Flow Equations for Electron-Phonon Interactions

Peter Lenz and Franz Wegner

Institut für Theoretische Physik
Ruprecht-Karls-Universität
D-69120 Heidelberg, Germany

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Abstract

A recently proposed method of continuous unitary transformations is used to eliminate the interaction between electrons and phonons. The differential equations for the couplings represent an infinitesimal formulation of a sequence of Fröhlich-transformations. The two approaches are compared. Our result will turn out to be less singular than Fröhlich’s. Furthermore the interaction between electrons belonging to a Cooper-pair will always be attractive in our approach. Even in the case where Fröhlich’s transformation is not defined (Fröhlich actually excluded these regions from the transformation), we obtain an elimination of the electron-phonon interaction. This is due to a sufficiently slow change of the phonon energies as a function of the flow parameter.

1New address: Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Kantstraße 55, 14513 Teltow, Germany
1 Introduction

Around 40 years ago Bardeen, Cooper and Schrieffer developed their famous theory of superconductivity [1]. Essential for their success was the interpretation of an effective interaction between electrons of a many-particle system [4]. This interaction was assumed to be present in addition to a Coulomb-interaction between the electrons. As Fröhlich showed 1952 [5] this effective electron-electron interaction can have its origin in the interaction between phonons and electrons. In this work Fröhlich eliminated the electron-phonon interaction by a unitary transformation. By doing so he was able to describe the interaction mediated by the lattice as an effective electron-electron interaction.

But Fröhlich’s approach contains some problems. He had to exclude certain regions in momentum space from the elimination since in these regions the transformation would become singular due to a vanishing energy-denominator.

In this paper we will apply an elimination procedure recently developed by one of the authors [9]. Instead of transforming the Hamiltonian in one step in this new approach the desired transformed Hamiltonian will be achieved step by step. Or more formally spoken instead of one unitary transformation a sequence of unitary transformations will be applied for diagonalization. In an infinitesimal formulation of this continuous transformation the renormalization of the coupling constants is described by the flow equations. In order to develop these differential equations some approximations will be necessary. By means of these transformations new types of interactions mainly involving larger numbers of particles will be generated. They will be neglected after normal-ordering. Fröhlich had to use similar approximations.

Our approach has the following advantages: (i) The original phonon-coupling can be completely eliminated, even when the states connected by this interaction are degenerate. The continuous transformation is chosen in such a way that the transformed Hamiltonian does not contain any interactions between one electron and the creation or annihilation of one phonon. These interactions are still present in Fröhlich’s approach due to normal ordering of generated interactions.
not taken into account. (ii) Singularities in the induced electron-electron interaction which appear in Fröhlich’s scheme, will either not appear in our approach or the divergencies will be less singular. In order to prove these properties the influence of the renormalization of the one-particle energies on the elimination of the electron-phonon coupling has to be taken into account. By doing so it is possible to make statements which cannot be obtained by perturbation theory. Within this approach the way the couplings reach their renormalized value can be determined. By discussing the consequences of this asymptotic behavior it becomes clear that our approach is superior to Fröhlich’s.

Our paper is organized as follows. In the following section a short review of Fröhlich’s approach will be given. In the Section 3 the flow equations describing the elimination of the electron-phonon interaction will be derived. In the next section the above mentioned approximations made by Fröhlich will be applied to the system of differential equations. The renormalized values will be calculated. Also the differences in the electron-electron interactions will be discussed. Section 5 contains the analysis of the behavior of our transformation in the asymptotic regime. The fundamental differential-equation for the phonon-energies will be discussed. In the next section the consequences of the asymptotic behavior of the couplings will be given. It will be shown that the electron-phonon coupling always is eliminated even in the case of degeneracies. The last section contains a short summary and outlook.

2 Fröhlich’s Transformation

In the following sections we will often refer to the above mentioned work of Fröhlich [5]. Thus for convenience a short summary of his results will be given here.

The Hamiltonian of the model will be written as

\[
H = \sum_q \omega_q : a^\dagger_q a_q : + \sum_k \varepsilon_k : c^\dagger_k c_k : + E + \sum_{k,q} M_q (a^\dagger_{-q} + a_q) c^\dagger_{k+q} c_k \\
\equiv H_0 + H_{e-p}.
\]  

(1)
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. \( a^{(t)} \) are bosonic creation respectively annihilation operators. \( c^{(t)} \) denote the corresponding fermionic operators. \( \ldots \) denotes normal-ordering and \( E \) is a constant energy. Further \( M_q \) is the coupling between electrons and phonons. Following the approach of Bloch [2] or Nordheim [8] it is independent of the electron momentum. If there is need to specify \( \varepsilon_k \) or \( \omega_q \) 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.

Fröhlich eliminated the electron-phonon interaction in Eq. (1) up to order \( |M_q(0)|^2 \) by expanding a unitary transformation with the Baker-Hausdorff formula

\[
H^F = e^{-S} H e^S = H + [H, S] + \frac{1}{2} [[H, S], S] + \ldots
\]

Fröhlich’s ansatz

\[
S := - \sum_{k, q} M_q \left( \frac{1}{\varepsilon_{k+q} - \varepsilon_k + \omega_q} a_{-q}^{\dagger} + \frac{1}{\varepsilon_{k+q} - \varepsilon_k - \omega_q} a_q \right) c_{k+q}^{\dagger} c_k,
\]

assures that the relation

\[
H_{e-p} + [H_0, S] = 0
\]

is fulfilled. If degeneracies can be excluded the transformed Hamiltonian becomes

\[
H^F = \sum_q \omega^F_q : a^\dagger_q a_q : + \sum_k (\varepsilon^F_k - 2 \sum_\delta n_{k+\delta} V^F_{k,k+\delta,\delta}) : c_k^{\dagger} c_k :
\]

\[
+ \sum_{k, k', \delta} V^F_{k,k',\delta} : c_{k+\delta}^{\dagger} c_{k' - \delta}^{\dagger} c_{k'} c_k :
\]

\[
+ E^F + \text{irrelevant Terms},
\]

where the irrelevant terms are either of order \( |M_q|^3 \) or represent other interactions not taken into account in Eq. (1). The occurring coefficients are given by:

\[
\varepsilon^F_k = \varepsilon_k - \sum_q |M_q|^2 \left( n_q \frac{1}{\varepsilon_{k+q} - \varepsilon_k - \omega_q} + (n_q + 1) \frac{1}{\varepsilon_{k+q} - \varepsilon_k + \omega_q} \right)
\]

\[
\omega^F_q = \omega_q - \sum_k |M_q|^2 \cdot n_k \left( \frac{1}{\varepsilon_{k+q} - \varepsilon_k + \omega_q} + \frac{1}{\varepsilon_{k+q} - \varepsilon_k - \omega_q} \right)
\]
\[ V_{k,k',q}^F = |M_q|^2 \frac{\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - \omega_q^2} \]

\[ E^F = E + \sum_k n_k(\varepsilon_k^F - \varepsilon_k) - \sum_{k,q} n_k n_{k+q} V_{k,k+q,q}^F \]

In the last equations the convention has been introduced that \( q \) denotes a phonon-wavevector, thus \( n_q \) is a bosonic occupation number whereas \( n_k \) and \( n_{k+q} \) denote the fermionic ones.

### 3 The Flow Equations

In order to eliminate the electron-phonon coupling by flow equations one divides \( H \)

\[ H = H^d + H^r, \]

into the phonon-number conserving part

\[ H^d = \sum_q \omega_q : a^\dagger_q a_q : + \sum_k (\varepsilon_k - 2 \sum_{\delta} n_{k+\delta} V_{k,k+\delta,\delta} : : c^\dagger_k c_k : + \sum_{k,k',\delta} V_{k,k',\delta} : : c^\dagger_{k+\delta} c^\dagger_{k' - \delta} c_{k'} c_k : + E \]

\[ \equiv H^{ph} + H^e + H^{e-e} + E \]

and the phonon-number violating part

\[ H^r \equiv H_{e-p} = \sum_{k,q} (M_{k,q} a^\dagger_{-q} + M^*_{k+q,-q} a_q)c^\dagger_{k+q} c_k. \]

All occurring coefficients have to be regarded as functions of the flow parameter \( l \). The initial conditions of the introduced new quantities are

\[ M_{k,q}(l = 0) = M^*_{k+q,-q}(l = 0) = M_q(0) \equiv M_q \]

\[ V_{k,k',\delta}(l = 0) = 0. \]

The generator of the continuous unitary transformation will be chosen as

\[ \eta := \sum_{k,q} (M_{k,q} \alpha_{k,q} a^\dagger_{-q} + M^*_{k+q,-q} \beta_{k,q} a_q)c^\dagger_{k+q} c_k. \]
where
\[ \alpha_{k,q} = \varepsilon_{k+q} - \varepsilon_k + \omega_q, \quad \beta_{k,q} = \varepsilon_{k+q} - \varepsilon_k - \omega_q. \]

By calculating the commutator \([\eta, H]\) one obtains for \(dH/dl\) besides terms of the type already presented in \(H^d\) contributions of the type \(W^{2ph}\), \(W^{e-2ph}\) and \(W^{2e-2ph}\). They are of the form

\[
\begin{align*}
W^{e-2ph} &\sim \sum_{k,q.q'} (a_{-q}^\dagger a_{-q}^\dagger : + a_{q} a_{q}^\dagger : c_{k+q,q}^\dagger c_{k}^\dagger : ) \quad (9) \\
W^{2e-2ph} &\sim \sum_{k,k',q,q'} (a_{-q}^\dagger + a_{q}^\dagger : c_{k+q,q}^\dagger c_{k'}^\dagger c_{k}^\dagger c_{k}^\dagger : ) \quad (10) \\
W^{2ph} &\sim \sum_{q} (a_{q}^\dagger a_{q}^\dagger + a_{-q} a_{-q}^\dagger ). \quad (11)
\end{align*}
\]

The interactions \(W^{e-2ph}\) and \(W^{2e-2ph}\) are not included in the original model Hamiltonian. They describe two-phonon-processes and the interaction of a phonon with two electrons. Although a more realistic Hamiltonian should contain such interactions, we will neglect them as Fröhlich did.

The interaction (11) describes the generation and annihilation of two phonons. It can be transformed away by introducing

\[
\begin{align*}
\tilde{H} = H + \sum_{q} \mu_{q} \left( a_{-q}^\dagger a_{q}^\dagger + a_{q} a_{q}^\dagger \right) \\
\tilde{\eta} = \eta + \eta^{(2)}, \\
\equiv \eta + \sum_{q} \xi_{q} \left( a_{q}^\dagger a_{-q}^\dagger - a_{q} a_{-q}^\dagger \right),
\end{align*}
\]

where \(\mu_{q}\) and \(\xi_{q}\) are real and \(\mu_{q}(l=0) = 0\).

These additional terms modify the equations for \(\omega_{q}, E, M_{k,q}\). Besides this one obtains the additional flow equation

\[
\frac{d\mu_{q}}{dl} = -2\omega_{q}\xi_{q} + \sum_{k} n_{k} \left( M_{k,q} M_{k+q,-q}\alpha_{k+q,-q} - M_{k-q,q} M_{k,-q}\alpha_{k,-q} \right).
\]

By choosing

\[
\xi_{q} = \frac{1}{2\omega_{q}} \sum_{k} n_{k} \left( M_{k,q} M_{k+q,-q}\alpha_{k+q,-q} - M_{k-q,q} M_{k,-q}\alpha_{k,-q} \right)
\]

it is assured that the interaction (11) will not be generated, i.e. one obtains for all flow-parameters \(l \in R_{0}^{+}\)

\[
\mu_{q}(l) = 0.
\]
Therefore the desired transformed Hamiltonian becomes

\[ H^d(\infty) = \sum_q \omega_q(\infty) : a_q^\dagger a_q : + \sum_k (\varepsilon_k(\infty) - 2 \sum_\delta n_{k+\delta} V_{k,k+\delta}\delta(\infty)) : c_k^\dagger c_k : \\
+ \sum_{k,k',\delta} V_{k,k',\delta}(\infty) : c_{k+\delta}^\dagger c_{k'-\delta}^\dagger c_{k'} c_k : + E(\infty) \\
+ \text{irrelevant terms}. \] (12)

The renormalization of the coefficients is described by the flow equations:

\[ \frac{dM_{k,q}}{dl} = -\alpha_{k,q}^2 M_{k,q} \\
-2 \cdot \sum_\delta V_{k,k+q+\delta,\delta} M_{k+\delta,q} \alpha_{k+\delta,q} \cdot (n_{k+q+\delta} - n_k) \\
-2 M_{k,q} \alpha_{k,q} \cdot \sum_\delta (n_{k+\delta} V_{k,k+\delta,\delta} - n_{k+q+\delta} V_{k,k+q+\delta,\delta}) \\
+2 \cdot \sum_{k'} V_{k,k'+q,\delta} M_{k',q} \alpha_{k',q} \cdot (n_{k'+q} - n_{k'}) \\
-\frac{M_{k+q,-q}}{\omega_q} \sum_{k'} M_{k',q} M_{k'+q,-q} \beta_{k',q} \cdot (n_{k'+q} - n_{k'}) \] (13)

\[ \frac{dV_{k',q}}{dl} = M_{k,q} M_{k'+q,-q} \beta_{k',q} - M_{k+q,-q}^* M_{k',-q} \alpha_{k',-q} \] (14)

\[ \frac{d\omega_q}{dl} = 2 \cdot \sum_k |M_{k,q}|^2 \alpha_{k,q} \cdot (n_{k+q} - n_k) \] (15)

\[ \frac{d\varepsilon_k}{dl} = -\sum_q (2 n_q |M_{k+q,-q}|^2 \beta_{k,q} + 2(n_q + 1)|M_{k,q}|^2 \alpha_{k,q}) \] (16)

\[ \frac{dE}{dl} = \sum_k n_k \frac{d\varepsilon_k}{dl} - \sum_{k,q} n_k n_{k+q} \frac{V_{k,k+q,q}}{dl}. \] (17)

The generated new interactions have been neglected. Thus the last equation does not describe correctly the renormalization of the ground state energy. Hence it will not be of further interest.

4 Comparison with Fröhlich’s Method I: The Non-Degenerate Case

In this first approach it will be assumed that \( \alpha_{k,q} \neq 0 \) holds for all \( k, q \). This could be realized by a finite system with appropriately chosen electron and phonon-
dispersion. In this case it is assured that the Fröhlich-transformation is well-defined.

In this section the flow equations will be compared with Fröhlich’s approach of Section 2. His results were only exact up to order $|M_q(0)|^2$. Thus in the flow equation approach terms of order $|M_q(0)|^3$ and higher might also be neglected. Because of the initial condition $V_{k,k',q}(0) = 0$ Eq. (14) shows that $V_{k,k',q}(l)$ is of the order $|M_q(0)|^2$. Thus the lines two to four in Eq. (13) become irrelevant. The same holds for the last line of this equation, i.e. is also of the order $|M_q(0)|^3$. Within the order given by this approximation Eq. (13) can be solved exactly

$$M_{k,q}(l) = M_q(0)e^{-(\varepsilon_{k+q}(0) - \varepsilon_k(0) + \omega_q(0))^2 l + \mathcal{O}(|M_q(0)|^3)}. \quad (18)$$

Using this solution the equations for $V_{k,k',q}(l)$, $\varepsilon_k(l)$ and $\omega_q(l)$ are easily integrated. Thus their renormalized values can be obtained. While $\varepsilon_k(\infty) = \varepsilon_k^F$ and $\omega_q(\infty) = \omega_q^F$ holds the interaction becomes

$$V_{k,k',q}(\infty) = |M_q(0)|^2 \left( \frac{\beta_{k',-q}}{\alpha_{k,q}^2 + \beta_{k',-q}^2} - \frac{\alpha_{k',-q}}{\beta_{k,q}^2 + \alpha_{k',-q}^2} \right). \quad (19)$$

Actually the last equation does not represent Fröhlich’s result. To illustrate this a look at the interaction between the electrons of a Cooper-pair will be taken ($k' = -k$):

In this case Fröhlich proposes (actually independently of this specialization)

$$V_{k,k',q}^F = V_{k,-k,q}^F = |M_q(0)|^2 \frac{\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - \omega_q^2}, \quad (20)$$

whereas the flow equations yield

$$V_{k,-k,q}(\infty) = -|M_q(0)|^2 \frac{\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 + \omega_q^2}. \quad (21)$$

Thus a remarkable difference between continuous unitary transformations and the Fröhlich transformation has arisen. Before discussing the origin of this difference it should be mentioned that the difference between the two interactions is independent of $M_q(0)$, i.e. holds even for arbitrarily weak coupling.
But it is easily seen that both approaches yield the same result for real processes. In this case the one-particle energy is conserved, i.e.

\[ \varepsilon_{k+q} - \varepsilon_k = \varepsilon_{k'} - \varepsilon_{k'-q}. \]  

(22)

For these processes the interaction becomes

\[ V_{k,k',q}^d = |M_q(0)|^2 \frac{\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - \omega_q^2} \text{ iff } \varepsilon_{k+q} - \varepsilon_k = \varepsilon_{k'} - \varepsilon_{k'-q}. \]

(23)

By introducing

\[ B := \{(k, k', q) : \varepsilon_{k+q} - \varepsilon_k = \varepsilon_{k'} - \varepsilon_{k'-q}\}, \]

the whole interaction can be written as

\[ H^{e-e} = \left( \sum_{(k, k', q) \in B} V_{k,k',q}^d + \sum_{(k, k', q) \notin B} V_{k,k',q}^r \right) : c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k :. \]

(24)

Both Fröhlich’s and the flow equation approach yield the same first term, i.e. both Eqs. (19) and (20) yield the result (23) for \( V_{k,k',q}^d \). Only the second term \( V_{k,k',q}^r \) in (24) differs. Thus the differences between the interactions (19) and (20) can be seen as a different generalization from processes with \((k, k', q) \in B\) to processes with \((k, k', q) \notin B\). The accordance in \( V_{k,k',q}^d \) grants the independence of the self-energy part of the one-particle energies.

Now the origin of the difference between the two interactions (19) and (20) has to be investigated. For that it is useful to formulate the transformation described by the flow equation as an \( l\)-independent transformation. To do so the flow equations

\[ \frac{dH}{dl} = [\eta, H] \]

will be interpreted as an infinitesimal formulation of the unitary transformation

\[ H(l) = U(l)H(0)U^\dagger(l), \]

where

\[ U(l) := T_\text{e}^{\int_0^l \eta(r)dr}. \]
Here l-ordering is defined in the same way as time-ordering.
Thus to get rid of the l-dependence one can introduce

\[ e^{-S} := U(\infty). \]

Then for \( S \) the following expansion holds

\[ S = S_1 + S_2 + \ldots \equiv -\int_0^\infty dl \eta(l) - \frac{1}{2} \int_0^\infty dl \int_0^l dl'[\eta(l), \eta(l')] + \ldots \quad (25) \]

and the neglected terms are again of order \( |M_q(0)|^3 \). Here \( \eta \) denotes again the choice (8). Using the solution (18) the first term of the last equation becomes the generator of the Fröhlich-transformation, while for the second term one obtains

\[
S_2 = -\frac{1}{2} \sum_{k,k',q} |M_q(0)|^2 \left\{ \frac{\alpha_{k,q}}{\beta_{k',-q}(\alpha_{k,q}^2 + \beta_{k',-q}^2)} - \frac{1}{\alpha_{k,q} \beta_{k',-q}} - \frac{\beta_{k,q}}{\alpha_{k',-q}(\beta_{k,q}^2 + \alpha_{k',-q}^2)} + \frac{1}{\beta_{k,q} \alpha_{k',-q}} \right\} \\
\times c_{k+q}^\dagger c_k^\dagger c_{k'-q} c_{k'-q} \\
+ \text{terms of the structure } a^\dagger ac. \quad (26)
\]

To derive the result (19) by using this modified Fröhlich-transformation up to order \( |M_q(0)|^2 \) only \( \left[ \sum_k \varepsilon_k c_k^\dagger c_k, S_2 \right] \) has to be taken into account. Again the generated interaction of the form (9) will be neglected. It is easily verified that

\[
\left[ \sum_k \varepsilon_k c_k^\dagger c_k, S_2 \right] = \sum_{k,k',q} \left( V_{k,k',q}(\infty) - V_{k,k',q}^F \right) c_{k+q}^\dagger c_{k'-q} c_{k'} c_k \quad (27)
\]

holds.

Thus the change in the effective electron-electron interaction is caused by a change of Fröhlich’s generator. This modification is produced by carrying out the l-ordering. Thus it is a consequence of the l-dependence of \( \eta \) respectively of the l-dependence of the coefficients of \( H \). Or more rigorously spoken it is the flow of the couplings which changes the unitary transformation.

\(^2\)Actually these terms together with \(-\int_0^\infty dl \eta^{(2)}(l)\) guarantee that \( H(\infty) \) does not contain any interactions of the form (11).
By comparing (19) and (20) it is obvious that the flow equations yield a result which is less singular, i.e. \( V_{k,k',q} \) diverges only for the special case \( \alpha_{k,q} = \beta_{k',-q} = 0 \). Nevertheless it is not clear which transformation is better with respect to the neglected interactions. Although the modification \( S_2 \) given above eliminates most of the singularities of Fröhlich’s result it is not clear by now if this modification \( S_2 \) is the best one can choose. By changing the coefficient of \( S_2 \) independent of any \( \eta \) a wide variety of possible corrections to \( V^F_{k,k',q} \) can be achieved. It is still an open question what the side-effect of these modifications will be. But one should be aware that modifications of \( S_2 \) are equivalent to modifications of the the unitary transformation. Only for real processes (where energy is conserved), one does not have a choice to modify the effective interaction in this perturbative approach.

5 The Asymptotic Behavior

By now the elimination of the electron-phonon coupling has been considered up to second order. A main advantage of the flow-equations is that in certain cases one can go beyond perturbation theory. Then the continuous change of the single particle energies has the interesting effect, that for processes which are real for a certain value of the flow parameter \( l \), this energy-conservation does no longer hold for other values of \( l \). As Kehrein, Mielke and Neu \[6\] have shown for the spin-boson-problem this allows a complete elimination of the coupling even if energy-conservation holds asymptotically, i.e. for \( l \) approaching infinity. The renormalization of the electron-energies \( \varepsilon_k \) will be neglected, assuming that the electron-phonon coupling is not strong enough to cause a significant change of \( \varepsilon_k \). This holds at least for weak electron-phonon coupling\[4\]. But special cases

\[3\]We will return to this point in Section 6.

\[4\]In deriving Eqs. (16) and (17) this assumption already has been used. There the \( l \)-dependence of the fermi-functions \( n_k \) has been neglected. This can be done for small differences \( V_{k,k',q}(\infty) - V_{k,k',q}(0) \). This assumption is consistent with the BCS-theory, where one neglects the self-energy.
like heavy fermions are excluded. Furthermore it is assumed that the influence of the lines two to five in Eq. (13) is negligible. Thus the dominating part of $M_{k,q}$ becomes

$$M_{k,q}(l) = M_q(0)e^{-\int_0^l d\nu(\epsilon_{k+q}+\omega_q(l'))^2}$$  \hspace{1cm} (28)$$

It should be emphasized that this ansatz corresponds to a highly non-perturbative behavior. By taking into account the change of $\omega_q$ in the order of $|M_q(0)|^2$ the Eq. (28) and hence the Eqs. (14) – (16) contain terms of any order of $|M_q(0)|^2$. This corresponds in the sense of perturbation theory to a summation over a particular subclass of diagrams.

With these approximations only the behavior of $\omega_q$ for large $l$ has to be examined. The key to the asymptotic regime lies in the interpretation of Eq. (15). 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 $\omega_q$ for large $l$ is determined only by the contributions coming from small $\alpha_{k,q}$.

To develop a more formal understanding of this point one replaces in Eq. (15) sums by integrals and introduces the quantity $\Gamma := 4\pi \cdot \frac{V}{(2\pi)^3}$. Specializing to three spatial dimensions and the case of quadratic electron-dispersion $\epsilon_k = \frac{k^2}{2m}$ one gets

$$\frac{d\omega_q}{dl} = -\Gamma \cdot |M_q(0)|^2$$

$$\times \left\{ \int_{-k_F}^{k_F} d\sigma (k_F^2 - \sigma^2) \cdot \left( \frac{-\sigma q}{m} + \epsilon_q + \omega_q \right) e^{-2\int_0^l d\nu(-\sigma_q/m+\epsilon_q+\omega_q)^2}$$

$$+ \int_{-k_F}^{k_F} d\sigma (k_F^2 - \sigma^2) \cdot \left( \frac{\sigma q}{m} + \epsilon_q - \omega_q \right) e^{-2\int_0^l d\nu(\sigma_q/m+\epsilon_q-\omega_q)^2} \right\},$$  \hspace{1cm} (29)$$

where $k_F$ stands for the fermi-momentum. By introducing $\overline{\omega}_q := \frac{1}{l} \int_0^l d\nu \omega_q(l')$ one can use

$$\exp\left(-2\int_0^l d\nu(-\sigma_q/m+\epsilon_q+\omega_q)^2\right) =$$

$$\exp\left(-2\int_0^l \omega_q^2(l')d\nu + \frac{2}{l} \left(\int_0^l \omega_q(l')d\nu\right)^2\right) \cdot \exp\left(-2(-\sigma_q/m+\epsilon_q+\overline{\omega}_q)^2 \cdot l\right).$$

\[5\] It can be seen by a self-consistent analysis that this assumption does not modify the results of this section, i.e. the asymptotic behavior of $\omega_q$. 

11
This allows to express the integral over $\sigma$ in terms of elementary functions and
the error integral. For large $l$ and for values of $q$ which are not too large the
integrals can be extended from $-\infty$ to $+\infty$. By neglecting the exponentially
decaying terms the result is

$$\frac{d \omega_q}{dl} = -2 \cdot \Gamma \cdot |M_q(0)|^2 \exp \left( -2 \int_0^l \omega_q^2(l')dl' + \frac{2}{7} \left( \int_0^l \omega_q(l')dl' \right)^2 \right)$$

$$\times \frac{m^2}{q} \sqrt{\frac{\pi}{2l}} \cdot [\omega_q(\omega_q - \omega_q) + \frac{1}{4l}].$$

(30)

It is worth mentioning that in leading order and besides a constant Eq. (30) is
identical with the integro-differential equation describing the asymptotic behavior
of the flow equations of the spin-boson problem [3]. Following the approach of
Kehrein, Mielke and Neu one can assume an asymptotic expansion of $\omega_q$, i.e. $\omega_q$
decays algebraically

$$\omega_q(l) \approx \omega_q(\infty) + c_q \cdot l^{-\nu}, \quad \nu > 0, \quad l \gg 1,$$

(31)

where $c_q$ is independent of $l$. Using $\omega_q - \omega_q \sim l^{-\nu}$ the integrals in Eq. (30)
are easily performed. The only consistent solution is the case with $\nu = 1/2$ and
$c_q = \pm 1/2$. Numerical studies suggest $\omega_q' \leq 0$, thus the ansatz (31) yields

$$\omega_q(l) \approx \omega_q(\infty) + \frac{1}{2\sqrt{l}}, \quad l \gg 1.$$

(32)

This solution implies that the approach to the $q$-dependent limit is independent
of $q$. We note however that $\omega_q(l)$ can be rescaled $\omega_q(l) = q \cdot c_s(lq^2)$ and $M_q(0) = \sqrt{q}M(0)$. Then Eq. (30) yields

$$\frac{dc_s(z)}{dz} = -2\Gamma \cdot |M(0)|^2 \cdot \exp(-2 \int_0^z c_s^2(z')dz' + 2z \cdot c_s^2(z'))$$

$$\times m^2 \sqrt{\frac{\pi}{2z}} \cdot [c_s(c_s - c_s) + \frac{1}{4z}]$$

with the asymptotic behavior

$$c_s(z) \approx c_s(\infty) + \frac{1}{2\sqrt{z}}.$$

Assuming that this asymptotic behavior holds for $z \gg z_1$ then Eq. (32) holds for
$l \gg l_1 = z_1/q^2$. Thus for small $q$ it is only reached for very large $l$. 12
To get a better understanding of the behaviour in the asymptotic regime a new approach has to be chosen. Therefore one has to go back to Eq. (30). If \( \omega_q \) decays weaker than \( l^{-1} \) than only the term \( \sim \omega_q(\infty)(\pi_q-\omega_q) \) has to be considered. Hence the other terms will be neglected. An a posteriori justification of this approximation will be given later. The remaining integro-differential equation can be transformed into a nonlinear differential equation. One simply differentiates the first term of (30) and expresses the new generated functions in terms of \( l, \omega_q, \omega_q' \). Introducing the function
\[
v(l) := \int_{l_0}^{l} \omega_q(l')dl' - l \cdot \omega_q(l),
\]
the result of this procedure becomes
\[
l^2 \left( v'' \cdot v - v'^2 \right) + \frac{1}{2} l \cdot v \cdot v' + 2 v^3 \cdot v' = 0,
\]
where \( v' = \frac{dv}{dl} \). Thus the integro-differential equation (30) has been replaced by a much more handable nonlinear differential-equation.

To make a first connection to the ansatz (31) one sees that (32) corresponds to \( v = \sqrt[l]{l} \). Thus the algebraic decay given above is a singular solution of the differential equation (33).

In order to solve the differential equation (33) one can make use of the fact that this equation is equidimensional. Thus the ansatz
\[
v(l) = \sqrt{l} \cdot \eta(\xi), \quad \xi = \log l/l_0
\]
yields the equation
\[
\eta \cdot \eta'' - \frac{1}{2} \eta \eta' - \eta^2 + 2 \eta^3 \eta' + \eta^4 - \frac{1}{4} \eta^2 = 0,
\]
which only implicitly depends on \( l \). Here is \( \eta' = \frac{d\eta}{d\xi} \). As a next step one can substitute
\[
\eta' = -\eta \gamma(x), \quad x = \eta^2 - \frac{1}{2} \log |\eta|,
\]
which yields for \( \gamma \neq 0 \)
\[
\gamma' = 1 - \frac{1}{2\gamma},
\]
\( ^{6} \)singular has to be understood as being unable to fulfill arbitrary initial conditions.
with $\gamma' = \frac{d\gamma}{dx}$. Interpreting this as a differential equation for the inverse function one gets for $\gamma \neq 1/2$

$$\frac{dx}{d\gamma} = \frac{2\gamma}{2\gamma - 1}. \tag{38}$$

By integrating the last equation one obtains

$$x = \gamma + \frac{1}{2} \log |2\gamma - 1| + C, \quad C := \text{const.} \tag{39}$$

Thus the applied transformations yield a first integral of the differential equation (33). Although the remaining Eq. (36) can only be solved in special cases it is possible to get an analytical understanding of the behavior of $\omega_q$ in the asymptotic regime. One only has to use the fact that $\gamma$ obeys the autonomous equation (37) and that the first integral (39) is known. The further discussion is organized as follows. First the solution $\gamma$ will be classified by phase space arguments. The properties of $\gamma$ determine the behavior of $\eta$. Thus the behavior of the general solution will become clear and a connection with the singular solution will be made. Finally the remaining Eq. (36) will be solved for some special cases.

If the function $\gamma : D \rightarrow R$ is a solution of a first order autonomous equation then it has exactly one of the following properties:

(i) $\gamma$ is constant and $D = R$.

(ii) $\gamma$ is injective and regular, i.e. $\gamma' \neq 0$ on $D$.

(iii) $\gamma$ is regular periodic, i.e. $D = R$ and $\gamma' \neq 0$ on $D$.

For a proof of this Theorem see for example [3].

While the singular solution (32) belongs to type (i) the solution for arbitrary initial conditions has to be classified now. For that the function $x$ will be interpreted as function of $\gamma$, as shown in Fig. 1. It follows from the definition (34) that $x \geq x_{min} := x(\frac{1}{2})$ (see also Fig. 2). Thus the value $\eta = 1/2$ corresponds to the minimum of the transformation $x = x(\eta)$. Because there exists a lower bound $x_{min}$ the image of the function $\gamma = \gamma(x)$ is also bounded. Therefore $\gamma$ cannot be bijective.

\footnote{In the following we will sometimes refer to the inverse function of $\gamma$, which has to be understood as local inverse function.}
Figure 1: x as function of γ to different initial conditions.

For general initial conditions the function \( x = x(\gamma) \) will be periodic, as can be easily seen by phase space arguments. Because of \( x = \eta^2 - \log|\eta|/2 \) the same holds for \( \eta = \eta(\log l/l_0) \).

Knowing that in general the function \( \eta \) will be periodic some more properties of the solution can be derived by using Fig. 1. First it should be mentioned that the singularities of the differential-equation (38) split the domain of \( x(\gamma) \) in two sections. The assumption \( \omega_q' < 0 \) implies \( \gamma < 1/2 \), as can be easily see from Eq. (34). Thus \( \gamma = 1/2 \) is the upper bound of the domain of \( x(\gamma) \).

Furthermore the point \( (\gamma = 0, x = x_{\text{min}}) \) in the phase space corresponds to a stable trajectory. This follows from the Eqs. (33) and (36), which imply \( \eta^{[n]} = 0, \ \forall n \). Therefore \( \eta = \text{const.} \), which means that also \( x \) and \( \gamma \) are constant. This stable trajectory is the singular solution (32).

If general initial conditions \( x(\gamma = 0) > x_{\text{min}} \) have to be fulfilled the relation \( x'(\gamma = 0) = 0 \) still holds. But the higher derivatives of \( x \) no longer vanish. Therefore a small deviation from the initial condition \( x(\gamma = 0) = x_{\text{min}} \) causes the solution \( \gamma = \gamma(x) \) to change from the behavior of type (i) to type (iii). The trajectory in the phase space is rather a curve than a point. This curve connects the two turning-points \( \gamma_l, \gamma_r \in \{ \gamma : x(\gamma) = x_{\text{min}} \} \). It corresponds to an oscillation...
of $x$ around $x_{\text{min}}$, i.e. of $\eta$ around $1/2$. For the turning-points the relation
\[
\frac{dx}{d\gamma} \bigg|_{\gamma_l, \gamma_r} \neq 0 \iff \frac{d\gamma}{dx} \bigg|_{x_l, x_r = x_{\text{min}}} \neq 0
\]
holds. This implies that an oscillating trajectory cannot turn into a constant one. To characterize the oscillation the following consideration is useful. In Fig. 2 a trajectory $x$ to the initial conditions $x(\gamma = 0) = C_1$ can be seen. This phase space curve corresponds to an oscillation of $\eta$ along the curve $x(\eta)$ in Fig. 2. Therefore the turning-points $\gamma_l, \gamma_r$ in the phase space correspond to the minimum at $\eta = 1/2$. While the point $x(\gamma = 0) = C_1$ represents the greatest elongation. Defining $\eta_{\pm} := x^{-1}(C_1)$, where $+$ denotes the right branch and $-$ left left branch of $x(\eta)$ the following relation holds:
\[
\eta_+ - \frac{1}{2} > \frac{1}{2} - \eta_-.
\]
Thus the amplitudes for the elongations $\eta > 1/2$ are greater than those for $\eta < 1/2$. On the other hand the 'time' for which the solution stays in the regime with $\eta < 1/2$ is longer than that for $\eta > 1/2$. This becomes clear by $|\eta'| = \eta \cdot |\gamma|$ and the fact that the image of $\gamma$ is independent of the branch. But $|\eta|$ is smaller in the left branch than in the right one. Therefore $|\eta'|$ is smaller in the left branch.
altogether the deformation of the oscillations in the Figs. 3-5 can be understood by now.

The above mentioned differences in amplitude and ‘remain-time’ in the cases \( \eta > 1/2 \) and \( \eta < 1/2 \) suggest that the relation \( \langle \eta^2 - 1/4 \rangle \equiv \langle \eta^2 \rangle - 1/4 = 0 \) holds. Here \( \langle \ldots \rangle \) denotes an average over one period. In analogy to the prove of the virial theorem one can try to find a periodic function \( \tilde{f}(\eta, \eta') \) fulfilling the relation

\[
\frac{d\tilde{f}}{d\xi} = \eta^2 - \frac{1}{4}.
\]

The condition (40) becomes easier to handle if again a change to the variables \( x \) and \( \gamma \) is made. Letting \( f(x, \gamma) = \tilde{f}(\eta, \eta') \), one has to fulfill the condition

\[
\frac{\partial f}{\partial \gamma} \cdot \left(1 - \frac{1}{2\gamma}\right) + \frac{\partial f}{\partial x} = -\frac{1}{2\gamma}.
\]

It is sufficient to take only analytical \( f \) into account:

\[
f(x, \gamma) = f_0(x) + f_1(x) \cdot \gamma + \frac{1}{2!} f_2(x) \cdot \gamma^2 + ...
\]

Therefore one obtains the recursional relations

\[
f_1 = 1
\]

\[
n f_n - \frac{1}{2} f_{n+1} + n \frac{df_{n-1}}{dx} = 0 \text{ for } n \geq 1.
\]
Figure 4: $\eta$ as function of $\log l/l_0$ to the initial conditions $\eta(\xi_1) = 1.2$, $\eta'(\xi_1) = 0$.

Figure 5: $\eta$ as function of $\log l/l_0$ to the initial conditions $\eta(\xi_1) = 1.8$, $\eta'(\xi_1) = 0$. The sequence of figures corresponds to a proceeding deviation from the singular solution.
The function $f_0(x)$ can be chosen arbitrarily. The ansatz $f_0(x) \sim x^m$, $m \geq 2$ implies that $f_n$ is a polynomial of degree $(m - 1)$ in $x$ for $n \geq 2$. In order to keep the analysis as simple as possible only the two following cases will be discussed:

1. **Case:** $f_0(x) = C = \text{const.}$: It follows easily by induction that $f_{n+1}(x) = 2^n \cdot n!$ holds for $n \geq 0$. Together with Eq. (42) this yields

$$f(x, \gamma) = C - \frac{1}{2} \log (1 - 2\gamma).$$  \hspace{1cm} (45)$$

Because of $\gamma < 1/2$ the last equation is welldefined.

2. **Case:** $f_0(x) = -x$: Here $f_n(x) \equiv 0$ holds for $n \geq 2$, and therefore

$$f(x, \gamma) = \gamma - x.$$  \hspace{1cm} (46)$$

Because of Eq. (39) the Eqs. (45) and (46) are actually identical. Thus the oscillating behavior of the function $\eta$ is completely determined by the first integral (39). Simultaneously it is shown that $\langle \eta^2 \rangle = 1/4$.

From the definition of $v$ and Eq. (34) one obtains

$$\frac{d\omega_q}{dl} = -l^{-3/2} \cdot (\frac{1}{2} \eta + \eta').$$

From this one can conclude

$$\omega_q(l) = \omega_q(\infty) + c_q \frac{1}{\sqrt{l}}, \quad l \gg 1.$$  \hspace{1cm} (47)$$

Here $c = c_q$ obeys the differential equation

$$\frac{c}{2} - c' = \frac{\eta}{2} + \eta', \quad c' = \frac{dc}{d\xi}.$$  \hspace{1cm} (48)$$

with the solution

$$c(\xi) = \exp(\xi/2) \int_{\xi}^{\infty} (\frac{\eta}{2} + \eta') \cdot \exp(-\xi/2)d\xi.$$  

Since $\eta$ is periodic in $\xi$, this also holds for $c$. One notes, that $\eta/2 + \gamma' = \eta(1/2 - \gamma)$ is positive, since both factors on the right hand side have this property. Thus $\omega_q$ decays monotonically as $l^{-1/2}$ and the term $(4l)^{-1}$ in Eq. (50) is asymptotically negligible. Thus the approximations leading to Eq. (53) are indeed justified.
For the following it will be of importance to show that the average of $c^2$ with respect to $\xi$ equals $1/4$. From the differential equation (48) one obtains

$$c^2 - \eta^2 = (c + \eta)(c - \eta) = 2(c' + \eta')(c + \eta) = \frac{d(c + \eta)^2}{d\xi}.$$  

Since the right hand side is a total derivative the averages of $c^2$ and $\eta^2$ coincide. Thus $\langle c^2 \rangle = 1/4$.

Finally two special solutions of Eq. (35) will be given.

**Nearly harmonic case:** Here it is assumed that $\eta$ deviates only weakly from the singular solution (corresponding to Fig. 3). By expanding the deviation of $\eta^2$ from $1/4$ in powers of the amplitude $A$ with $A \ll 1$ the Eq. (35) yields the solution

$$\eta(\xi)^2 = \frac{1}{4} + A \cdot \cos \left(\frac{1}{\sqrt{2}}y\right) + A^2 \cdot \left[-\frac{\sqrt{2}}{3} \sin \left(\frac{2}{\sqrt{2}}y\right) + \frac{4}{3} \cos \left(\frac{2}{\sqrt{2}}y\right)\right] + A^3 \cdot \left[\frac{5}{4} \cos \left(\frac{3}{\sqrt{2}}y\right) - \sqrt{2} \sin \left(\frac{3}{\sqrt{2}}y\right)\right] + \mathcal{O}(A^4),$$

$$y = \varphi + \xi \cdot \{1 - A^2 + \mathcal{O}(A^4)\}$$

Thus stronger deviations from the singular solution correspond to smaller frequencies. Observe, that the term proportional to $A^2$ does not contain a constant. The same applies for the term proportional to $A^4$ which is not given here. This was a first indication for us, that the average of $\eta^2$ might be $1/4$ independent of the amplitude $A$.

Instead of averaging the solution the algebraic decay of $\omega_\eta$ can be characterized in first order in $A$ by the decay-exponents $\nu = \frac{1}{2}, \frac{1}{2} \pm \frac{i}{\sqrt{2}}$. Hence harmonic oscillations correspond to complex decay-exponents.

**Strongly non-harmonic case:** Here the solution is characterized by a strong deviation from the singular solution (corresponding to Fig. 3). For the case $\eta \ll 1/2$ Eq. (35) can be expanded in powers of $\varepsilon$ if $\eta$ is assumed to be of order $\varepsilon$. In this case the solution is

$$\eta(\xi) = \varepsilon \exp\left\{-\frac{1}{2} \xi + C \cdot e^{\xi/2}\right\} + \mathcal{O}(\varepsilon^2), \quad C = \text{const.},$$
where \( C \) must be positive to assure that \( \eta \) has a positive slope.

The case \( \eta \gg 1/2 \) is not so easy to handle. Here \( \eta \) can be expanded at its maximum \( M = \eta_{\text{max}}^2 - \frac{1}{2} \log \eta_{\text{max}} \approx \eta_{\text{max}}^2 \). In the vicinity of this maximum \( \gamma = \sqrt{M^2 - \eta^2} \) holds as can be seen by expanding Eq. (39). Thus a good approximation for this regime is

\[
\eta(\xi) = \frac{2Me^{-M(\xi-\xi_0)}}{1 + e^{-2M(\xi-\xi_0)}}.
\]

6 Comparison with Fröhlich’s Method II: The Degenerate Case

If systems with many electrons and phonons are considered in general it will be not possible to avoid that the energy difference \( \alpha_{k,q} \) becomes zero. More precisely there will exist electron and phonon momenta satisfying the relation

\[
\frac{kq \cos \theta}{m} \pm v_s q = 0,
\]

where \( \theta \) denotes the angle between \( k \) and \( q \) and \( v_s \) the velocity of sound. The Fröhlich-transformation is not defined for these \( k, q \). Thus the corresponding couplings \( M_{k,q} \) are not eliminated in this approach.

But even in these cases the elimination described by the flow equations works. To verify this the asymptotic behavior of \( \omega_q \) has to be taken into account.

For \( \alpha_{k,q} \) the following asymptotic expansion holds:

\[
\alpha_{k,q}(l) \approx \alpha_{k,q}(\infty) + c_q \cdot \frac{1}{\sqrt{l}}, \quad l \gg 1.
\]

Thus for \( \alpha_{k,q}(\infty) = 0 \) one obtains

\[
M_{k,q} \approx C \cdot \left( \frac{1}{l} \right)^{\frac{3}{4}} = C \cdot \left( \frac{1}{l} \right)^{1/4},
\]

with an appropriate constant \( C \). In this case the decay is rather algebraic than exponential.

Hence it is not important that \( \alpha_{k,q} \) becomes zero for some special \( l \). It is only
important that it is not zero for all $l$. Thus the elimination of $M_{k,q}$ is a direct consequence of the renormalization of $\omega_q$.

A similar argumentation was used by Kehrein, Mielke and Neu [6] for the spin-boson model. There the authors argued that the coupling to the bosonic bath always is eliminated because of the renormalization of the tunneling frequency.

A final remark shall be made on the remaining singularities of the electron-electron interaction (19). By taking the renormalization of $\omega_q$ into account only the special values $\alpha_{k,q}(\infty) = \beta_{k',-q}(\infty) = 0$ are critical. It is easily seen that in this case

$$V_{k,k',q}(l) = V_{k,k',q}(l_0) + D \cdot \log l/l_0, \quad D := \text{const.}$$

holds for $l \gg 1$. Thus there will remain some singularities in our approach. But as long as these special values are multiplied with functions which stay finite for $l \to \infty$ they will have no influence.

7 Conclusions

It has been shown that it is possible to eliminate the electron-phonon interaction by using continuous unitary transformations. This elimination causes the renormalization of the coupling functions of the Hamiltonian described by the flow equations. This change of the couplings corresponds to the renormalization of the one-particle energies and to the generation of an effective electron-electron interaction. In order to set up these differential equation the generated new interactions have to be neglected.

By analyzing these flow equations some different approaches can be chosen. First it is possible to apply the approximation used by Fröhlich. In this case terms of higher order than $|M(0)|^2$ can be neglected. Furthermore the possibility of degeneracies has to be excluded. By doing so the flow equations can be solved exactly. By comparing the results with Fröhlich’s one sees that the induced electron-electron interactions differ. The origin of this difference lies in the fact

\footnote{This will typically happen if one calculates averages of observables.}
that in our approach all couplings depend on $l$. Thus by going over to a formulation similar to Fröhlich’s, i.e. carrying out the $l$-ordering of $\eta$, it can be seen that the flow of the coefficients changes the generator of the unitary transformation. Our result looks much friendlier than Fröhlich’s interaction. But nevertheless it is not clear by now in which sense our result is ’better’ or even ’the best’ one can obtain.

It is worth mentioning that Kehrein and Mielke obtain similar modifications by eliminating the hybridization term in the single impurity Anderson model by continuous unitary transformations \([7\). The authors show that their approach generates a spin-spin interaction which differs from the one obtained by the famous Schrieffer-Wolff transformation. Their induced interaction is also less singular. But even more important their result shows the right high-energy cutoff. Thus at least for this model a physical criterion exists to decide which interaction is ’better’.

Besides this direct comparison with Fröhlich’s results it is possible to prove that our approach indeed eliminates the interactions between one phonon and one electron. For this purpose the influence of the renormalization of $\omega_q$ on the elimination of $M_{k,q}$ has to be taken into account. By doing so the renormalization of $\omega_q$ in the asymptotic regime is described by an integro-differential equation. This equation can be transformed into a differential-equation which is much easier to analyze. By using its first integral the behavior of $\omega_q$ for large $l$ can be characterized. As a consequence of the properties of $\omega_q$ the electron-phonon coupling is always eliminated even in the case of degeneracies. Furthermore it is shown that the remaining singularities in the electron-electron interaction are of a very weak nature.

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