

# WANNIER FORMULATION OF THE LEE–LOW–PINES TRANSFORMATION

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**Abstract.** A 2nd quantized version of the Lee–Low–Pines transformation (LLPT) is presented in a one-band Wannier base which offers itself to multiparticle applications. It is first applied to a translationally invariant coupled electron–phonon system. Later it is generalized to arbitrary Abelian Hamiltonians. In the one-electron case the transformation achieves diagonalization of the respective Hamiltonians with regard to the electronic subspace. This is even achieved in the case when the electron–phonon interaction is nonlinear. Also, in a multiparticle case the LLPT can be fully performed. An illustrative example is given. For future application it may further be noted that the multiparticle LLPT establishes effective electron–electron interaction terms of non-Fröhlich type, which may also have an impact onto superconductivity.

**Key words:** electron–phonon systems, diagonalization operator.

## 1. TRANSLATIONALLY INVARIANT (CYCLIC) SYSTEMS

We introduce a unitary multiparticle operator which in a one-particle case reduces to the LLP operator [1]. We limit the electronic Hilbert space to a one-band Wannier base  $c_m^\dagger |\text{vac}\rangle = |m\rangle$ . Then our multiparticle LLP operator reads:

$$U_{\text{LLP}} = \exp \left[ -\frac{2i\pi}{N} \sum_{m=1}^N m c_m^\dagger c_m \sum_{q=1}^N q b_q^\dagger b_q \right]. \tag{1}$$

In a one-particle case Expr. (1) may be written as

$$U_{\text{LLP}} = \sum_{m=1}^N c_m^\dagger c_m (R_1(Q))^m, \quad (c_m c_n = 0), \tag{2}$$

where we have introduced the translation operators

$$R_r = R_1^r, \quad R_l = R_1(Q) \cdot R_1^{(cl)}, \quad R_l c_m = c_{m+1} R_l,$$

$$R_1(Q)Q_q = e^{i\frac{2\pi}{N}q}Q_qR_1(Q). \quad (3)$$

The electron-phonon model is represented by the Hamiltonian

$$H = H_{ph} + W, \quad H_{ph} = \frac{1}{2} \sum_{\gamma=1}^N (P_{\gamma}^{\dagger} P_{\gamma} + \Omega_{\gamma}^2 Q_{\gamma}^{\dagger} Q_{\gamma}), \quad W = \sum_{m,n=1}^N c_m^{\dagger} c_n A_{mn}(Q). \quad (4)$$

Thus the transformed Hamiltonian reads

$$T_{LLP} : H = U_{LLP}^{\dagger} H U_{LLP} = H_{ph} + \sum_{m=1}^N \sum_{r=1}^N c_m^{\dagger} c_{m+r} A_{N,r}(Q) R_1^r(Q) + \text{multiparticle terms.} \quad (5)$$

In order to complete the diagonalization of electronic one-particle terms we introduce the Bloch-transformed electron operators  $c_k$  by

$$c_m = N^{-1/2} \sum_{k=1}^N \exp\left[\frac{2i\pi}{N}mk\right] c_k. \quad (6)$$

By means of (6) the transformed Hamiltonian reads

$$T_{LLP} : H = H_{ph} + \sum_{k=1}^N c_k^{\dagger} c_k \sum_{r=1}^N \exp\left[\frac{2i\pi}{N}kr\right] A_{N,r}(Q) R_1^r(Q) + \text{multiparticle terms,} \quad (7)$$

which is diagonal in the electronic subspace.

## 2. GENERAL ABELIAN SYSTEMS

Due to a lemma given in the book of Lomont [2], each Abelian group may be divided into a product of cyclic subgroups. Therefore Expr. (1) may be written as a product of unitary operators, each of them referring to a single cyclic subspace. The multiparticle LLP operator thus reads

$$U_{LLP} = \prod_{\lambda=1}^{\Lambda} U_{\lambda},$$

$$U_{\lambda} = \exp \left[ -2\pi i \sum_{m_1=1}^{N_1} \cdots \sum_{m_{\Lambda}=1}^{N_{\Lambda}} c_{m_1, \dots, m_{\Lambda}}^{\dagger} c_{m_1, \dots, m_{\Lambda}} \sum_{q_1=1}^{N_1} \cdots \right. \quad (8)$$

$$\left. \cdots \sum_{q_{\Lambda}=1}^{N_{\Lambda}} \frac{m_{\lambda} q_{\lambda}}{N_{\lambda}} b_{q_1, \dots, q_{\Lambda}}^{\dagger} b_{q_1, \dots, q_{\Lambda}} \right].$$

We note that the single set of the indices  $\{m\}$  is now transmuted into a multiple set  $\{m_1\}, \dots, \{m_{\Lambda}\}$  if there are  $\Lambda$  cyclic subgroups. The same holds for the phonon indices  $\{q\}$ .

### 3. EXAMPLE: N-SITE-FRÖHLICH PROBLEM WITH SPINFLIPS

As an example we treat an extended 2nd quantized form of the Fröhlich Hamiltonian [3] by adding spin coordinates to the electronic operators (see also [4]). Therefore the system is no longer mono-cyclic but still Abelian:

$$\begin{aligned}
 H_F = & \sum_{q=1}^N \hbar\Omega(q)b_q^\dagger b_q + \sum_{m=1}^N \sum_{d=0}^{N-1} \sum_{\sigma=\uparrow,\downarrow} [T^{(d)}c_{m,\sigma}^\dagger c_{m+d,\sigma} + \text{h.c.}] + \\
 & + \sum_{m=1}^N \sum_{d=0}^{N-1} \sum_{\rho \neq \sigma=\uparrow,\downarrow} [T_{sf}^{(d)}c_{m,\rho}^\dagger c_{m+d,\sigma} + \text{h.c.}] + \\
 & + \sum_{q=1}^N \sum_{m=1}^N \sum_{d=0}^{N-1} \sum_{\sigma=\uparrow,\downarrow} [D_q^{(d)} \exp\left[\frac{2i\pi}{N}qm\right] (b_q + b_{-q}^\dagger) c_{m,\sigma}^\dagger c_{m+d,\sigma} + \text{h.c.}]. \quad (9)
 \end{aligned}$$

We allow spinflip dynamics in the transfer terms and introduce the spinflip transfer energy  $T_{sf}^{(d)}$  which is usually much smaller than the transfer energy  $T^{(d)}$  without spinflips. Since the phonon modes are independent of the spin, Expr. (8) in this particular case assumes the form

$$U_{LLP} = \exp\left[-\frac{2i\pi}{N} \sum_{m=1}^N \sum_{\sigma=\uparrow,\downarrow} m c_{m,\sigma}^\dagger c_{m,\sigma} \sum_{q=1}^N q b_q^\dagger b_q\right]. \quad (10)$$

The transformed fundamental operators of the problem are given by

$$T_{LLP} : c_{m,\sigma} = c_{m,\sigma} \cdot \exp\left[-\frac{2i\pi}{N} m \sum_{k=1}^N k b_k^\dagger b_k\right], \quad (11)$$

$$T_{LLP} : b_k = b_k \cdot \exp\left[-\frac{2i\pi}{N} km\right].$$

Again we introduce the Bloch-transformed electronic operators  $c_{k,p_\sigma}$ :

$$c_{m,\sigma} = (2N)^{-1/2} \sum_{k=1}^N \sum_{p_\sigma=1}^2 \exp\left[\frac{2i\pi}{N}mk\right] \exp\left[i\pi\sigma p_\sigma\right] c_{k,p_\sigma}, \quad (12)$$

where in the exponent on the right-hand side  $\sigma$  is represented by integers 1, 2, such that  $\sigma = 1 \hat{=} \text{spin } \uparrow$  and  $\sigma = 2 \hat{=} \text{spin } \downarrow$ , ( $\sigma = 3 \hat{=} \sigma = 1$ ).

In the transformed picture the two spin indices are denoted by  $p_\sigma = \pm 1$ , which alludes to the physical meaning of a "spin-parity". We find the transformed Hamiltonian

$$T_{LLP} : H_F = \sum_{q=1}^N \hbar\Omega(q)b_q^\dagger b_q +$$

$$\begin{aligned}
& + \sum_{k=1}^N \sum_{d=0}^{N-1} \sum_{p_\sigma=1}^2 \left[ T^{(d)} \exp \left[ \frac{2i\pi}{N} d \left( k - \sum_{q=1}^N q b_q^\dagger b_q \right) \right] c_{k,p_\sigma}^\dagger c_{k,p_\sigma} + \text{h.c.} \right] + \\
& + \sum_{k=1}^N \sum_{d=0}^{N-1} \sum_{p_\sigma=1}^2 \left[ T_{sf}^{(d)} \exp \left[ \frac{2i\pi}{N} d \left( k - \sum_{q=1}^N q b_q^\dagger b_q \right) \right] e^{i\pi p_\sigma} c_{k,p_\sigma}^\dagger c_{k,p_\sigma} + \right. \\
& \left. + \text{h.c.} \right] + \sum_{d=0}^{N-1} \sum_{q=1}^N \sum_{k=1}^N \sum_{p_\sigma=1}^2 \left[ D_q^{(d)} \exp \left[ \frac{2i\pi}{N} d \left( k - \sum_{q=1}^N q b_q^\dagger b_q \right) \right] \times \right. \\
& \left. \times \left( b_q + b_{-q}^\dagger \right) c_{k,p_\sigma}^\dagger c_{k,p_\sigma} + \text{h.c.} \right] + \text{multiparticle terms,} \quad (13)
\end{aligned}$$

which indeed is of a diagonal form in one-electron terms.

#### 4. RESULTS AND CONCLUSIONS

- A 2nd quantized LLP-type unitary operator in the exponential form is introduced.
- It achieves diagonalization of one-electron terms in Abelian electron-phonon systems; this is true even for nonlinear electron-phonon coupling.
- As an illustrative example its application to a generalized Fröhlich Hamiltonian with spinflips is given, including the transformed fundamental operators.
- Its applications to multiparticle systems are possible due to its exponential form. The concrete calculation of multiparticle terms for the presented example as well as for other systems is straightforward and supposed to be examined in future works.

#### REFERENCES

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## LEE-LOW'-PINESI TEISENDUSE WANNIER' FORMULATSIION

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On esitatud Lee-Low'-Pinesi teisenduse sekundaarkvantimise versioon ühetsoonilisel Wannier' baasil ja vaadeldud selle mitmeosakeselisi rakendusi. Esmalt on teisendust rakendatud translatsioonivariantsele elektron-foonon-seosega süsteemile. Seejärel on seda üldistatud meelevaldsete Abeli hamiltoniaanide tarvis. Üheelektronilisel juhul diagonaliseerib see teisendus vastava hamiltoniaani elektronide alamruumis. See on võimalik isegi mittelineaarse elektron-foonon-interaktsiooni korral. Ka mitmeosakeselisel juhul on vaadeldav teisendus täielikult teostatav. Sel puhul määrab teisendus efektiivsed elektron-elektron-interaktsiooni liikmed, mis võivad olla rakendatavad ülijuhtivuses.

## ФОРМУЛИРОВКА ВАНЬЕ-ПРЕОБРАЗОВАНИЯ ЛИ-ЛОУ-ПАЙНСА

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Представлена вторично-квантованная версия преобразования Ли-Лоу-Пайнса (ПЛЛП) на однозонном базисе Ванье и рассмотрены ее многочастичные применения. Сначала она применена для трансляционно-инвариантной системы с электрон-фононной связью, затем обобщена для произвольных абелевых гамильтонианов. В одноэлектронном случае это преобразование диагонализует соответствующий гамильтониан в электронном подпространстве. Это возможно даже при нелинейном электрон-фононном взаимодействии. В многочастичном случае ПЛЛП также полностью осуществимо. Многочастичное ПЛЛП определяет эффективные члены электрон-электронного взаимодействия, которые могут использоваться в теории сверхпроводимости.