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Peierls–Fröhlich Instability and Kohn Anomaly

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A mathematical basis is given to the Peierls–Fröhlich instability and the Kohn anomaly. The techniques and ideas are based on the recently developed mathematical theory of quantum fluctuations and response theory. We prove that there exists a unique resonant one-mode interaction between electrons and phonons which is responsible for the Peierls–Fröhlich instability and the phase transition in the Mattis–Langer model. We prove also that the softening of this phonon mode at the critical temperature (Kohn anomaly) is a consequence of the critical slowing down of the dynamics of the lattice distortion fluctuations. It is the result of the linear dependence of two fluctuation operators corresponding to the frozen charge density wave and the distortion order parameter.

KEY WORDS: Electron–phonon systems; quantum fluctuations; Peierls instability; Kohn anomaly.

1. INTRODUCTION

The physics of low-dimensional systems with electron–phonon interaction is quite nontrivial. The Peierls–Fröhlich (PF) instability[1,2] together with the Kohn anomaly[3] are probably the most important phenomena predicted and then discovered in the physics of quasi-one-dimensional conductors. For a review see, e.g., refs. 4 and 5.

Peierls[1] argued that a one-dimensional fermion system living on the periodic soft lattice $\mathbb{Z}_a$ with period a becomes unstable if the Fermi surface $\pm k_F$ coincides with $\pm\pi/2a$ (half-filled band). That is, lattice distortion which doubles periodicity to $\mathbb{Z}_{2a}$ creates a gap in the electron spectrum. Then the energy of the half-filled band is lowered because the energies of

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the occupied levels are lowered, whereas the energies of the unoccupied ones are raised.

This argument was for zero temperature and it did not take into account the cost of the lattice energy required to create the lattice distortion. It is Fröhlich[2] who showed that the Peierls instability persists if the (classical) lattice restoring forces are weak enough and the temperature is sufficiently low.

For the classical lattice the Peierls–Fröhlich instability can be settled as the variational problem of finding the minimum of the thermodynamic functional for the electron–lattice system. In this form the Peierls–Fröhlich problem has attracted the attention of mathematical physicists, who have discovered its relation to the problems of "integrable systems."[6-9] The next important observation was made by Kohn[3]: he showed that, as a consequence of the lattice undergoing a Fröhlich distortion, the lattice vibrations with the wavevectors close to $\pm 2k_F$ can be significantly reduced. This softening of the phonon frequency is known now as the Kohn anomaly.

The quantum statistical mechanics treatment of the Peierls–Fröhlich instability (but not the Kohn anomaly) was initiated by Mattis and Langer,[10] who argued that the one-mode model should be exactly solvable. Rigorous work was done in ref. 11 by the approximating Hamiltonian method for the free-energy density. This method made possible the rigorous analysis of the Mattis–Langer model for electrons interacting via a Bardeen–Cooper–Schriefer potential.[12] This analysis was important in connection with the idea[13] that the modification of the electron spectrum caused by the Peierls–Fröhlich instability could give an essential increase in the critical temperature for the superconductor phase transitions in the electron subsystem.

In the present paper we consider the quantum nature of the Peierls–Fröhlich instability and Kohn anomaly. The aim of the paper is twofold: (1) to give a rigorous motivation for the one-mode Mattis–Langer Hamiltonian[10] and to extend ref. 11 to the level of the Gibbs states; and (2) to give a mathematical treatment of the Kohn anomaly. In both points we essentially use the recent theory of quantum fluctuation operators and the response theory.[14-16]

The paper is organized as follows. In Section 2 the nature of the resonant mode $2k_F$ is clarified on the basis of the response theory.[16] The equilibrium states are described in Section 3 as a solution of the limiting Gibbs state correlation inequalities.[17] The phase transition in the model breaks the $\mathbb{Z}_a$ lattice symmetry down to the $\mathbb{Z}_{2a}$ one and gives two conjugate order parameters: the frozen charge-density wave and the lattice distortion; see Section 4. In Section 5 we show that the Kohn anomaly softening of the phonon mode is a direct consequence of the critical slowing down of the dynamics of the distortion quantum fluctuations. The mathematical mechanism yields a linear correlation of the fluctuation operators corresponding to the above order parameters.

2. PEIERLS–FRÖHLICH INSTABILITY

In refs. 1 and 2 it is argued on the basis of perturbation theory that the PF instability is an instability of the electronic system against any arbitrary small deformations of the one-dimensional lattice with the wavevector $2k_F$ (k_F = Fermi momentum). Here we apply recent results on the exactness of the linear response theory[16] in order to give a rigorous proof of this phenomenon. In other words, we prove that the perturbation arguments of refs. 1 and 2 (see also refs. 4 and 5) can be turned into exact arguments.

Now the one-dimensional electronic system is a system of fermions enclosed in the lattice interval $\Lambda = [-la, -(l-1)a, ..., la]$ with one-particle wave functions the elements in $l^2(\Lambda) = \mathbb{C}^{2l+1}$, a being the lattice distance. The one-particle kinetic energy operator is then

$$h_\Lambda = -\tfrac{1}{2}\varepsilon_0 \Delta - \varepsilon_0, \qquad \varepsilon_0 > 0$$

where

$$(\Delta f)(x) = f(x+a) - 2f(x) + f(x-a)$$

with periodic boundary conditions. Let

$$\varepsilon(k) = -\varepsilon_0 \cos ka - \mu$$

Then h_Λ has as eigenfunctions $\varphi_k(x) = (1/\sqrt{V})\, e^{ikx}$, where $V = 2l+1$, the volume of Λ, with eigenvalues $\varepsilon(k)$ and

$$k \in \Lambda^* = \{n\pi/la;\, n = -l, ..., l\}$$

The free electron Hamiltonian $T_\Lambda = d\Gamma(h_\Lambda)$ is then

$$T_\Lambda = \sum_{k \in \Lambda^*} \varepsilon(k)\, a_k^* a_k \tag{1}$$

where

$$a_k^* = \frac{1}{\sqrt{V}} \sum_{x \in \Lambda} e^{ikx} a^*(x)$$

satisfying the anticommutation relations

$$\{a(x), a^*(y)\} = \delta_{x,y}$$
$$\{a(x), a(y)\} = 0$$

The unique equilibrium state $\omega_\beta^{0,\Lambda}$ at $\beta = 1/kT$ and chemical potential μ for T_Λ is known to be the quasi-free state[18] with the following two-point function:

$$\omega_{\beta,\mu}^{0,\Lambda}(a_k^* a_{k'}) = \delta_{k,k'} n_k(\beta, \mu) \tag{2}$$

where

$$n_k(\beta, \mu) = \frac{1}{1 + e^{\beta\varepsilon(k)}}$$

Remark that the thermodynamic limit (i.e., $\Lambda \to \mathbb{Z}$) of this equilibrium state does exist as the well-known electron state $\omega_{\beta,\mu}^0$, where

$$\omega_{\beta,\mu}^0(a_k^* a_{k'}) = \delta(k - k')\, n_k(\beta, \mu) \tag{3}$$

Now we compute the total response on the electron system due to a perturbation of the fluctuation type. Thermodynamically the free electron Hamiltonian (1) is an extensive quantity of the order of the volume V. The perturbation will be of the order $V^{1/2}$, and hence very small. It does not change the thermodynamics of the system (i.e., it does not alter the bulk properties of the system), but the perturbation will have an effect on the fluctuations around the equilibrium.

We take the following perturbation:

$$P_\Lambda(q) = \frac{1}{\sqrt{V}} \sum_{k \in \Lambda^*} (a_k^* a_{k+q} + a_{k+q}^* a_k) \tag{4}$$

Clearly $P_\Lambda(q)$ is a density fluctuation of wavelength q. Due to the fact that the free fermion state (3) is exponentially clustering, it follows from ref. 16 that, for all finite temperatures, the equilibrium state of the perturbed system $T_\Lambda + P_\Lambda(q)$ exists and can be expressed explicitly in terms of the unperturbed state. The bulk properties of this state coincide with those of the unperturbed state, but the perturbation is effective and nontrivial on the level of the fluctuation observables. Denote this state by $\omega_{\beta,\mu}^{P_\Lambda}$; then by Theorem 4.1 of ref. 16 one has the following formula, expressing the expectation value of the perturbation in the perturbed state, i.e., the isothermal susceptibility:

$$\chi(q, \beta) = \lim_{\lambda \to 0} \lim_{\Lambda} \frac{\omega_{\beta,\mu}^{\lambda P_\Lambda}(P_\Lambda(q)) - \omega_{\beta,\mu}^0(P_\Lambda(q))}{\lambda}$$

$$= \lim_{\Lambda} [\omega_{\beta,\mu}^{P_\Lambda}(P_\Lambda(q)) - \omega_{\beta,\mu}^0(P_\Lambda(q))]$$

$$= \lim_{\Lambda} (-\beta) \int_0^1 \int_0^1 ds\, \omega_{\beta,\mu}^0([e^{\beta s[T_\Lambda, \cdot]} P_\Lambda(q)]\, P_\Lambda(q)) \tag{5}$$

This is the total response against the perturbation (4).

Theorem 2.1. Let the Fermi level wavevector k_F be fixed by $\mu = -\varepsilon_0 \cos ak_F$; then the isothermal susceptibility $\chi(q, \beta)$ in (5) exists and has the following properties:

(i) If $\beta < \infty$, then $\chi(q, \beta)$ is finite for all q.

(ii) $\lim_{\beta \to \infty} \chi(q, \beta)$ is finite for $q \neq \pm 2k_F$ and is divergent for $q = \pm 2k_F$.

Proof. The proof of the existence and the first part of equality (5) is the most difficult part of the statement. Technically it reduces to the linear response proof of ref. 16 and we omit it here. The right-hand side of formula (5) can be computed explicitly, yielding

$$\chi(q, \beta) = \frac{a}{\pi} \int_{-\pi/a}^{\pi/a} dk \frac{1}{\varepsilon(k) - \varepsilon(k+q)} \left(\frac{1}{1 + e^{\beta\varepsilon(k+q)}} - \frac{1}{1 + e^{\beta\varepsilon(k)}} \right)$$

$$= \frac{a}{\pi} \int_{-\pi/a}^{\pi/a} dk \frac{e^{\beta(\varepsilon(k) - \varepsilon(k+q))} - 1}{\varepsilon(k) - \varepsilon(k+q)} \frac{e^{\beta\varepsilon(k+q)}}{(e^{\beta\varepsilon(k)} + 1)(e^{\beta\varepsilon(k+q)} + 1)}$$

Clearly for finite β, the singularity at $\varepsilon(k) = \varepsilon(k+q)$ is integrable. Now we look at the limit $\beta \to \infty$, i.e.,

$$\lim_{\beta \to \infty} \chi(q, \beta) = \lim_{\beta \to \infty} \frac{a}{2\pi\varepsilon_0} \int_{-\pi/a}^{\pi/a} \frac{-dk}{\sin(qa/2)\sin(k + q/2)a} \times [n_{k+q}(\beta, \mu) - n_k(\beta, \mu)]$$

By the definition of the Fermi level k_F one gets

$$\lim_{\beta \to \infty} \chi(q, \beta) = \frac{a}{2\pi\varepsilon_0 \sin(qa/2)} \left(-\int_{-k_F - q}^{-k_F} + \int_{k_F - q}^{k_F} \right) \frac{dk}{\sin(k + q/2)a}$$

Clearly

$$\lim_{q \to \pm 2k_F} \chi(q, \infty) = -\infty$$

but $|\chi(q, \infty)| < \infty$ if $q \neq \pm 2k_F$. ∎

We should note that as a consequence of ref. 16, we are able to compute the total dynamical response (Kubo formula). This gives a more canonical meaning to earlier derivations. In fact, we prove that the total dynamical response of the free electron system to a density fluctuation of momentum $q \neq 2k_F$ is finite for all temperatures, including $T=0$. However, if $q = \pm 2k_F$, the system is unstable under these perturbations in the ground state. This constitutes a rigorous setting of the well-known Peierls instability. For one of the first mathematical results in this direction see ref. 19, where a mean-field version is discussed.

Theorem 2.1 demonstrates the necessity of taking into account (as most important) the interaction between the electron system and the lattice fluctuations with the specially tuned value of the transfer momentum $q = \pm 2k_F$. In fact we shall study the Peierls–Fröhlich instability in the standard setting of the tight-binding model[4,5] in solid-state physics.

3. LIMIT GIBBS STATES OF THE TIGHT-BINDING MODEL

We consider the limit Gibbs states of the tight-binding model by means of the correlation inequalities for states on the algebra of observables.[17] It has some advantages for our aims in the sense that one can see better and use more efficiently the fact that the equilibrium states are determined solely by the commutator with the Hamiltonian.

Let us first formulate the model. Denote by $\mathscr{H} = l^2(\mathbb{Z}_a)$ and $\mathscr{A}_\pm = \mathscr{A}_\pm(\mathscr{H})$ the CAR $(+)$ and the CCR $(-)$ algebras, respectively, for the one-particle lattice space $\mathscr{H}$. We shall use the obvious notation $\mathscr{A}^\Lambda_\pm = \mathscr{A}_\pm(l^2(\Lambda))$. The algebra of observables for the infinitely extended system is

$$\mathscr{A} = \mathscr{A}_+ \otimes \mathscr{A}_-$$

and for the finite subsystems

$$\mathscr{A}_\Lambda = \mathscr{A}^\Lambda_+ \otimes \mathscr{A}^\Lambda_-$$

$\mathscr{A}_+$ contains the observables of the electrons and $\mathscr{A}_-$ the observables of the lattice vibrations. The latter are generated by the Fock boson creation and annihilation operators $b^\#(x)$, $x \in \mathbb{Z}_a$:

$$[b(x), b^\#(y)] = \delta_{x,y}; \qquad x, y \in \mathbb{Z}_a$$

$$[b(x), b(y)] = 0$$

The local Hamiltonian of the model is given by

$$H_\Lambda = T^0_\Lambda \otimes \mathbb{1} + \lambda B_\Lambda \otimes b_\Lambda + \bar{\lambda} B^*_\Lambda \otimes b^*_\Lambda + \mathbb{1} \otimes \Omega b^*_\Lambda b_\Lambda$$

$$+ \mathbb{1} \otimes \sum_{p \in \Lambda^* \setminus q} \Omega_p b^*_{p,\Lambda} b_{p,\Lambda} \tag{6}$$

Here the sum of the last two terms corresponds to the Hamiltonian H_Λ^{ph} of the harmonic lattice $\mathbb{Z}_a$.[10] Furthermore,

$$b_\Lambda = \frac{1}{\sqrt{V}} \sum_{x \in \Lambda} e^{iqx} b(x) \equiv b_{-q,\Lambda}$$

$$B_\Lambda = \frac{1}{\sqrt{V}} \sum_{k \in \Lambda^*} a_k^* a_{k+q}$$

with the special choice of $q = \pm 2k_F$ for which the PH instability was demonstrated in the previous section. Moreover, from now on we limit our discussion to the case of chemical potential $\mu = 0$, i.e., to the most unstable case of the *half-filled band*.[4,5] From above it follows that then q is chosen to be $q = \pi/a$.

The equilibrium state, denoted by ω_β, of the infinitely extended system defined by H_Λ in (6) is any solution of the set of correlation inequalities[17]

$$\lim_\Lambda \beta \omega_\beta(A^*[H_\Lambda, A]) \geqslant \omega_\beta(A^*A) \ln \frac{\omega_\rho(A^*A)}{\omega_\beta(AA^*)} \tag{7}$$

for all local $A \in \bigcup_\Lambda \mathscr{A}_\Lambda$.

Up to an isomorphism the CAR fermion algebra $\mathscr{A}_+$ has the following structure:

$$\mathscr{A}_+ = \bigotimes_{n \in \mathbb{Z}_a} \mathscr{A}_+(\mathbb{C}) = \bigotimes_{n \in \mathbb{Z}_{2a}} \mathscr{A}_+(\mathbb{C}^2)$$

Because of the last representation and since the operator b_Λ is $\mathbb{Z}_{2a}$-permutation invariant, due to the fact that $q = \pi/a$, one can use the result of ref. 20 and write the equilibrium state ω_β, the solution of (7), as an integral over equilibrium product states on the product algebra $\mathscr{A} = \mathscr{A}_+ \otimes \mathscr{A}_-$:

$$\omega_\beta = \int \mu(d\tau)\, \eta_{\beta,\tau} \otimes \tilde{\eta}_{\beta,\tau} \tag{8}$$

Here $\eta_{\beta,\tau}$ is a state on $\mathscr{A}_+$ and $\tilde{\eta}_{\beta,\tau}$ is an extremal $\mathbb{Z}_{2a}$-*permutation-invariant* state on $\mathscr{A}_-$, labeled by an index τ, which we drop for notational convenience. Furthermore, η_β and $\tilde{\eta}_\beta$ are limit states of the finite-volume states η_β^Λ and $\tilde{\eta}_\beta^\Lambda$, respectively, satisfying: (i)

$$\beta \eta_\beta^\Lambda(X^*[H_{+,\Lambda}^{\text{eff}}, X]) \geqslant \eta_\beta^\Lambda(X^*X) \ln \frac{\eta_\beta^\Lambda(X^*X)}{\eta_\beta^\Lambda(XX^*)}$$

for $X \in \mathscr{A}_+^{\Lambda}$ with effective electron Hamiltonian

$$H_{+,\Lambda}^{\text{eff}} = T_\Lambda^0 + \left(\gamma_\Lambda \lambda \sum_{k \in \Lambda^*} a_k^* a_{k+q} + \text{h.c.}\right)$$

$$\gamma_\Lambda = \tilde{\eta}_\beta^\Lambda \left(\frac{b_\Lambda}{\sqrt{V}}\right)$$

(ii) For $Y \in \mathscr{A}_-^{\Lambda}$:

$$\beta \tilde{\eta}_\beta^\Lambda(Y^*[H_{-,\Lambda}^{\text{eff}}, Y]) \geqslant \tilde{\eta}_\beta^\Lambda(Y^*Y) \ln \frac{\tilde{\eta}_\beta^\Lambda(Y^*Y)}{\tilde{\eta}_\beta^\Lambda(YY^*)}$$

with effective boson Hamiltonian

$$H_{-,\Lambda}^{\text{eff}} = \sum_{p \in \Lambda^*} \Omega_p b_{p,\Lambda}^* b_{p,\Lambda} + (\lambda \alpha_\Lambda b_\Lambda + \text{h.c.})$$

$$\alpha_\Lambda = \eta_\beta^\Lambda(B_\Lambda)$$

(iii) The time invariance of the equilibrium states yields for each finite volume Λ

$$\eta_\beta^\Lambda \otimes \tilde{\eta}_\beta^\Lambda([H_\Lambda^{\text{eff}}, b_\Lambda]) = 0$$

with

$$H_\Lambda^{\text{eff}} = H_{+,\Lambda}^{\text{eff}} \otimes \mathbb{1} + \mathbb{1} \otimes H_{-,\Lambda}^{\text{eff}} \tag{9}$$

An easy computation leads to the equation

$$\Omega \gamma_\Lambda = -\bar{\lambda} \frac{\bar{\alpha}_\Lambda}{\sqrt{V}} \tag{10}$$

Because of (i) and (ii), the states η_β^Λ and $\tilde{\eta}_\beta^\Lambda$ are Gibbs states for the effective Hamiltonians $H_{\pm,\Lambda}^{\text{eff}}$, and $\eta_\beta^\Lambda \otimes \tilde{\eta}_\beta^\Lambda$ for the H_Λ^{eff} in (9).

Furthermore, on all local observables,

$$\lim_\Lambda \eta_\beta^\Lambda \otimes \tilde{\eta}_\beta^\Lambda = \eta_\beta \otimes \tilde{\eta}_\beta$$

with the limit state in the support of the measure μ in (8).

Equation (10) relates the boson to the fermion states.

Because of pure symmetry arguments (the $\mathbb{Z}_{2a}$ permutation symmetry), the systems H_Λ of (6) and H_Λ^{eff} of (9) have the same equilibrium expectation values in the thermodynamic limit for all quasilocal observables.

Therefore the states η_β and $\tilde{\eta}_\beta$ are the equilibrium states for the effective Hamiltonians H_+^{eff} and H_-^{eff}, respectively. The major advantage of this is that all correlations for these states are computable. For this reason the model is sometimes called soluble.

In particular, because of the $\mathbb{Z}_{2a}$ symmetry

$$\gamma = \lim_{\Lambda} \gamma_\Lambda = \tilde{\eta}_\beta \left(\frac{b(0) - b(1)}{2} \right)$$

As $B_\Lambda/\sqrt{V}$ is a lattice average, the following thermodynamic limit exists:

$$\xi = \lim_{\Lambda} \frac{\alpha_\Lambda}{\sqrt{V}}$$

and Eq. (10) becomes

$$\Omega\gamma = -\bar{\lambda}\xi \tag{11}$$

This is a self-consistency equation relating the states η_β and $\tilde{\eta}_\beta$. The parameter τ in the expression can be taken as $\tau = \xi$ and then μ of (8) is any probability measure on $\mathbb{C}$.

Furthermore, as the free energy density functional on the set of states is an affine functional, we have that

$$f(\omega_\beta) = f(\eta_\beta \otimes \tilde{\eta}_\beta)$$

for all $\eta_\beta \otimes \tilde{\eta}_\beta$ in the support of μ in (8). We compute it in Section 6.

4. THE PEIERLS TRANSITION

From the analysis above, the system described by the tight-binding model behaves like a coupled fermion–boson model. If one looks at the effective Hamiltonian (9), it consists of the sum of the fermion part and the boson part. In this section we treat the phase transition, and the corresponding order parameters in both subsystems will be a *frozen charge-density wave* and a *lattice distortion* below the critical temperature.

The analysis of the self-consistency equation is done in the following lemma.

Lemma 4.1. Equation (11) can be expressed explicitly in terms of $\sigma = 2 \operatorname{Re} \lambda\gamma$:

$$\frac{\pi\Omega}{2\,|\lambda|^2}\sigma = \sigma \int_{-\pi/2a}^{\pi/2a} \frac{\operatorname{th}(\beta/2)\,E(k)}{E(k)}\,dk \tag{12}$$

where

$$E(k) = [\varepsilon(k)^2 + \sigma^2]^{1/2} \operatorname{sign} \varepsilon(k)$$

Proof. First we have to compute

$$\lim_{\Lambda} \eta_\beta^\Lambda \left(-\frac{\bar{\lambda}}{V} \sum_{k \in \Lambda^*} a_{k+q}^* a_k \right), \qquad q = \frac{\pi}{a}$$

where η_β^Λ is the equilibrium state for $H_{+,\Lambda}^{\text{eff}}$.

We diagonalize this Hamiltonian. Remark that we can write

$$H_{+,\Lambda}^{\text{eff}} = \sum_{k \in \tilde{\Lambda}^*} \{\varepsilon(k)\, a_k^* a_k + \varepsilon(k+q)\, a_{k+q}^* a_{k+q} + \sigma_\Lambda (a_k^* a_{k+q} + a_{k+q}^* a_k)\}$$

where

$$\tilde{\Lambda}^* = \left\{ \frac{n\pi}{la} \,\middle|\, n = -l+1, \ldots, 0 \right\}$$

and

$$\sigma_\Lambda = 2 \operatorname{Re} \lambda \gamma_\Lambda$$

Therefore it is sufficient to diagonalize a Hamiltonian of the type

$$\varepsilon_1 a_1^* a_1 + \varepsilon_2 a_2^* a_2 + \sigma (a_1^* a_2 + A_2^* a_1)$$

where the $a_i^\#$ are fermion creation and annihilation operators; clearly $a_1 = a_k$, $a_2 = a_{k+q}$.

This being a standard exercise, we give the result

$$H_{+,\Lambda}^{\text{eff}} = \sum_{k \in \Lambda^*} E(k)\, c_k^* c_k$$

where

$$E(k) = [\varepsilon(k)^2 + \sigma_\Lambda^2]^{1/2} \operatorname{sign} \varepsilon(k)$$

$$E(k+q) = -E(k)$$

and the $c_k^\#$ are again fermion operators defined by the Bogoliubov transformation:

$$a_1 = u c_1 + v c_2$$

$$a_2 = \bar{v} c_1 - \bar{u} c_2$$

$$uv = \frac{\sigma_\Lambda}{2E(k)}; \qquad |u|^2 + |v|^2 = 1$$

Using this form of the Hamiltonian, one gets straightforwardly that η^{Λ}_{β} is a quasi-free state with the two-point function

$$\eta^{\Lambda}_{\beta}(c^*_k c_{k'}) = \frac{\delta_{k,k'}}{1+e^{\beta E(k)}}$$

and

$$\begin{aligned}\Omega\sigma_{\Lambda} &= \Omega(\lambda\gamma_{\Lambda} + \bar{\lambda}\bar{\gamma}_{\Lambda}) \\ &= \frac{-|\lambda|^2}{V}\eta^{\Lambda}_{\beta}\left(\sum_{k\in\Lambda^*}(a^*_{k+q}a_k + a^*_k a_{k+q})\right) \\ &= \frac{-2|\lambda|^2}{V}\sigma_{\Lambda}\eta^{\Lambda}_{\beta}\left(\sum_{k\in\Lambda^*}\frac{c^*_k c_k}{E(k)}\right) \\ &= \frac{-2|\lambda|^2}{V}\sigma_{\Lambda}\sum_{k\in\Lambda^*}\frac{1}{E(k)}\frac{1}{1+e^{\beta E(k)}}\end{aligned}$$

In the limit $\Lambda \to \mathbb{Z}_a$

$$\Omega\sigma = -\frac{|\lambda|^2}{\pi}\sigma\int_{-\pi/a}^{\pi/a}\frac{dk}{E(k)(1+e^{\beta E(k)})} \qquad \blacksquare$$

Denote

$$\mathscr{G}(\beta,\sigma) = \int_{-\pi/a}^{\pi/a}\frac{dk}{E(k)(1+e^{\beta E(k)})}$$

and remark that $E(k) \geqslant 0$ for $k \in [\pi/2a, \pi/a]$. The main result of this section is:

Theorem 4.2. For λ large (Ω small) enough, there exists a critical temperature T_c such that:

(i) For $T \geqslant T_c$, the only solution of (12) is $\sigma = 0$.

(ii) For $T < T_c$, Eq. (12) has the solutions $\sigma = 0$ and $\sigma_0 \neq 0$, where σ_0 is given by

$$\mathscr{G}(\beta,\sigma_0) = \frac{\pi\Omega}{2|\lambda|^2}$$

In this case the spectrum $E(k)$ has a gap at $k = \pi/2a$, because for $\sigma_0 > 0$

$$\lim_{k\to\pm\pi/2a} E(k) = \pm 2\sigma_0$$

Proof. Clearly $\sigma=0$ is always a solution of (12). For $\sigma\neq 0$, (12) becomes

$$\frac{\pi\Omega}{2\,|\lambda|^2}=\mathscr{G}(\beta,\sigma)$$

If $\sigma\to 0$, then $\mathscr{G}(\beta,\sigma)\to\mathscr{G}(\beta,0)$, with the property that $\mathscr{G}(\beta,0)$ is divergent for large β (see proof of Theorem 2.1). Therefore, there is a T_c such that $\mathscr{G}(\beta_c,0)=\pi\Omega/2\,|\lambda|^2$.

On the other hand, $\mathscr{G}$ is a monotonically decreasing function of σ and $\mathscr{G}(\beta,\sigma)\to 0$ if $\sigma\to\infty$. Hence for $T<T_c$ there is $\sigma_0>0$ such that

$$\mathscr{G}(\beta,\sigma_0)=\frac{\pi\Omega}{2\,|\lambda|^2};\qquad \sigma_0=\sigma_0(T)$$

if λ is large enough.

The rest is clear from the definition of $E(k)$. ∎

Therefore the ground state of the system (6) is always unstable with respect to the creation of the gap in the electron spectrum,[1] while for $T>0$ the system is unstable (phase transition) only if $\pi\Omega/2\,|\lambda|^2<\max_\sigma\mathscr{G}(\beta,\sigma)$, i.e., if the lattice is soft for the frequency Ω or if the coupling constant λ is large.[2]

This settles the existence of the phase transition and the electronic spectrum of the model. Next one should analyze the phonon or boson properties of the model. Of course, here one has to look at the boson part of the Hamiltonian H_Λ^{eff}. The latter has $\mathbb{Z}_{2a}$-permutation symmetry but $\mathbb{Z}_a$-translation symmetry. In the following theorem we indicate the spontaneous breaking of this symmetry below the critical point, while the $\mathbb{Z}_{2a}$-permutation symmetry is not broken.

Theorem 4.3. At $T=T_c$ the lattice in the tight-binding model (6) changes the translation symmetry from $\mathbb{Z}_a$ (for $T\geqslant T_c$) to $\mathbb{Z}_{2a}$ (for $T<T_c$), i.e., a displacement phase transition at T_c.

Proof. By definition,

$$Q_x=\frac{1}{\sqrt{V}}\sum_{p\in\Lambda^*}e^{ipx}\left(\frac{1}{2\Omega_p}\right)^{1/2}(b_{p,\Lambda}+b^*_{-p,\Lambda})\tag{13}$$

is the operator of displacement at the site $x\in\Lambda$. Then by (10) and Theorem 4.2 one gets

$$\lim_{\Lambda}\tilde{\eta}_\beta^\Lambda(Q_x)=(-e^{iqx})\left(\frac{1}{2\Omega}\right)^{1/2}\frac{\sigma_0(T)}{|\lambda|}\tag{14}$$

This means that $\tilde{\eta}_{\beta\leqslant\beta_c}(Q_x)=0$ and $\tilde{\eta}_{\beta>\beta_c}(Q_x)=(-1)\,\tilde{\eta}_{\beta>\beta_c}(Q_{x+a})$. ∎

Corollary 4.4. For $T \geqslant T_c$ the state $\eta_\beta \otimes \tilde{\eta}_\beta$ corresponds to the tight-binding model (6) with $\lambda = 0$, i.e., it has the symmetry of the lattice $\mathbb{Z}_a$. For $T < T_c$ the state $\eta_\beta \otimes \tilde{\eta}_\beta$ reduces the symmetry to $\mathbb{Z}_{2a}$. ∎

In the low-temperature phase the electron subsystem: (1) has a gap in the spectrum, $\sigma_0 \neq 0$, splitting the conducting half-filled band into filled and empty ones (metal–insulator phase transition); and (2) the order parameter is $\lim_\Lambda \eta^\Lambda_{\beta > \beta_c}(\alpha_\Lambda/\sqrt{V}) \neq 0$ (frozen charge-density wave with the wave vector $q = \pi/a$).

The phonon subsystem manifests: (1) the Bose condensation of the phonon mode with $p = q$ $[\lim_\Lambda \tilde{\eta}^\Lambda_{\beta > \beta_c}(b_\Lambda/\sqrt{V}) \neq 0]$; (2) or, equivalently, deformation of the lattice from $\mathbb{Z}_a$ to $\mathbb{Z}_{2a}$ symmetry, i.e., a structural (displacement) phase transition.

As is known from ref. 21, the displacement phase transition in the lattice (Bose condensation of the q-phonon mode) is connected with a nontrivial algebra of fluctuations.

From the analysis in Section 3 [see (10) and (11)], it is clear that $\alpha_\Lambda = O(V^{1/2})$, such that one cannot expect a reasonable behavior for $H^{\text{eff}}_{-,\Lambda}$. Looking somewhat more closely at α_Λ, one remarks that it is not an intensive quantity, but a fluctuation. With this in mind we apply the theory of fluctuation operators[14,15] to examine the boson part of the model.

5. FLUCTUATION DYNAMICS

In order to make the mathematical scheme clear, first we introduce some generalities about the system of fluctuations carried by a microscopic dynamical system, here given by the triplet $(\mathcal{A}, \omega_\beta, \alpha_t)$, where $\mathcal{A}$ is the algebra of observables, ω_β is an equilibrium state of the system, and α_t is the dynamics defined by the model (6).

As in refs. 10 and 11, here we have a lattice ($\mathbb{Z}_a$) quantum system. It is proved in refs. 14 and 15 that one can give a mathematical meaning to the limit of operators

$$F_\delta(A) = \lim_V \frac{1}{V^{1/2+\delta}} \sum_{i \in \Lambda} (A_i - \langle A \rangle) \tag{15}$$

where A_i is a copy of a local observable A in $i \in \mathbb{Z}_a$. The limit is taken in the sense of a central limit theorem with respect to the equilibrium state ω_β or its local approximations $\eta^\Lambda_\beta \otimes \tilde{\eta}^\Lambda_\beta$,

$$\langle A \rangle = \omega_\beta(A) \qquad \text{or} \qquad \langle A \rangle = \eta^\Lambda_\beta \otimes \tilde{\eta}^\Lambda_\beta(A)$$

The parameter δ in formula (15) has to be chosen such that the limit exists and is not trivial. If $\delta = 0$, one has a normal fluctuation; if $\delta \neq 0$, one has a critical fluctuation; δ depends on the observable A, on the state, etc. In fact, one proves that the set $\mathscr{F} = \{F_\delta(A)\}$, where A belongs to some subspace $\mathscr{A}_0$ of $\mathscr{A}$, is a set of operators, called fluctuation operators. They generate a representation of the canonical commutation relations induced by a state $\tilde{\omega}$ defined by

$$\lim_{\Lambda} \left\langle \exp\left[i\lambda \frac{1}{V^{1/2+\delta}} \sum_{i\in\Lambda} (A_i - \langle A \rangle) \right] \right\rangle = \tilde{\omega}(e^{i\lambda F_\delta(A)}) \qquad (16)$$

for all $A \in \mathscr{A}_0$ if $\mathscr{A}_0$ is quasilocal. The fluctuation operators satisfy the commutation relations

$$[F_\delta(A), F_{\delta'}(B)] = \begin{cases} \omega_\beta([A, B]) & \text{if} \quad \delta + \delta' = 0 \\ 0 & \text{if} \quad \delta + \delta' > 0 \\ \text{undefined} & \text{if} \quad \delta + \delta' < 0 \end{cases}$$

These commutation relations indicate the classical and/or quantum character of the fluctuation operators algebra.

Clearly the fluctuation operators act on the GNS representation space $\tilde{\mathscr{H}}$, generated by all polynomials P of elements of $\mathscr{F}$, with scalar product

$$(P(\mathscr{F}), P(\mathscr{F})) = \tilde{\omega}(P(\mathscr{F})^* P(\mathscr{F}))$$

In particular, two fluctuation operators $F_\delta(A)$ and $F_{\delta'}(B)$ are equal if

$$\tilde{\omega}([F_\delta(A) - F_{\delta'}(B)]^* [F_\delta(A) - F_{\delta'}(B)]) = 0 \qquad (17)$$

Finally one can look at the dynamics $\tilde{\alpha}_t$ of the fluctuation operator algebra generated by the set $\mathscr{F}$. It is defined in the Heisenberg picture, induced by the microdynamics α_t, by the formula

$$\tilde{\alpha}_t F_\delta(A) = F_\delta(\alpha_t A) \qquad (18)$$

To conclude this overview of the picture developed in ref. 15, one can state that the microsystem carries a macrosystem of fluctuations determined by the fluctuation algebra of observables, the state $\tilde{\omega}$, and the dynamics $\tilde{\alpha}_t$. We apply all this to the tight-binding model (6).

As remarked before, the operators b_Λ and B_Λ in formula (6) are local fluctuations; we denote

$$b_\Lambda = F_0^\Lambda(b)$$

$$B_\Lambda = F_0^\Lambda(\rho)$$

i.e., b_Λ is the fluctuation of the local phonon operator $b(x)$, $x \in \mathbb{Z}_a$, and B_Λ is the fluctuation of the local electron density $\rho = a^*(x)\, a(x)$, $x \in \mathbb{Z}_a$, with the wavevector $q = \pi/a$.

Denote by ω_Λ the Gibbs state for the model Hamiltonian H_Λ of (6); we prove the following important property.

Lemma 5.1. The limit

$$\lim_\Lambda \omega_\Lambda\left(\left(b_\Lambda + \frac{\lambda}{\Omega} B_\Lambda\right)^* \left(b_\Lambda + \frac{\lambda}{\Omega} B_\Lambda\right)\right) \equiv \tilde{\omega}\left(F_0\left(b + \frac{\lambda}{\Omega}\rho\right)^* F_0\left(b + \frac{\lambda}{\Omega}\rho\right)\right)$$

is bounded by a constant for all temperatures.

Proof. Clearly

$$\begin{aligned}
&\omega_\Lambda\left(F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^* F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right) \\
&\quad = \frac{1}{2}\omega_\Lambda\left(\left[F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^*, F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right]\right) \\
&\quad\quad + \frac{1}{2}\omega_\Lambda\left(\left\{F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^*, F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right\}\right) \qquad (*)
\end{aligned}$$

where $\{\cdot, \cdot\}$ stands for the anticommutator.

In our case, because $q = \pi/\alpha$, we have $B_\Lambda^* = B_\Lambda$, hence

$$\left[F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^*, F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right] = -1$$

Now using the inequality of Harris,[22] one gets for $(*)$

$$\begin{aligned}
&\omega_\Lambda\left(F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^* F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right) \\
&\quad \leqslant -1 + \left(F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right), F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)\right)_\sim \\
&\quad\quad + \frac{\beta}{3}\omega_\Lambda\left(\left[\left[F_0^\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right), H_\Lambda\right], F_\Lambda\left(b + \frac{\lambda}{\Omega}\rho\right)^*\right]\right)
\end{aligned}$$

where $(\cdot, \cdot)_\sim$ is the Duhamel two-point function[23]

$$(A, B)_\sim = \frac{1}{\beta}\int_0^\beta d\tau \, \frac{\operatorname{tr} e^{-(\beta-\tau) H_\Lambda} A^* e^{-\tau H_\Lambda} B}{\operatorname{tr} e^{-\beta H_\Lambda}}$$

Remark that

$$\frac{d}{i\,dt} b_\Lambda = [H_\Lambda, b_\Lambda] = -\Omega b_\Lambda^* - \bar{\lambda} B_\Lambda^*$$

and compute

$$\begin{aligned}
&\left(F_0^\Lambda\left(b+\frac{\lambda}{\Omega}\rho\right), F_0^\Lambda\left(b+\frac{\lambda}{\Omega}\rho\right)\right)_\sim \\
&\quad = \frac{1}{\Omega^2}([b_\Lambda, H_\Lambda], [b_\Lambda, H_\Lambda])_\sim \\
&\quad = \frac{\beta}{\Omega^2}\omega_\Lambda([b_\Lambda, [H_\Lambda, b_\Lambda^*]]) \\
&\quad = \frac{\beta}{\Omega}
\end{aligned}$$

Furthermore, a straightforward computation yields

$$\begin{aligned}
&\omega_\Lambda\left(\left[\left[F_0^\Lambda\left(b+\frac{\lambda}{\Omega}\rho\right), H_\Lambda\right], F_\Lambda\left(b+\frac{\lambda}{\Omega}\rho\right)^*\right]\right) \\
&\quad = \Omega + \frac{\lambda}{\Omega}\frac{1}{V}\sum_k (2\varepsilon(k) - \varepsilon(k+q) - \varepsilon(k-q))\,\omega_\Lambda(a_{k-q}^* a_{k+q})
\end{aligned}$$

Using the fact that

$$|\omega_\Lambda(a_{k-q}^* a_{k+q})| \leqslant 1$$

one gets that this term is bounded by the constant

$$\Omega + \frac{\lambda}{2\pi\Omega}\int_{-\pi/a}^{\pi/a} dk\, 4\,|\varepsilon(k)|$$

All these bounds together prove the lemma. ∎

This lemma proves the existence of the fluctuation operator $F_0(b+(\lambda/\Omega)\rho)$, together with the fact that it is normal, i.e., $\delta = 0$. An important consequence of this fact is that

$$F_\delta\left(b+\frac{\lambda}{\Omega}\rho\right) = 0 \qquad \text{if} \quad \delta > 0 \tag{19}$$

This lemma does not prove that the fluctuations $F_0(b)$ and/or $F_0(\rho)$ exist. In fact, one can show that these fluctuation operators exist if $T > T_c$.

This is quite immediate from the fact that above T_c the limit state of ω_Λ is the product state $\eta_\beta \otimes \tilde{\eta}_\beta$ (see Sections 3 and 4). We have no proof of the existence of $F_\delta(b)$ and $F_{\delta'}(\rho)$ if $T < T_c$.

Now we treat the case $T \geqslant T_c$ in the spirit of the Ginzburg–Landau theory. It should be remarked that this is just one way to obtain a possible value of δ at the critical point. There are of course many other approaches possible, but we are convinced of the fact the critical value δ is independent of these approaches. However, we have no proof of this. Anyway, in order to prove our main result, we need only to prove that $\delta > 0$ at T_c.

For $T > T_c$ we have a proof which is already rather too involved to be presented here. To this end, we need the free energy density functional defined on the product states $\eta_\beta \otimes \tilde{\eta}_\beta$, determined by the parameter

$$\tau = \lim_\Lambda \frac{1}{V} \eta_\beta \left(\sum_k a_k^* a_{k+q} \right)$$

and with $\sigma = (2\lambda^2/\Omega)\tau$; if $T \geqslant T_c$, the value $\tau = 0$ is the solution of the self-consistency equation (11). A straightforward computation in the case of uniform density of the electron states in the band yields

$$f(T, \tau) = \frac{\lambda^2}{\Omega} \tau^2 - \frac{T}{2\varepsilon_0} \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon \ln 2 \operatorname{ch} \frac{\beta}{2} (\varepsilon^2 + \sigma^2)^{1/2} \tag{20}$$

and the variational problem of statistical mechanics gives

$$\inf_\tau f(T, \tau) = f(T, 0)$$

for all $T \geqslant T_c$, with T_c defined by

$$\frac{2\lambda^2}{\Omega \varepsilon_0} \int_0^{\varepsilon_0} d\varepsilon \frac{\operatorname{th} \beta_c \varepsilon}{\varepsilon} = 1$$

(see Theorem 4.2).

Clearly $\tau \to f(T, \tau)$ is analytic at $\tau = 0$ with

$$f'(T) = \left. \frac{\partial f(T, \tau)}{\partial \tau} \right|_{\tau = 0} = 0$$

$$f''(T) = \left. \frac{\partial^2 f(T, \tau)}{\partial \tau^2} \right|_{\tau = 0} \begin{cases} > 0 & \text{if} \quad T > T_c \\ = 0 & \text{if} \quad T = T_c \end{cases}$$

and

$$f^{(4)}(T_c) = \left. \frac{\partial^4 f(T_c, \tau)}{\partial \tau^4} \right|_{\tau = 0} > 0$$

We consider the electronic density fluctuation $F_\delta(\rho)$. Then

$$F_\delta^\Lambda(\rho)=\frac{1}{V^{1/2+\delta}}\sum_{x\in\Lambda}(a_x^*a_x-\eta_\beta(a_x^*a_x))\,e^{iqx}$$
$$=\frac{1}{V^{1/2+\delta}}\sum_k a_k^*a_{k+q}$$

Remark that

$$\eta_\beta\left(\frac{1}{V^{1/2+\delta}}\sum_k a_k^*a_{k+q}\right)=V^{1/2-\delta}\tau$$

We compute

$$\phi_\delta(t)=\lim_\Lambda\frac{\int_{\mathbb{R}}d\tau\exp[-\beta Vf(T,\tau)]\exp(itV^{1/2-\delta}\tau)}{\int_{\mathbb{R}}d\tau\exp[-\beta Vf(T,\tau)]} \tag{21}$$

i.e., we are looking for δ such that the random variable τ has a finite variance and a nontrivial distribution (see also ref. 24). Because the function $\tau\to f(T,\tau)$ reaches its minimum at the equilibrium value $\tau=0$, the equilibrium state yields the bulk contribution to the limit (21). This formula is reminiscent of the Ginzburg–Landau approach for critical phenomena.[25]

Lemma 5.2. For $T>T_c$, $\delta=0$ and

$$\phi_0(t)=\exp[-t^2/\beta f''(T)]$$

For $T=T_c$, $\delta=1/4$ and

$$\phi_{1/4}(t)=\frac{\int d\tau\exp[-\beta f^{(4)}(T_c)\,\tau^4+it\tau]}{\int d\tau\exp[-\beta f^{(4)}(T_c)\,\tau^4]}$$

Proof. Consider the expansion around $\tau=0$ for $T\geqslant T_c$:

$$f(T,\tau)=f(T,0)+\frac{f''}{2}(T)\,\tau^2+\frac{1}{4!}f^{(4)}(T)\,\tau^4+O(T^6)$$

For $T>T_c$, $f''(T)>0$, using the change of variables $\tau'=V^{1/2}\tau$, one gets a nontrivial limit for (21) if and only if $\delta=0$. For $T=T_c$, $f''(T_c)=0$, but $f^{(4)}(T_c)>0$.

By the change of variables $\tau'=V^{1/4}\tau$ one gets a nontrivial limit for (21) if and only if $\delta=1/4$.

Both limits are formulated in the lemma. ∎

This lemma proves that if the fluctuation operator $F_\delta(\rho)$ of the electronic density exists at T_c, then $\delta = 1/4$. This result, together with the result of Lemma 5.1, implies that if the fluctuation operator $F_\delta(b)$ of the lattice vibrations exists at T_c, then $\delta = 1/4$.

Above T_c, Lema 5.2 reproduces the existence of the fluctuation operators $F_0(\rho)$ and $F_0(b)$.

Now we turn to the dynamics $\tilde{\alpha}_t$ [see (18)] of the boson mode $F_\delta(b)$. We start with the first time derivative

$$\frac{d}{i\,dt} b_\Lambda = [H_\Lambda, b_\Lambda] = -\Omega b_\Lambda^* - \bar{\lambda} B_\Lambda^*$$

By taking the fluctuation limit of both sides of this equation, we obtain the following equation for the fluctuation operators:

$$\frac{d}{i\,dt} F_\delta(b) = -\Omega F_\delta(b^*) - \bar{\lambda} F_\delta(\rho)^*$$

It is clear that the boson mode is coupled to the fermion density fluctuation. Therefore we have to know the time dependence of the latter:

$$\frac{d}{i\,dt} B_\Lambda = [H_\Lambda, B_\Lambda] = \frac{2}{\sqrt{V}} \sum_k \varepsilon(k)\, a_k^* a_{k+q}$$

A new fluctuation operator appears in the right-hand side of this equation. It is essentially the fluctuation of the one-step jump operator $a^*(x)\, a(x+1) + \text{h.c.}$, which we denote by j_1. Hence, taking again the fluctuation limit in the equilibrium state yields the following equation for fluctuation operators:

$$\frac{d}{i\,dt} F_\delta(\rho) = 2\varepsilon_0 F_\delta(j_1)$$

Now we have to examine the time evolution of the right-hand side:

$$\frac{d}{i\,dt}\left(\frac{1}{\sqrt{V}} \sum_k \varepsilon(k)\, a_k^* a_{k+q}\right)$$
$$= 2\frac{1}{\sqrt{V}} \sum_k \varepsilon(k)^2\, a_k^* a_{k+q} - 2\lambda B_\Lambda \frac{1}{V} \sum_k \varepsilon(k)\, a_k^* a_k$$

Once again a new operator appears, this time the fluctuation of the two-step jump operator $j_2 = a^*(x)\, a(x+2) + \text{h.c.}$ This is easily seen by remarking that (let $a = 1$)

$$\varepsilon(k)^2 = \varepsilon_0^2 \cos^2 k = \frac{\varepsilon_0^2}{2}(1 + \cos 2k)$$

Then

$$\frac{d}{i\,dt}\left(\frac{1}{\sqrt{V}}\sum_k \varepsilon(k)\, a_k^* a_{k+q}\right)$$
$$= \varepsilon_0^2 \frac{1}{\sqrt{V}} \sum_k (1+\cos 2k)\, a_k^* a_{k+q} - 2\lambda B_\Lambda \frac{1}{V}\sum_k \varepsilon(k)\, a_k^* a_k$$

In the fluctuation limit one gets

$$\varepsilon_0 \frac{d}{i\,dt} F_\delta(j_1) = \varepsilon_0^2 F_\delta(\rho) + \varepsilon_0^2 F_\delta(j_2) - 2\lambda h_0 F_\delta(\rho)$$

where

$$h_0 = \lim_\Lambda \eta_\beta\left(\frac{H_\Lambda^0}{V}\right)$$

is the electronic kinetic energy density.

Again the time derivative now of $F_\delta(j_2)$ has to be considered, etc. It is clear that this procedure has to be repeated indefinitely, that is, one never gets a finite closed system of equations. Instead one obtains an infinite set of coupled equations because at each step a new operator is introduced. The dynamics of the system is given by the solution of the following infinite set of evolution equations:

(i) $$\frac{d}{i\,dt} F_\delta(b) = -\Omega F_\delta(b)^* - \bar{\lambda} F_\delta(\rho)^*$$

(ii) $$\frac{d}{i\,dt} F_\delta(\rho) = 2\varepsilon_0 F_\delta(j_1)$$

(iii) $$\frac{d}{i\,dt} \varepsilon_0 F_\delta(j_1) = \varepsilon_0^2 F_\delta(\rho) + \varepsilon_0^2 F_\delta(j_2) - 2\lambda F_\delta(\rho)\, h_0$$

...

...

We are unable to solve this set of equations. We strongly believe that the model is not soluble in this sense. On the other hand, the situation at $T = T_c$ is essentially simpler. We are able to prove the following rigorous form of the Kohn anomaly,[3-5] expressing the physically so-called softening of the mode of the lattice vibrations at the critical point.

Theorem 5.3 (Kohn anomaly). For all temperatures β for which $\delta > 0$, the fluctuation operator $F_\delta(b)$ is a constant of the motion, in other words, this fluctuation oscillates with zero frequency.

Proof. By Lemma 5.1, for all temperatures $T > 0$, there exists a finite constant R such that

$$0 \leqslant \tilde{\omega}\left(F_0\left(b+\frac{\lambda}{\Omega}\rho\right)^* F_0\left(b+\frac{\lambda}{\Omega}\rho\right)\right) \leqslant R$$

If $\delta > 0$, this implies that

$$0 \leqslant \tilde{\omega}\left(F_\delta\left(b+\frac{\lambda}{\Omega}\rho\right)^* F_\delta\left(b+\frac{\lambda}{\Omega}\rho\right)\right) \leqslant \lim_V \frac{R}{V^{2\delta}} = 0$$

By (17) this means that

$$F_\delta\left(b+\frac{\lambda}{\Omega}\rho\right) = 0$$

Substituting this in the evolution equation (i), one gets

$$\frac{d}{i\,dt} F_\delta(b) = -\Omega F_\delta^*\left(b+\frac{\lambda}{\Omega}\rho\right) = 0$$

which proves the theorem. ▮

In Lemma 5.2 it is proved that the lattice vibration fluctuation $F_\delta(b)$ is (abnormally) critical only at the critical point T_c with critical index $\delta = 1/4$. Therefore the Kohn anomaly is a typical phenomenon of the phase transition. It is interesting to note that

$$0 = F_\delta\left(b+\frac{\lambda}{\Omega}\rho\right)$$

i.e., the boson mode fluctuation $F_\delta(b)$ and the fermion density fluctuation $F_\delta(\rho)$ are coherent with correlation coefficient equal to -1, or the two fluctuations become linearly dependent at $T = T_c$.

Furthermore, as a consequence of the hierarchy of the time evolution equations and the Kohn anomaly at $T = T_c$, one gets also that

$$\frac{d}{i\,dt} F_\delta(\rho) = 0$$

i.e., the dynamics of the charge density fluctuations $F_\delta(\rho)$ is also "frozen." Also

$$\frac{d}{i\,dt} F_\delta(j_1) = 0, \quad \text{etc.}$$

at $T = T_c$. Therefore the hierarchy of equations (i), (ii), (iii),... describing the time evolution reduces to linear algebraic correlations between the fluctuation operators. One gets that the soft lattice crystallizes completely at $T = T_c$.

Mathematically this phenomenon at $T = T_c$ manifests an infinite set of constants of the motion. It resembles the classical analog of the PF instability as an integrable system.[6–9]

6. CONCLUDING REMARKS

The paper contains rigorous results about two well-known physical phenomena, namely the Peierls–Fröhlich instability and the softening of the mode in the tight-binding model. The latter is also known as the Kohn anomaly. As far as the Peierls–Fröhlich instability is concerned, our contribution consists in providing a rigorous and canonical proof of the phenomenon. We use the word canonical because we have succeeded in giving a formulation of it in which it is clear that the instability is a property of any electronic system on a lattice whose electrons are allowed to hop from one lattice site to an other. The lattice structure is essential, but the particular type of interaction with the lattice vibrations is irrelevant, i.e., the Peierls argument.

We studied also the Peierls transition in the tight-binding model, describing a linear interaction between the electronic density and the lattice vibrations. Because the free energy of this model can be calculated exactly, it is often believed that this model is completely soluble. However, if one looks at the dynamical equations in Section 5, they appear far from soluble. They constitute an infinite set of coupled differential equations. We were able to prove one property, namely that the frequency of the fluctuation operators involved in the evolution equations is exactly zero at the critical point. This gives in particular a rigorous proof of the Kohn anomaly. Mathematically, it amounts to the fact that because of the appearance of critical fluctuations, the equation for the lattice distortion fluctuation is decoupled from the rest of the infinite set of algebraic relations between fluctuation operators. Outside of the critical point one cannot say very much. Here our only contribution is a rigorous formulation of the dynamics, such that the problem is ready for further study. In the dynamical sense the model is far from solved.

We would also like to point out that our proof of the Kohn anomaly is very much dependent on the proof of Lemma 5.2, where we compute the critical index $\delta = 1/4$ at $T = T_c$. One might guess that this index which we computed depends on the type of Ginzburg–Landau approach we used. We have definite indications that a computation in the Gibbs state does give the same index. We did not include these computations, which are long and of a much more involved nature. On the other hand, we also have definite indications that the distribution obtained in Lemma 5.2 does depend on our approach. This distribution, however, is not used.

Finally, the model which we studied is fairly well known for its applicability as a prototype for a metal–insulator transition. In this paper we did not discuss this aspect. However, we come back to this in a future contribution, where we discuss the important extension to values of the chemical potential μ different from zero. The results we present here will also enable us to give a rigorous computation of the conductivity.

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