}{l_0} - \frac{(\sqrt{l+l_0}-\sqrt{l_0})^2}{l} \quad (44)$$

with the average frequency

$$\overline{\omega}_q = \frac{1}{l}\int_0^l dl' \omega_q(l') = \omega_q(\infty) + \frac{1}{l}\left(\sqrt{l+l_0}-\sqrt{l_0}\right). \quad (45)$$

Then with

$$f(l) := \left(\frac{l_0}{l_0+l}\right)^{1/4} e^{\left(\frac{l+2l_0-2\sqrt{l+l_0}\sqrt{l_0}}{l}\right)} \quad (46)$$

we have

$$\begin{aligned} K_{1,2}(l,l') &= \pm\frac{\Gamma M_q^2}{2} f(l)f(l') \times \int_{-k_F}^{k_F} d\sigma (k_F^2-\sigma^2)\Big[\alpha_q\big(\sigma,\omega_q(l)\big)\alpha_q\big(\sigma,\pm\omega_q(l')\big) \\ &\quad \times e^{-l\alpha_q^2(\sigma,\overline{\omega}_q(l)) - l'\alpha_q^2\left(\sigma,\pm\overline{\omega}_q(l')\right)} - \{\omega\to-\omega\}\Big] \\ &= \pm\frac{\Gamma M_q^2}{2} f(l)f(l') e^{-\frac{ll'}{l+l'}\left(\overline{\omega}_q(l)\mp\overline{\omega}_q(l')\right)^2} \times \int_{-k_F}^{k_F} d\sigma (k_F^2-\sigma^2)\Big[\alpha_q\big(\sigma,\omega_q(l)\big)\alpha_q\big(\sigma,\pm\omega_q(l')\big) \\ &\quad \times e^{-(l+l')\alpha_q^2\left(\sigma,b_\pm(l,l')\right)} - \{\omega\to-\omega, b\to-b\}\Big] \end{aligned} \quad (47)$$

where the upper sign holds for K_1 and the lower one for K_2 and

$$b_\pm(l,l') = \frac{l\overline{\omega}_q(l) \pm l'\overline{\omega}_q(l')}{l+l'}. \quad (48)$$

We substitute $\alpha = \alpha_q(\sigma,b)$ as new variable for integration, realize, that only those terms of the polynomial in front of the Gaussian contribute, which are even in α and odd in ω and b. Then only the contributions of $k_F^2-\sigma^2$ which are linear in α or $b_\pm$ contribute and the integral reduces to

$$\frac{2m^2}{q}\int d\alpha(\alpha - b_\pm(l,l'))(\alpha+\omega_q(l)-b_\pm(l,l')) \times (\alpha\pm\omega_q(l') - b_\pm(l,l'))e^{-(l+l')\alpha^2}. \quad (49)$$

One obtains

$$\begin{aligned} K_{1,2}(l,l') = &\mp\frac{\Gamma M_q^2 m^2}{q}\sqrt{\frac{\pi}{l+l'}} f(l)f(l') e^{-\frac{ll'}{l+l'}\left(\overline{\omega}_q(l)\mp\overline{\omega}_q(l')\right)^2} \\ &\times\Big[b_\pm(l,l')\big(b_\pm(l,l')-\omega_q(l)\big)\big(b_\pm(l,l')\mp\omega_q(l')\big) \\ &+\frac{1}{2(l+l')}\big(3b_\pm(l,l')-\omega_q(l)\mp\omega_q(l')\big)\Big]. \end{aligned} \quad (50)$$

It is easy to see, that in the limit $l_0\to\infty$ both kernels $K_1(l,l')$ and $K_2(l,l')$ turn into the corresponding expressions (40,41) since the relation $\omega_q(l)\to\omega_q(\infty)$ is fulfilled in this limit as well.

We will now discuss the behavior of the kernel K_1 and K_2 and the solutions of the equations for large l,

$$l \gg l_0. \quad (51)$$

First of all one observes that the kernel $K_2(l,l')$ is exponentially suppressed in comparison to $K_1(l,l')$ with the damping factor

$$\exp\left(-\frac{4\omega_q(\infty)^2 ll'}{l+l'}\right) \quad (52)$$

which is the same as in equation (41). Thus for large l this kernel can contribute only for small l'. In this limit one obtains for K_2

$$K_2(l,l') = \frac{m^2 M_q^2 \Gamma \sqrt{\pi} l_0^{1/4} \omega_q^2}{q l^{5/4}} e^{1-4\omega_q^2 l'}. \quad (53)$$

Thus for large l there will be a contribution to $d\mu_q/dl$ decaying like $l^{-5/4}$, yielding a contribution to μ_q decaying like $l^{-1/4}$. We will see below, that the self-consistent contribution from K_1 to μ_q decays slower, so that the contribution from K_2 can be neglected. Then the equations for $\nu_q(l')$ and $\mu_q(l')$ decouple in the asymptotic regime,

$$\frac{d\mu_q(l)}{dl} = \int_0^l dl' K_1(l,l') \mu_q(l'). \quad (54)$$

Next we consider K_1 in the limit of large l. In this limit the leading contribution to K_1 yields

$$K_1(l,l') = - \frac{m^2 M_q^2 \Gamma \sqrt{\pi} \omega_q(\infty) e^2}{q} \frac{\sqrt{l_0}}{(l\cdot l')^{1/4}} \exp\left(\frac{2\sqrt{l\cdot l'}}{l+l'} - 1\right) \times \left(\frac{2\sqrt{l\cdot l'}}{(l+l')^{5/2}} + \frac{1}{2(l+l')^{3/2}} - \frac{1}{4\sqrt{l}\sqrt{l'}\sqrt{l+l'}}\right). \quad (55)$$

We see, that the function $f(l)f(l')$ which comes from the variation of ω_q as a function of l influences in a crucial manner the behavior of the integral equation (54). Asymptotically this additional term causes a factor $1/(l\,l')^{1/4}$, which produces the same powers of l on both sides of equation (54), if one makes the ansatz of an algebraic decay

$$\mu_q(l) = c_q l^\kappa. \quad (56)$$

With this ansatz one obtains the following transcendent equation for κ, if one substitutes $l' = lx$

$$\kappa = g \int_0^1 dx \frac{x^{\kappa - \frac{3}{4}}}{\sqrt{x+1}} \exp\left(\frac{2\sqrt{x}}{1+x} - 1\right) \times \left(\frac{2x}{(1+x)^2} + \frac{\sqrt{x}}{2(x+1)} - \frac{1}{4}\right). \quad (57)$$

Moreover one realizes using equation (26) that no q-dependence is contained in the factor in front of the integral in the last equation. This factor equals a constant coupling $g = -(1/2)\sqrt{2}$, which does not depend on the electron-phonon coupling M_q. A numerical solution of equation (57) yields

$$\kappa = -0.07. \quad (58)$$

The exponent κ as a function of the coupling g from equation (57) is shown in Figure 1 and can be read of from this figure. This solution is universal, *i.e.* the exponent κ does

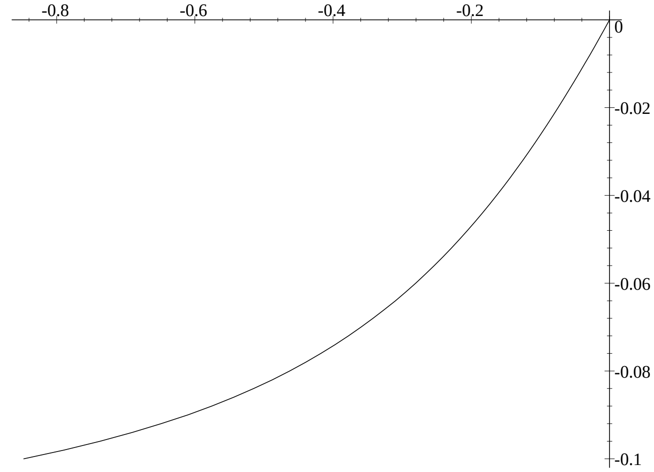

Fig. 1. κ as a function of the coupling g.

not depend on physical quantities like the electron-phonon coupling. The power decay (56) is valid only for large l, (51). For small l μ will only vary slowly. Since the crossover to the power law is expected at $l \approx l_0$ we assume roughly

$$\mu_q(l) = c_q (l + l_0)^\kappa, \quad (59)$$

taking into account, that $\mu_q(l)$ stays finite for small l, actually tends to 1.

We can use this expression to integrate the differential equations for $\gamma_{k,q}$, where we realize, that it depends only on q and $\varepsilon_k - \varepsilon_{k-q}$

$$\gamma_{k,q}(\infty) = \gamma_q(\varepsilon_k - \varepsilon_{k-q}), \quad (60)$$

$$\gamma_q(\delta\varepsilon) = -M_q \int_0^\infty dl e^{-\int_0^l dl' \left(\delta\varepsilon + \omega_q(l')\right)^2} \left(\delta\varepsilon + \omega_q(l)\right) \mu_q(l). \quad (61)$$

First we assume $\delta\varepsilon$ to be far away from the resonance $-\omega_q(l)$. Then the exponential function will decay much faster than $\mu_q(l)$, so that we replace $\mu_q(l)$ by 1, which yields

$$c_q = \frac{1}{l_0^\kappa} \quad (62)$$

and

$$\gamma_q(\delta\varepsilon) = -\frac{M_q}{\delta\varepsilon + \omega_q(\infty)} \cdot \quad (63)$$

The case of degeneracies and nearly degeneracies $\delta\varepsilon + \omega_q(\infty) \approx 0$ will be discussed in the next section.

5 The spectral function

In order to determine the damping of phonons in a solid one has to calculate the phonon correlation function or its Fourier transform, the spectral function. The latter quantity can directly be inferred by neutron scattering experiments. Furthermore it is closely connected to the imaginary part of the retarded Greens function. The phonon correlation function can be defined as

$$C(q,t) = \langle a_q(t)a_q^\dagger(0) - a_q^\dagger(0)a_q(t)\rangle = Tr\left(\rho_{eq}[a_q(t), a_q^\dagger(0)]\right), \quad (64)$$

where

$$\rho_{eq} = \exp(-\beta H)/Tr\big(\exp(-\beta H)\big). \quad (65)$$

It is useful to calculate the correlation function at $l = \infty$ since in this limit the phonons are decoupled from the electrons. Unfortunately in our case the Hamiltonian is only block-diagonal. However if we limit our considerations to non-superconducting systems we can neglect the electron-electron interaction. This means we will consider the solid in the state above T_c. Calculating the thermodynamic expectation value one obtains

$$C(q,t) = \sum_{k,k'} \gamma_{k,q}\gamma_{k',q} e^{it(\varepsilon_{k-q}-\varepsilon_k)} \langle [: c_{k-q}^\dagger c_k :, : c_{k'}^\dagger c_{k'-q} :]\rangle \quad (66)$$

$$= \sum_k \gamma_{k,q}^2 e^{it(\varepsilon_{k-q}-\varepsilon_k)}(n_{k-q} - n_k). \quad (67)$$

For simplicities sake we will use n_k at $T = 0$. If we again replace the sum by the corresponding integral then we obtain

$$C(q,t) = \frac{\Gamma}{2}\int_{-k_F}^{k_F} d\sigma(k_F^2 - \sigma^2) \times\left[-\gamma_q^2\left(\frac{\sigma q}{m} - \frac{q^2}{2m}\right)e^{it\left(-\frac{\sigma q}{m}+\frac{q^2}{2m}\right)} + \gamma_q^2\left(\frac{\sigma q}{m} + \frac{q^2}{2m}\right)e^{it\left(-\frac{\sigma q}{m}-\frac{q^2}{2m}\right)}\right]. \quad (68)$$

If one defines the spectral function

$$B(q,\omega) = \int_{-\infty}^{\infty} dt C(q,t)e^{-i\omega t} \quad (69)$$

then one obtains the following expression

$$B(q,\omega) = \frac{\Gamma m}{2q} \times \left\{\left[k_F^2 - \left(\frac{|\omega - q^2/2m|m}{q}\right)^2\right] \times\Theta\left(k_F - \frac{|\omega - q^2/2m|m}{q}\right) - \left[k_F^2 - \left(\frac{|\omega + q^2/2m|m}{q}\right)^2\right] \times\Theta\left(k_F - \frac{|\omega + q^2/2m|m}{q}\right)\right\}\gamma_q^2(-\omega). \quad (70)$$

For ω sufficiently small the condition $\omega \ll (v_F/c)\omega_q$ is fulfilled, where v_F is the Fermi-velocity and c is the speed of sound. Using this condition both Θ-functions equal 1 and we obtain

$$B(q,\omega) = \frac{m^2 V}{\pi q}\omega\gamma_q^2(-\omega). \quad (71)$$

From equation (63) we conclude that for large values of ω the spectral function behaves like $\omega(\omega - \omega_q)^{-2}$. In the general case we obtain using equations (59, 61, 71)

$$B(q,\omega) = \frac{\sqrt{2\pi}c_q^2\omega}{2\sqrt{l_0}\omega_q(\infty)e^2} \times\left[\int_0^\infty dl\left(\omega - \omega_q(\infty) - \frac{1}{2\sqrt{l+l_0}}\right) \times\left(\frac{l_0}{l+l_0}\right)^{1/4}(l+l_0)^\kappa \exp\Big(-\big(\omega-\omega_q(\infty)\big)^2 l + 2\big(\omega - \omega_q(\infty)\big)\left[\sqrt{l+l_0} - \sqrt{l_0}\right]\Big)\right]^2. \quad (72)$$

Rescaling equation (72) we get an analytical understanding of the dependence of the spectral function on the coupling

$$B(q,\omega) = \frac{\sqrt{2\pi}\sqrt{l_0}|l_0^\kappa|^2 c_q^2\omega}{2e^2\omega_q(\infty)} \times\left|\int_0^\infty dx\left(\delta\omega\sqrt{l_0} - \frac{1}{2\sqrt{x+1}}\right) \times\left(\frac{1}{x+1}\right)^{1/4}(x+1)^\kappa \exp\Big(-(\delta\omega)^2 l_0 x + 2\delta\omega\sqrt{l_0}(\sqrt{x+1}-1)\Big)\right|^2, \quad (73)$$

where we have set $\delta\omega = \omega - \omega_q(\infty)$. If we substitute $1+x = y/(\delta\omega^2 l_0)$ and use equation (62) then B can be rewritten in terms of a scaling function $\hat{B}(\delta\omega\sqrt{l_0})$.

$$B(q,\omega) = \frac{\sqrt{l_0}\omega}{\omega_q(\infty)}\hat{B}\left(\delta\omega\sqrt{l_0}\right), \quad (74)$$

$$\hat{B}(\nu) = \frac{\sqrt{2\pi}}{2e^2|\nu|^{1+4\kappa}}\left|\int_{\nu^2}^\infty dy\left(\pm 1 - \frac{1}{2\sqrt{y}}\right) \times y^{\kappa-\frac{1}{4}}\exp\left(-y \pm 2\sqrt{y}\right)\right|^2, \quad (75)$$

where the upper sign stands for positive $\nu = \delta\omega\sqrt{l_0}$ and the lower sign for negative ν, respectively. The function $\hat{B}(\nu)$ is plotted in Figure 2. From this relation we observe that the width of the spectral function grows linearly with $1/\sqrt{l_0}$ or M_q^2. Simultaneously the height of this function scales like $\sqrt{l_0}$.

Finally we examine the behavior of $B(q,\omega)$ for very small and for very large $\delta\omega$. In the first case, that is for $\delta\omega \ll 1/\sqrt{l_0}$ we may replace the lower limit of the integral in (75) by 0 which yields the values for the integrals $C_+ = 2.63$ for positive $\delta\omega$ and $C_- = -2.24$ for negative $\delta\omega$.

$$B(q,\omega) = \frac{\sqrt{2\pi}\sqrt{l_0}C_\pm^2}{2e^2\left(|\delta\omega|\sqrt{l_0}\right)^{1+4\kappa}}\cdot \quad (76)$$

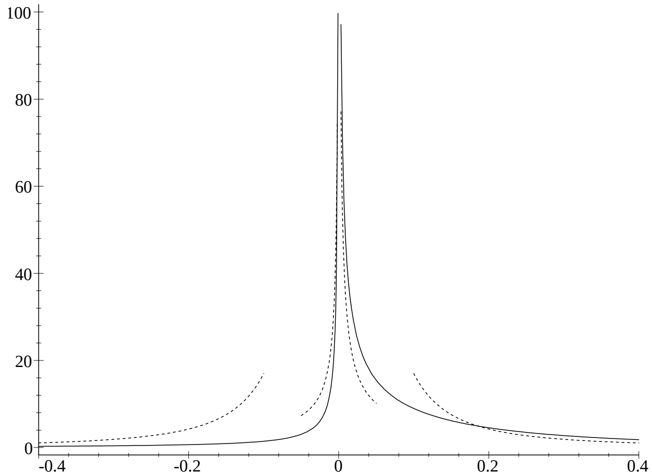

Fig. 2. The rescaled spectral function $\hat{B}(\nu)$ *versus* ν from the numerical solution (solid line) and from the approximate solutions (dashed line).

The corresponding asymptotic behavior is shown in figure 2. There is however a large correction for finite $\delta\omega$, yielding $C_\pm + [(|\delta\omega|\sqrt{l_0})^{2\kappa+1/2}]/(2\kappa+1/2)$ for the integral. In the case of large $\delta\omega \gg 1/\sqrt{l_0}$ one concludes from equation (63)

$$B(q,\omega) = \frac{\sqrt{2\pi}\omega}{2e^2\sqrt{l_0}\omega_q(\infty)(\delta\omega)^2}\,. \tag{77}$$

The crossover between the two types of behavior equations (76, 77) occurs at $|\delta\omega| \approx 1/\sqrt{l_0}$.

The conventional result given in reference [1] yields (for $|\delta\omega| \ll \omega$) a Lorentzian damping

$$B(q,\omega) = \frac{2\gamma_1}{(\delta\omega)^2 + \gamma_1^2} \tag{78}$$

with a width γ_1 which is related to our quantities by

$$\frac{1}{\sqrt{l_0}} = \sqrt{\frac{8}{\pi}}e^2\gamma_1. \tag{79}$$

Thus the width of the spectral function is the same in both approaches. Moreover there is agreement with the behaviour for $|\delta\omega| \gg \gamma_1$. For small $\delta\omega$, however, we obtain a different behaviour.

6 Discussion and conclusion

Let us sum up the main results of this paper. We have examined the dynamics of the electron-phonon problem using continuous unitary transformations. This transformation was designed as to eliminate the electron-phonon coupling [16], the main results of which were summarized in Section 2. The good agreement of T_c with the Eliashberg theory was found in [5,6] and summarized here in Section 1. Here we were interested in the dynamics of the phonons. Therefore the main part of this paper is dedicated to the transformation of the creation and annihilation operators for phonons. Under the flow of these operators due to the unitary transformation they decay into electronic particle-hole excitations. The approximations used are similar to those performed in [11–15]. The decay of the operators is described by a linear integro-differential equation of the Volterra-type. The equation can be solved analytically if one neglects the flow of the electron energies ε_k and takes into account the l-dependence of the phonon frequencies ω_q. We obtained an algebraic decay of the bosonic operators, see equations (58, 59). Surprisingly the spectral function (previous section) turned out to be universal in the sense that the exponent κ, which describes the behavior of the spectral function for small $\delta\omega = \omega - \omega_q(\infty)$ does not depend on physical quantities like the electron-phonon coupling. We cannot exclude, however, that taking into account more complex excitations like those appearing in equation (29) will have some effect on the exponent κ. The scaling function equation (75) is universal as long as the coupling is not too strong (see the discussion after Eq. (43)). The electron-phonon coupling enters only in the scales. The width of the spectral function is the same as obtained in the conventional approach [1]. For small $\delta\omega$ the spectral function decays with $\delta\omega^{-1-4\kappa}$ with $\kappa = -0.07$, whereas for large $\delta\omega$ it decreases with the conventional $\delta\omega^{-2}$. This paper shows that the method of flow equations can also be used to investigate the dynamics due to the electron-phonon interaction.

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References

1. A.A. Abrikosov, L.P. Gorkov, I.E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice Hall, 1963), Sect. 21.2.
2. J. Bardeen, L.N. Cooper, J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
3. F. Bloch, Z. Phys. **52**, 555 (1928).
4. H. Fröhlich, Proc. Roy. Soc. A **215**, 291 (1952).
5. A. Mielke, Ann. Phys. (Leipzig) **6**, 215 (1997).
6. A. Mielke, Europhys. Lett. **40**, 195 (1997).
7. S.D. Glazek, K.G. Wilson, Phys. Rev. D **49**, 4214 (1994).
8. G.M. Eliashberg, Zh. Eksp. Teor. Fiz. **28**, 966 (1960); *ibid* 1437 (1960) (Sovj. Phys. JETP **11**, 696 (1960); **12**, 1000 (1960)).
9. P.B. Allen, R.C. Dynes, Phys. Rev. B **12**, 905 (1975).
10. W. Mac Millan, Phys. Rev. **167** 331, (1968).
11. S.K. Kehrein, A. Mielke, J. Phys. A, Math. Gen. **27**, 4259 (1994); corrigendum **27**, 5705 (1994).
12. S.K. Kehrein, A. Mielke, P. Neu, Z. Phys. B **99**, 269 (1996).
13. S.K. Kehrein, A. Mielke, Ann. Phys. (NY) **252**, 1 (1996).
14. S.K. Kehrein, A. Mielke, Phys. Lett. A **219**, 313 (1996).
15. S.K. Kehrein, A. Mielke, Ann. Physik (Leipzig) **6**, 90 (1997).
16. P. Lenz, F. Wegner, Nucl. Phys. B **482**[FS] 693 (1996).
17. L. Nordheim, Ann. Physik (Leipzig) **9**, 607 (1931).
18. F. Wegner, Ann. Physik (Leipzig) **3**, 77 (1994).