REVISITING THE FRÖHLICH-TYPE TRANSFORMATION
WHEN DEGENERATE STATES ARE PRESENT.

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Abstract

We focus on the definition of the unitary transformation leading to an effective second order Hamiltonian, inside degenerate eigensubspaces of the non-perturbed Hamiltonian. We shall prove, by working out in detail the Su-Schrieffer-Heeger Hamiltonian case, that the presence of degenerate states, including fermions and bosons, which might seemingly pose an obstacle towards the determination of such "Fröhlich-transformed" Hamiltonian, in fact does not: we explicitly show how degenerate states may be harmlessly included in the treatment, as they contribute with vanishing matrix elements to the effective Hamiltonian matrix. In such a way, one can use without difficulty the eigenvalues of the effective Hamiltonian to describe the renormalized energies of the real excitations in the interacting system. Our argument applies also to few-body systems where one may not invoke the thermodynamic limit to get rid of the "dangerous" perturbation terms.
I. INTRODUCTION.

Effective Hamiltonians obtained by unitary transformations truncated to second order in the perturbation, which here we shall label as of “Fröhlich-type”, are ubiquitous in condensed matter physics. Given a starting Hamiltonian $H = H_0 + I$, with a basic part $H_0$ and a perturbation $I$, one may write the unitary transformed Hamiltonian neglecting terms of third or higher order in the perturbation as:

$$H \equiv e^R(H_0 + I)e^{-R} = H_0 + I + [R, H_0] + [R, I] + \frac{1}{2}[R, [R, H_0]] + O(I^3)$$ (1)

The antihermitian generator $R$ of the unitary transformation $e^R$ is determined by imposing the vanishing of the first-order terms

$$I + [R, H_0] = 0$$ (2)

so that the transformed second-order Hamiltonian $H^{(2)}$ reads

$$H^{(2)} = H_0 + \frac{1}{2}[R, I] + O(I^3)$$ (3)

To solve Eq.2 for $R$, one may explicitate it on a complete set of orthonormal eigenstates $|X_\alpha\rangle$ of $H_0$:

$$H_0|X_\alpha\rangle = \mathcal{E}_\alpha|X_\alpha\rangle \quad 1 = \sum_\alpha |X_\alpha\rangle\langle X_\alpha|$$ (4)

yielding the basic equation to determine the matrix elements of $R$

$$\langle X_\beta|I|X_\alpha\rangle = (\mathcal{E}_\beta - \mathcal{E}_\alpha)\langle X_\beta|R|X_\alpha\rangle$$ (5)

In solving Eq.5 one has to distinguish between the cases of non-degenerate or degenerate eigenstates. For non-degenerate cases, the matrix elements of $R$ are directly obtained and the second-order Hamiltonian is straightforwardly derived, as usually done. The presence of degenerate eigenstates of $H_0$ requires a special analysis. Namely, if $\mathcal{E}_\alpha = \mathcal{E}_\beta$ the right hand side of the equation vanishes identically for any finite $\langle X_\beta|R|X_\alpha\rangle$, and two possibilities appear, depending on the perturbation $I$. If also $\langle X_\beta|I|X_\alpha\rangle = 0$, the left-hand side vanishes as well, and one gets no condition for the corresponding matrix element of $R$ between these degenerate states. On the other hand, for $\langle X_\beta|I|X_\alpha\rangle \neq 0$, Eq.5 would make no sense except for the case of a divergent $\langle X_\beta|R|X_\alpha\rangle$. We will focus on this problem, and explicitly show
by working out in detail a non-trivial example that a well defined unitary transformation can nonetheless be defined when degenerate eigenstates are present (as first observed in general by Wagner\cite{2}) , and through it the second-order Hamiltonian be obtained. To fix ideas, we will consider the case of a non-perturbed Hamiltonian $H_0$ describing a system of non-interacting bosons and fermions, in particular the Su-Schrieffer-Heeger electron-phonon Hamiltonian. The degenerate states $|X_\alpha\rangle$ and $|X_\beta\rangle$ might differ in having one more, or one less, boson, which is created or destroyed in a real (as opposed to virtual) scattering process with the fermions, as described by perturbation $I$, conserving the total energy between initial and final states. We show how the generator $\mathcal{R}$ can be defined, such that the frequently used procedure of identifying renormalized excitation energies of the real interacting bosons with eigenvalues of their effective Hamiltonian, obtained by averaging over the fermion wavefunction, can be applied without difficulties.

II. THE SU-SCHRIEFFER-HEEGER ELECTRON-PHONON HAMILTONIAN

Let us work out in detail a specific example based on the Su-Schrieffer-Heeger electron-phonon Hamiltonian\cite{1}, for which the non-interacting Hamiltonian reads:

$$H_0 = \sum_{k\sigma} E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_q \hbar \Omega_q \left( b_q^\dagger b_q + \frac{1}{2} \right)$$

(6)

Introducing the number operators $n_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma}$, for itinerant electrons in states characterized by: crystal momentum $k$, spin $\sigma$, and energy $E_k$, and $\nu_q = b_q^\dagger b_q$, for phonons in states characterized by crystal momentum $q$ and energy $\Omega_q$, the generic eigenstate $|X_\alpha\rangle = |X_{k,q,\sigma}\rangle$ of $H_0$ may be written as a product of fermionic and bosonic orthonormal eigenstates:

$$|X_{k,q,\sigma}\rangle = |..n_{k\sigma},n_{k+q,\sigma},n_{k-q,\sigma},\cdots\rangle|..\nu_q,\nu_{-q},\cdots\rangle$$

Above, we have explicitly written only the occupation numbers of the states of interest for our discussion. For instance, the boson state indicated simply as $|\nu_q\rangle$, denotes the following $N$-phonon state in occupation number representation ($N$ different wavevectors):

$$|\nu_q\rangle \iff \left[ \frac{1}{\sqrt{\langle \nu_q \rangle}} (b_q^\dagger)^{\nu_q} \prod_{p \neq q} \frac{1}{\sqrt{\langle \nu_p \rangle}} (b_p^\dagger)^{\nu_p} \right] |0\rangle$$

(7)

while the orthonormal boson states ($\langle \nu_q | \nu_p \rangle = \delta_{pq}$) are such that:

$$b_q |\nu_q\rangle = \sqrt{\langle \nu_q \rangle} |\nu_q - 1\rangle \quad b_q^\dagger |\nu_q\rangle = \sqrt{\langle \nu_q \rangle + 1} |\nu_q + 1\rangle$$

(8)
The exact eigenenergy $\mathcal{E}_{kq\sigma}$ of $|X_{kq\sigma}\rangle$ is:

$$
\mathcal{E}_{kq\sigma} = E_{k\sigma} \langle n_{k\sigma} \rangle + E_{k+q,\sigma} \langle n_{k+q,\sigma} \rangle + E_{k-q,\sigma} \langle n_{k-q,\sigma} \rangle + \hbar \Omega_q \langle \nu_q \rangle
+ \sum_{p \neq (k,k\pm q)} E_{p\sigma} \langle n_{p\sigma} \rangle + \sum_{r \neq q} \hbar \Omega_r \langle \nu_r \rangle
$$

(9)

For this Hamiltonian, the perturbation term $I$ reads:

$$
I = \frac{1}{\sqrt{N}} \sum_{kq\sigma} \Gamma_{k,\sigma} \sum_{kq\sigma} \langle c_{k\sigma}^\dagger c_{k-q,\sigma} \rangle (b_{-q}^\dagger + b_q)
$$

(10)

where the bond-stretching interaction amplitude, resulting from a modulation of the electron hopping $t_{ij}$, for a lattice with a centre of inversion is:

$$
\Gamma_{k,k-q} = i \sum_{(ij)} g_{ij} \{ \sin [(k-q) \Delta_{ij}] - \sin [k \Delta_{ij}] \}
$$

(11)

Notice $\Gamma_{k,k-q} = -\Gamma_{k,k-q}^*$. Thus, rewriting $\sum_{kq\sigma} \Gamma_{k,k-q}^* c_{k\sigma}^\dagger c_{k-q,\sigma} b_{-q}^\dagger = \sum_{kq\sigma} \Gamma_{k,k-q}^* c_{k\sigma}^\dagger c_{k,q,\sigma} b_q^\dagger$, we can decompose the perturbation as

$$
I = \frac{1}{\sqrt{N}} \sum_{kq\sigma} (I_{kq\sigma}^+ + I_{kq\sigma}^-)
$$

(12)

where

$$
I_{kq\sigma}^+ = \Gamma_{k,k-q}^* c_{k-q,\sigma}^\dagger c_{k,\sigma} b_q^\dagger
I_{kq\sigma}^- = \Gamma_{k,k-q} c_{k-q,\sigma}^\dagger c_{k,\sigma} b_q
$$

(13)

A given perturbation term $I_{kq,\sigma}^\pm$ yields non-vanishing results only when applied to the specific state $|A_{kq,\sigma}^\pm\rangle$ where:

$$
|A_{kq,\sigma}^+\rangle = |1_{k\sigma}, n_{k+q,\sigma}, 0_{k-q,\sigma}, \cdots \rangle |\nu_q, \nu_{-q}, \cdots \rangle
|A_{kq,\sigma}^-\rangle = |0_{k\sigma}, 1_{k-q,\sigma}, n_{k+q,\sigma}, \cdots \rangle |\nu_q, \nu_{-q}, \cdots \rangle
$$

(14)

Namely,

$$
I_{kq\sigma}^+ |A_{kq,\sigma}^+\rangle = \Gamma_{k,k-q}^* \sqrt{\langle \nu_q \rangle} + 1 |0_{k\sigma}, n_{k+q,\sigma}, 1_{k-q,\sigma}, 0_{k-q,\sigma}, \cdots \rangle |\nu_q, 1_{k-q,\sigma}, \nu_{-q}, \cdots \rangle
$$

(15)

$$
I_{kq\sigma}^- |A_{kq,\sigma}^-\rangle = \Gamma_{k,k-q} \sqrt{\langle \nu_q \rangle} |1_{k\sigma}, n_{k+q,\sigma}, 0_{k-q,\sigma}, \cdots \rangle |\nu_q, 1, \nu_{-q}, \cdots \rangle
$$

(16)

where we have introduced the notation $|B_{kq,\sigma}^\pm\rangle$ for the states resulting from applying the perturbation. Notice also that: $I_{k,q,\sigma}^\pm A_{k,q,\sigma}^\mp = 0$, and that states $|A_{kq,\sigma}^+\rangle$ and $|B_{kq,\sigma}^+\rangle$ are orthogonal:

$$
\langle A_{kq,\sigma}^+ | B_{kq,\sigma}^+ \rangle = \frac{1}{\Gamma_{k,k-q}^*} \langle A_{kq,\sigma}^+ | I_{kq,\sigma}^+ A_{kq,\sigma}^+ \rangle = 0
$$

(17)

To fix ideas, in the following we will solve in detail the problem for the case of two degenerate eigenstates of the unperturbed Hamiltonian. The argumentation can be straightforwardly extended for larger size of the degenerate eigensubspace, without altering the conclusions.
III. THE CASE OF TWO DEGENERATE STATES.

Let us now assume that the spectrum of non-interacting energies of the system is such that, given the state \(|A^+_{kq\sigma}\rangle = |1_{k\sigma}, n_{k+q,\sigma}, 0_{k-q,\sigma}\rangle|\nu_q, \nu_{-q}\rangle\) with energy \(\mathcal{E}^A_{kq\sigma}\), a phonon exists such that \(|A^+_{kq\sigma}\rangle\) is degenerate with the state \(|B^+_{kq\sigma}\rangle = \sqrt{\langle \nu_q \rangle + 1}|0_{k\sigma}, n_{k+q,\sigma}, 1_{k-q,\sigma}\rangle|\nu_q + 1, \nu_{-q}\rangle\). Thus \(\mathcal{E}^B_{kq\sigma} = \mathcal{E}^A_{kq\sigma}\), which implies \(E_k = E_{k-q} + \hbar \Omega_q\). In this case, we might be in trouble with Eq.5, as mentioned in the Introduction.

To tackle the problem, it is convenient to rewrite the condition for the transformation generator \(\mathcal{R}\), Eq.2, specifically isolating in \(I\) the "dangerous" terms \(I^+_k + I^-_k\):  

\[
I = \frac{1}{\sqrt{N}} \sum_{pr\tau} (I^+_pr\tau + I^-_pr\tau) (1 - \delta_{pk}\delta_{rq}\delta_{\tau\sigma}) + \frac{1}{\sqrt{N}} (I^+_k + I^-_k) \equiv I_1 + I_{kq\sigma}
\]  

(18)

Analogously, we write for the generator: \(\mathcal{R} = \mathcal{R}_1 + \mathcal{R}_{kq\sigma}\), explicating its restriction to the degenerate subspace in last term. Notice that the commutators \([I_1, I_{kq\sigma}]\), \([\mathcal{R}_1, \mathcal{R}_{kq\sigma}]\), \([\mathcal{R}_1, I_{kq\sigma}]\) and \([I_1, \mathcal{R}_{kq\sigma}]\) vanish, since the operators to be commuted involve different wavevectors. Thus, the transformed Hamiltonian of Eq.1 now reads:  

\[
H \equiv e^{(\mathcal{R}_1 + \mathcal{R}_{kq\sigma})}(H_0 + I_1 + I_{kq\sigma})e^{-(\mathcal{R}_1 + \mathcal{R}_{kq\sigma})} = \\
= H_0 + I_1 + I_{kq\sigma} + ([\mathcal{R}_1 + \mathcal{R}_{kq\sigma}], H_0) + [\mathcal{R}_1, I_1] + [\mathcal{R}_{kq\sigma}, I_{kq\sigma}] + \frac{1}{2} [\mathcal{R}_1, [\mathcal{R}_1, H_0]] + \frac{1}{2} [\mathcal{R}_{kq\sigma}, [\mathcal{R}_1, H_0]] + \frac{1}{2} [\mathcal{R}_{kq\sigma}, [\mathcal{R}_{kq\sigma}, H_0]] + O(1^3)
\]  

(19)

The condition to be imposed in order to eliminate the terms linear in the perturbation takes the form:  

\[
I_1 + I_{kq\sigma} + ([\mathcal{R}_1 + \mathcal{R}_{kq\sigma}], H_0) = 0
\]  

(20)

The above equation for \(\mathcal{R}\) can further be split into two independent constraints  

\[
I_1 + [\mathcal{R}_1, H_0] = 0 \quad \Rightarrow \quad [\mathcal{R}_1, H_0] = -I_1
\]  

(21)

\[
I_{kq\sigma} + [\mathcal{R}_{kq\sigma}, H_0] = 0 \quad \Rightarrow \quad [\mathcal{R}_{kq\sigma}, H_0] = -I_{kq\sigma}
\]  

(22)

Therefore, using these two constraints in Eq.19 and dropping all vanishing commutators, it follows that to second order one has:  

\[
H^{(2)} = H_0 + \frac{1}{2} [\mathcal{R}_1, I_1] + \frac{1}{2} [\mathcal{R}_{kq\sigma}, I_{kq\sigma}] + O(1^3)
\]  

(23)

where the matrix elements of commutator \([\mathcal{R}_1, I_1]\) can be evaluated safely even over the pair of degenerate states. In the following, we shall focus on the matrix elements of the potentially "dangerous" commutator \([\mathcal{R}_{kq\sigma}, I_{kq\sigma}]\).
A. The action of the perturbation on the degenerate states.

As $|B^+_{kq\sigma}\rangle$ is not normalized, let’s introduce the corresponding normalized eigenstate $|B^+_{kq\sigma}\rangle$ as:

$$|B^+_{kq\sigma}\rangle = \frac{1}{\sqrt{\langle \nu_q \rangle + 1}} |B^+_{kq\sigma}\rangle = |0_{k\sigma}, n_{k+q,\sigma}, 1_{k-q,\sigma}\rangle |\nu_q + 1, \nu_q\rangle$$  \hspace{1cm} (24)

Let us evaluate the matrix elements of $(I^+_{kq\sigma} + I^-_{kq\sigma})$ inside the degenerate subspace spanned by: $|A^+_{kq\sigma}\rangle$, $|B^+_{kq\sigma}\rangle$. The diagonal elements vanish by orthogonality:

$$\langle A^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | A^+_{kq\sigma}\rangle = \langle B^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | B^+_{kq\sigma}\rangle = 0$$  \hspace{1cm} since the perturbation changes the number of bosons, while:

$$\langle B^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | A^+_{kq\sigma}\rangle = \Gamma^*_{k,k-q} \sqrt{\langle \nu_q \rangle + 1} = \left[ \langle A^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | B^+_{kq\sigma}\rangle \right]^*$$  \hspace{1cm} (25)

B. The perturbation-split equivalent states and the corresponding matrix elements.

By a rotation inside the degenerate subspace, we now diagonalize the restriction of the perturbation $\frac{1}{\sqrt{N}}(I^+_{kq\sigma} + I^-_{kq\sigma})$, there. From its eigenvalues, we obtain the respective eigenenergies of the Hamiltonian including first-order perturbative corrections:

$$E_{kq\sigma}^{\pm} = E_{kq\sigma}^A \pm |\langle B^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | A^+_{kq\sigma}\rangle| = E_{kq\sigma}^A \pm \frac{1}{\sqrt{N}} |\Gamma_{k,k-q}| \sqrt{\langle \nu_q \rangle + 1}$$  \hspace{1cm} (26)

with respective orthonormal eigenvectors of $H_0$:

$$|\psi^+_{kq\sigma}\rangle = \frac{1}{\sqrt{2}} \left[ |\lambda |A^+_{kq\sigma}\rangle + |B^+_{kq\sigma}\rangle \right] \hspace{1cm} |\psi^-_{kq\sigma}\rangle = \frac{1}{\sqrt{2}} \left[ |\lambda |A^+_{kq\sigma}\rangle - |B^+_{kq\sigma}\rangle \right]$$  \hspace{1cm} (27)

$$\lambda \equiv \frac{\Gamma_{k,k-q}}{\Gamma_{k,k-q}} = i \lambda' \hspace{.5cm} \text{where} \hspace{.5cm} \lambda' \equiv sgn \left[ \sum_{\langle ij \rangle} g_{ij} \left\{ \sin [(k - q) \Delta_{ij}] - \sin [k \Delta_{ij}] \right\} \right]$$  \hspace{1cm} (28)

The diagonal matrix elements of ”dangerous” perturbation terms in the $|\psi^\pm_{kq\sigma}\rangle$ subspace are:

$$\langle \psi^+_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | \psi^+_{kq\sigma}\rangle = -|\Gamma_{k,k-q}| \sqrt{\langle \nu_q \rangle + 1}$$

$$\langle \psi^-_{kq\sigma} | (I^+_{kq\sigma} + I^-_{kq\sigma}) | \psi^-_{kq\sigma}\rangle = |\Gamma_{k,k-q}| \sqrt{\langle \nu_q \rangle + 1}$$  \hspace{1cm} (29)

while the off-diagonal ones vanish.
C. Matrix elements of the effective Hamiltonian in the $|\psi_{kq\sigma}^+\rangle$, $|\psi_{kq\sigma}^-\rangle$ subspace.

Of interest is the effect that the "dangerous" perturbation term might have on the matrix elements of $H^{(2)}$ of Eq. 23. We will show that, with an appropriate definition of $R$, all matrix elements of $[R_{kq\sigma}, I_{kq\sigma}]$ in the subspace spanned by $|\psi_{kq\sigma}^+\rangle$ and $|\psi_{kq\sigma}^-\rangle$ vanish.

For the evaluation of the off-diagonal elements of $[R_{kq\sigma}, I_{kq\sigma}]$ it will be convenient to use the following decomposition of the identity operator:

$$1 = \sum_{pr\sigma} |X_{pr\sigma}\rangle\langle X_{pr\sigma}| (1 - \langle A_{pr\sigma}^+|X_{pr\sigma}\rangle) (1 - \langle B_{pr\sigma}^+|X_{pr\sigma}\rangle)$$

$$+ |\psi_{kq\sigma}^+\rangle\langle \psi_{kq\sigma}^+| + |\psi_{kq\sigma}^-\rangle\langle \psi_{kq\sigma}^-|$$

where use has been made of the equality: $|\psi_{kq\sigma}^+\rangle\langle \psi_{kq\sigma}^+| + |\psi_{kq\sigma}^-\rangle\langle \psi_{kq\sigma}^-| = |A_{kq\sigma}^+\rangle\langle A_{kq\sigma}^+| + |B_{kq\sigma}^-\rangle\langle B_{kq\sigma}^-|$. For simplicity, in the following we will assume that except for the subspace explicitated above, $H_0$ possesses no other degenerate eigenstates.

We have:

$$\langle \psi_{kq\sigma}^+ | [R_{kq\sigma}, I_{kq\sigma}] | \psi_{kq\sigma}^- \rangle =$$

$$= \frac{1}{\sqrt{N}} \left[ \langle \psi_{kq\sigma}^+ | R_{kq\sigma} (I_{kq\sigma}^+ + I_{kq\sigma}^-) | \psi_{kq\sigma}^- \rangle - \langle \psi_{kq\sigma}^+ | (I_{kq\sigma}^+ + I_{kq\sigma}^-) R_{kq\sigma} | \psi_{kq\sigma}^- \rangle \right]$$

Inserting the identity operator $1$, the first contribution to the rhs of Eq.31 , reads:

$$\langle \psi_{kq\sigma}^+ | R_{kq\sigma} (I_{kq\sigma}^+ + I_{kq\sigma}^-) | \psi_{kq\sigma}^- \rangle =$$

$$= \sum_{pr\sigma} \left( 1 - \langle A_{pr\sigma}^+|X_{pr\sigma}\rangle \right) \left( 1 - \langle B_{pr\sigma}^+|X_{pr\sigma}\rangle \right) \langle \psi_{kq\sigma}^+|X_{pr\sigma}\rangle \langle X_{pr\sigma}|(I_{kq\sigma}^+ + I_{kq\sigma}^-)|\psi_{kq\sigma}^-\rangle +$$

$$+ \langle \psi_{kq\sigma}^+|R_{kq\sigma}|\psi_{kq\sigma}^+\rangle\langle \psi_{kq\sigma}^-|X_{pr\sigma}\rangle \langle X_{pr\sigma}|(I_{kq\sigma}^+ + I_{kq\sigma}^-)|\psi_{kq\sigma}^-\rangle \langle \psi_{kq\sigma}^-| \psi_{kq\sigma}^- \rangle$$

For the first term, notice that $\sum_{pr\sigma}$ involves only eigenstates outside the degenerate subspace specified, while, using Eqs.15 , 24 and 25, one has:

$$\langle X_{pr\sigma}|(I_{kq\sigma}^+ + I_{kq\sigma}^-)|\psi_{kq\sigma}^-\rangle =$$

$$= \frac{\lambda}{\sqrt{2}} \Gamma_{k, k-\mathbf{q}} \sqrt{\langle \psi_{\mathbf{q}}^- \rangle + 1} \langle X_{pr\sigma}|B_{kq\sigma}^+\rangle - \frac{1}{\sqrt{2}} \Gamma_{k, k-\mathbf{q}} \sqrt{\langle \psi_{\mathbf{q}}^- \rangle + 1} \langle X_{pr\sigma}|A_{kq\sigma}^+\rangle \equiv 0$$

where the last equality follows from orthogonality, in both scalar products.
The next term in Eq.32 vanishes because \[ \langle \psi^+_{kq\sigma} | (I^{+}_{kq\sigma} + I^{-}_{kq\sigma}) | \psi^-_{kq\sigma} \rangle = 0 \]. The last term in Eq.32, due to Eq.29, reads:

\[
\langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle \langle \psi^-_{kq\sigma} | (I^{+}_{kq\sigma} + I^{-}_{kq\sigma}) | \psi^-_{kq\sigma} \rangle = 0
\]

The off-diagonal matrix elements of \( R_{kq\sigma} \) are required to satisfy the condition given by Eq.5. But due to the diagonalization of the perturbation performed, and \( H_0 | \psi^\pm_{kq\sigma} \rangle = E^A_{kq\sigma} | \psi^\pm_{kq\sigma} \rangle \), one is in the case in which both sides of Eq.5 are identically zero. Thus, one in fact has the freedom to choose the value of \( \langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle \) as zero, in particular. In the following, we will justify this choice as a reasonable and most convenient one.

First, one can justify that choice by an analytical continuity argument. Having performed the diagonalization of the perturbation, \( \langle \psi^+_{kq\sigma} | (I^{+}_{kq\sigma} + I^{-}_{kq\sigma}) | \psi^-_{kq\sigma} \rangle = 0 \) holds exactly for any value of \( |\Gamma_{k,k-q}| \geq 0 \). If in Eq.5 one would replace the zero-order (degenerate, here) eigenenergies difference by the vanishing perturbation limit of the first-order eigenenergies splitting,

\[
0 = \lim_{|\Gamma| \to 0} \left( E^+_{kq\sigma} - E^-_{kq\sigma} \right) \langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle = \lim_{|\Gamma| \to 0} \frac{1}{N} \sqrt{\langle \nu_q \rangle + 1} \langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle \quad (|\Gamma_{k,k-q}| \geq 0) \quad (35)
\]

one would see that in the whole neighbourhood of \( |\Gamma_{k,k-q}| = 0 \) the consistent definition of the transformation would be:

\[
\langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle = 0 \quad (|\Gamma_{k,k-q}| > 0) \quad (36)
\]

By continuity, it thus seems reasonable to choose \( \langle \psi^+_{kq\sigma} | R_{kq\sigma} | \psi^-_{kq\sigma} \rangle = 0 \), also for \( |\Gamma_{k,k-q}| = 0 \).

Further, as a hand-waving argument, one could also mention that since \( R_{kq\sigma} \) has the same operatorial structure as \( (I^{+}_{kq\sigma} + I^{-}_{kq\sigma}) \), one might expect the two objects to have similarly vanishing off-diagonal matrix elements in the \( |\psi^\pm_{kq\sigma} \rangle \) subspace.

Going back to Eq.31, with our choice we thus have a vanishing contribution for the first term of the commutator. To evaluate the second term of the commutator we again introduce the identity decomposition previously used, yielding:

\[
\langle \psi^+_{kq\sigma} | (I^{+}_{kq\sigma} + I^{-}_{kq\sigma}) (1) R_{kq\sigma} | \psi^-_{kq\sigma} \rangle =
\]
\[
= \sum_{pr\sigma} \left( 1 - \langle A^+_{pr\sigma} | X_{pr\sigma} \rangle \right) \left( 1 - \langle B^+_{pr\sigma} | X_{pr\sigma} \rangle \right) \langle \psi^+_k q \rangle \left( I^+_k q + I^-_k q \right) | X_{pr\sigma} \rangle \langle X_{pr\sigma} | R_{kq\sigma} | \psi^-_k q \rangle + \\
+ \langle \psi^+_k q \rangle \left( I^+_k q + I^-_k q \right) | \psi^-_k q \rangle \langle R_{kq\sigma} | \psi^-_k q \rangle + \langle \psi^+_k q \rangle \left( I^+_k q + I^-_k q \right) | \psi^-_k q \rangle \rangle R_{kq\sigma} | \psi^-_k q \rangle 
\]

(37)

Here, the first term is zero by orthogonality, analogously to Eq.33, and having chosen to define: \( \langle \psi^+_k q | R_{kq\sigma} | \psi^-_k q \rangle = 0 \), the second term of Eq.37 vanishes as well. Finally, the last term also vanishes, because \( |\psi^+_k q\rangle \) are orthogonal eigenvectors of the perturbation.

Therefore, Eq.31 yields vanishing off-diagonal matrix elements of \( [R_{kq\sigma}, I_{kq\sigma}] \).

Let us now evaluate its diagonal elements. We have to consider

\[
\langle \psi^+_k q | [R_{kq\sigma}, I_{kq\sigma}] | \psi^+_k q \rangle = \\
= \frac{1}{\sqrt{N}} \left[ \langle \psi^+_k q | R_{kq\sigma} \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle - \langle \psi^+_k q \rangle \left( I^+_k q + I^-_k q \right) R_{kq\sigma} | \psi^+_k q \rangle \right] 
\]

(38)

Again, inserting the identity decomposition, the first contribution to the commutator in Eq.38 reads:

\[
\langle \psi^+_k q | R_{kq\sigma} \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle = \langle \psi^+_k q | R_{kq\sigma} \left( 1 \right) \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle = \\
= \sum_{pr\sigma} \left( 1 - \langle A^+_{pr\sigma} | X_{pr\sigma} \rangle \right) \left( 1 - \langle B^+_{pr\sigma} | X_{pr\sigma} \rangle \right) \langle \psi^+_k q \rangle \langle R_{kq\sigma} | X_{pr\sigma} \rangle \langle X_{pr\sigma} | \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle + \\
+ \langle \psi^+_k q \rangle \langle R_{kq\sigma} | \psi^+_k q \rangle \langle \psi^+_k q \rangle \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle 
\]

(39)

The last equality follows since in the first term the matrix elements \( \langle X_{pr\sigma} | \left( I^+_k q + I^-_k q \right) | \psi^+_k q \rangle \) vanish by orthogonality condition, as we have shown when evaluating the off-diagonal matrix elements; in the second term the diagonal element \( \langle \psi^+_k q | R_{kq\sigma} | \psi^+_k q \rangle = 0 \), due to antihermiticity of \( R_{kq\sigma} \); and, in the last contribution, the perturbation diagonalization yields \( \langle \psi^+_k q | \left( I^+_k q + I^-_k q \right) | \psi^-_k q \rangle = 0 \).

Analogously, it is immediate to demonstrate that the second term of the commutator also vanishes, leading to:

\[
\langle \psi^+_k q | [R_{kq\sigma}, \left( I^+_k q + I^-_k q \right)] | \psi^+_k q \rangle = 0 
\]

(40)

Using the same arguments, one can easily show that also the other diagonal element vanishes: \( \langle \psi^-_k q | [R_{kq\sigma}, \left( I^+_k q + I^-_k q \right)] | \psi^-_k q \rangle = 0 \).
In conclusion, all contributions of the "dangerous" perturbation terms to the second-order transformed Hamiltonian have vanishing matrix elements inside the degenerate subspace, if one avails oneself of the freedom one has to complete the definition of generator $R$ and chooses that its restriction to the degenerate subspace is diagonal in the same basis of eigenvectors of the perturbation, there. This conclusion is clearly not dependent on the size of the degenerate eigensubspace. In our example, the choice is: $\langle \psi_{kq\sigma}^+ | R_{kq\sigma} | \psi_{kq\sigma}^- \rangle = 0$, where $|\psi_{kq\sigma}^\pm\rangle$ diagonalize the perturbation restriction to the two-dimensional degenerate subspace. Therefore, the eigenvalues of the complete Hamiltonian in the degenerate subspace only have contributions from the "innocuous" commutator $[R_1, I_1]$. Using Eq.23, we can indeed write:

$$\langle \psi_{kq\sigma}^\alpha | H^{(2)} | \psi_{kq\sigma}^\beta \rangle = \langle \psi_{kq\sigma}^\alpha | \left( H_0 + \frac{1}{2} [R_1, I_1] + \frac{1}{2\sqrt{N}} [R_{kq\sigma}, (I_{kq\sigma}^+ + I_{kq\sigma}^-)] \right) | \psi_{kq\sigma}^\beta \rangle =$$

$$= \langle \psi_{kq\sigma}^\alpha | \left( H_0 + \frac{1}{2} [R_1, I_1] \right) | \psi_{kq\sigma}^\beta \rangle = \mathcal{E}^A \delta_{\alpha\beta} + \frac{1}{2} \langle \psi_{kq\sigma}^\alpha | [R_1, I_1] | \psi_{kq\sigma}^\beta \rangle \quad (\alpha, \beta = \pm) \quad (41)$$

IV. DIAGONALIZATION OF $H^{(2)}$ IN THE DEGENERATE $|\psi_{kq\sigma}^\pm\rangle$ SUBSPACE.

At this stage, to use the "Fröhlich"-transformed Hamiltonian in the presence of degenerate states of $H_0$ it would seem necessary to actually determine the eigenvectors which diagonalize the perturbation inside each degenerate subspace. We will now show that this is not the case: in fact, that one can work with the transformed Hamiltonian only knowing an eigenvector basis of the unperturbed Hamiltonian $H_0$, as is usually the case.

To show this, we will explicitly diagonalize $H^{(2)}$ in the degenerate subspace, spanned by $|\psi_{kq\sigma}^\pm\rangle$ in our example. Its matrix elements are:

$$\langle \psi_{kq\sigma}^+ | H^{(2)} | \psi_{kq\sigma}^+ \rangle =$$

$$= \mathcal{E}_{kq\sigma}^A + \frac{1}{4} \left\{ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle + \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right\} - \frac{\lambda^2}{2} Im \langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \quad (42)$$

$$\langle \psi_{kq\sigma}^- | H^{(2)} | \psi_{kq\sigma}^- \rangle =$$

$$= \mathcal{E}_{kq\sigma}^A + \frac{1}{4} \left\{ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle + \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right\} + \frac{\lambda^2}{2} Im \langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \quad (43)$$

$$\langle \psi_{kq\sigma}^+ | H^{(2)} | \psi_{kq\sigma}^- \rangle =$$

$$= \mathcal{E}_{kq\sigma}^A + \frac{1}{4} \left\{ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle + \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right\} + \frac{\lambda^2}{2} Im \langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \quad (44)$$
$$\langle \psi_{kq\sigma}^- | H^{(2)} | \psi_{kq\sigma}^+ \rangle =$$

$$= \frac{1}{4} \left[ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle - \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right] + \frac{i\lambda'}{2} \text{Re} \langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$$

(44)

$$\langle \psi_{kq\sigma}^- | H^{(2)} | \psi_{kq\sigma}^+ \rangle =$$

$$= \frac{1}{4} \left[ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle - \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right] - \frac{i\lambda'}{2} \text{Re} \langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$$

(45)

Now, the terms in $[R_1, I_1]$ can not transform $|A_{kq\sigma}^+ \rangle$ into $|B_{kq\sigma}^+ \rangle$ because neither $R_1$ nor $I_1$ change the number of $|q\rangle$ phonons, this being instead the effect of $[R_{kq\sigma}, (I_{kq\sigma}^+ + I_{kq\sigma}^-)]$. Therefore, off-diagonal matrix elements $\langle A_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$ vanish. Conversely, the diagonal elements $\langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle$, $\langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$ do not vanish because $[R_1, I_1]$ includes diagonal terms like $b_p^\dagger b_p (1 - n_{r-p,\sigma}) n_{r\sigma} (1 - \delta_{pq}\delta_{rk})$ which do not necessarily vanish in the $|A_{kq\sigma}^+ \rangle$, $|B_{kq\sigma}^+ \rangle$ states. It follows that:

$$\langle \psi_{kq\sigma}^+ | H^{(2)} | \psi_{kq\sigma}^- \rangle = \langle \psi_{kq\sigma}^- | H^{(2)} | \psi_{kq\sigma}^- \rangle =$$

$$= \mathcal{E}_{kq\sigma}^A + \frac{1}{4} \left\{ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle + \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right\}$$

(46)

$$\langle \psi_{kq\sigma}^+ | H^{(2)} | \psi_{kq\sigma}^+ \rangle = \langle \psi_{kq\sigma}^- | H^{(2)} | \psi_{kq\sigma}^- \rangle =$$

$$= \frac{1}{4} \left[ \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle - \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle \right]$$

(47)

Thus, diagonalization of $H^{(2)}$ in the degenerate subspace leads to the following secular equation:

$$\det \begin{bmatrix} \mathcal{E}_{kq\sigma}^A + (A + B) - \lambda & (A - B) \\ (A - B) & \mathcal{E}_{kq\sigma}^A + (A + B) - \lambda \end{bmatrix} = 0$$

(48)

where

$$A \equiv \frac{1}{4} \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle , \quad B \equiv \frac{1}{4} \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$$

(49)

Therefore, the eigenvalues are:

$$\eta_A = \mathcal{E}_{kq\sigma}^A + 2A = \mathcal{E}_{kq\sigma}^A + \frac{1}{2} \langle A_{kq\sigma}^+ | [R_1, I_1] | A_{kq\sigma}^+ \rangle$$

$$\eta_B = \mathcal{E}_{kq\sigma}^A + 2B = \mathcal{E}_{kq\sigma}^A + \frac{1}{2} \langle B_{kq\sigma}^+ | [R_1, I_1] | B_{kq\sigma}^+ \rangle$$

(50)

The eigenstate $|\Phi_{kq\sigma}^\pm \rangle = a|\psi_{kq\sigma}^+ \rangle + b|\psi_{kq\sigma}^- \rangle$ has coefficients set by

$$\left[ \mathcal{E}_{kq\sigma}^A + (A + B) - \eta_{A,B} \right] a + (A - B) b = 0$$

(51)
or, $a = \pm b$ yielding $a = 1/\sqrt{2}$ corresponding to the normalized eigenvectors

$$\langle \Phi_{kq}\rangle \mid = \mid \Phi_{kq}\rangle \rangle = \mid A_{kq}\rangle \rangle$$

$$\langle \Phi_{kq}\rangle \rangle = \mid \Phi_{kq}\rangle \rangle$$

Our final result is:

$$\langle A_{kq} \mid H \mid A_{kq} \rangle = \langle B_{kq} \mid H \mid B_{kq} \rangle$$

The conclusion is that, in evaluating the spectrum of $H^{(2)}$ one can use the eigenstates of $H_0$ and simply ignore the "dangerous terms" $\mid R_{kq}, I_{kq} \rangle \rangle$, because only the "innocuous terms" $\mid R_{kq}, I_{kq} \rangle \rangle$ will modify the non-interacting spectrum.

V. CONCLUSIONS.

We have explicitly shown by working out in detail an example based on the Su-Schrieffer-Heeger Hamiltonian, how to complete the definition of the transformation generator when degenerate eigenstates of the non-perturbed Hamiltonian are present. Namely, these states, which would apparently cause a divergence in the effective pairing between fermions and bosons generated by transforming "à la Fröhlich" an interacting Hamiltonian, actually contribute vanishing matrix elements to the effective Hamiltonian matrix. The matrix elements of the latter can therefore be evaluated by using the eigenstates of the basic $H_0$, and ignoring the "dangerous terms". The conclusions do not depend on the size of the degenerate eigensubspace, as our argumentation can be straightforwardly generalized for the case of more than two degenerate states. Notice that, even if we have explicitated the eigenstates $\mid X_{kq} \rangle$ as product of separate fermionic and bosonic eigenfunctions, actually our reasoning holds for any structure of $\mid X_{kq} \rangle$. For non-factorized eigenstates, the numerical coefficients in the formulae above would be different, but the conclusion would still be the same. The procedure has been successfully applied also to other complex fermion-boson Hamiltonians, e.g. the one for interacting ferromagnetic spin waves and electrons considered in$^3$. Thus, at low temperatures renormalized excitation energies of the real interacting bosons can be
described by the eigenvalues of the effective second-order boson Hamiltonian, obtained by averaging over the fermion ground state wavefunction.

As a final observation, notice that when we isolate the dangerous term in the perturbation (Eq.18) it comes weighed by a factor $1/\sqrt{N}$. So in the infinite-lattice limit this part might be assumed to give in any case an irrelevant contribution. In recent times, a great deal of work has been done on finite or low-dimensional systems (mesoscopic, quantum dots etc.) where such a justification for neglecting the dangerous terms would not hold. Our demonstration, however, holds even for a single-particle system, because it concerns the matrix elements, irrespective of the kind of system where they are evaluated.

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