QUANTUM FLUCTUATIONS EFFECTS ON THE 1-D PEIERLS INSTABILITY

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ABSTRACT

The influence of quantum lattice fluctuations on the one-dimensional molecular crystal Peierls instability is analyzed through the renormalization group and the functional integral techniques. The analysis is made for spinless electrons in the half-filled band case including the effect of electron-electron interaction. The comparaison with Monte Carlo simulations is also briefly discussed.

INTRODUCTION

Recently different approaches have been used to study the continuous suppression of the zero temperature 1-D Peierls order parameter in presence of quantum lattice fluctuations [1,2]. The functional integral approach coupled to the renormalization group technique is particularly interesting for this problem since it allows a continuous control of the validity of the Peierls order paramater (in the Landau sense) as a function of the phonon frequency. Here we will briefly illustrate it for the 1-D Molecular Crystal (MC) model in the spinless half-filled band case where for non-interacting electrons numerical simulations are avaiable [2].

RENORMALIZATION GROUP RESULTS

As shown in ref.[1a], the functional integral representation of the partition function Z=Tr exp(-βH) for the interacting MC model can be written as :

$$Z=\int D\psi^* D\psi D\phi \ \exp(S[\psi^*,\psi,\phi]) = \int D\psi^* D\psi D\phi \ \exp(S^o[\phi]+S^o[\psi^*,\psi]+S_I[\psi^*,\psi]+S_\lambda[\psi^*,\psi,\phi])$$

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where the various parts of the euclidean action S functional of Grassmann (ψ) and c-number phonon (ϕ) fields are given by:

$$S^{o}[\phi]=\sum_{(q,\omega_m)}[D^{o}(\omega_m)]^{-1}|\phi(q,\omega_m)|^2;\quad S^{o}[\psi^*,\psi]=\sum_{(p,k,\omega)}[G^{o}_p(k,\omega_n)]^{-1}\psi^*_p(k,\omega_n)\psi_p(k,\omega_n)$$

$$S_I[\psi^*,\psi]=g_2T/2L\sum_{(p,k,\omega)}\psi^*_p(k+q,\omega_n+\omega_m)\psi^*_{-p}(k'-q,\omega_{n'}-\omega_m)\psi_p(k,\omega_n)\psi_{-p}(k',\omega_{n'});$$

$$S_\lambda[\psi^*,\psi,\phi]=\lambda\sqrt{T/L}\sum_{(p,k,\omega)}\Big[[\psi^*_+(k,\omega_n)\psi_-(k-2k_F-q,\omega_n-\omega_m)\phi(2k_F+q,\omega_m)+c.c]$$
$$\psi^*_p(k,\omega_n)\psi_p(k-q,\ \omega_n-\omega_m)\phi(q,\omega_m)\Big].\qquad(1)$$

where $D^{o}(\omega_m)=-M^{-1}(\omega_m^2+\omega_o^2)^{-1}$ and $G^{o}_p(k,\omega_n)=[i\omega_n-v_F(pk-k_F)]^{-1}$ are the bare phonon and electron propagators with ω_m and ω_n as their respective Matsubara frequencies. $\omega_o=\sqrt{K/M}$ is the molecular phonon frequency, K is the elastic constant and M the ionic mass. The electronic spectrum has been linearized around the Fermi level where p=± stands for right (+) and left (-) moving electrons, $v_F=2t(k_F)$ is the Fermi velocity (momentum) and $E_F=v_Fk_F$ ($E_o=4t$) is the Fermi energy (band width). For the interacting parts S_I and S_λ, g_2 and λ correspond to the forward scattering and to the electron-phonon coupling constants respectively. Note that the coupling to phonons near $2k_F$ and $q\simeq0$ is considered. We apply a Kadanoff-Wilson type of transformation for Z [1a] where we integrate the fermion ($\bar\psi$) degrees of freedom inside an outer energy shell of thickness $E_o(\ell)d\ell/2$ at the p=± band edges and for all ω_n by keeping the ϕ's fixed with $E_o(\ell)=E_oe^{-\ell}$ as the scaled band width. Considering S_I and S_λ as perturbations, this can be formally written as:

$$Z=\int_{E_o(\ell)}D\psi^*D\psi D\phi\ e^{S^{o}[\phi]}\int_{os}D\bar\psi^*D\bar\psi\ e^{S^{o}[\bar\psi^*,\ \bar\psi]}(e^{S_I[\bar\psi^*,\bar\psi,\psi^*,\psi,\phi]}+S_\lambda[\bar\psi^*,\bar\psi,\psi^*,\psi,\phi])$$
$$=\int_{E_o(\ell)}D\psi^*D\psi D\phi\ \exp\Big\{S[\psi^*,\psi,\phi])+\delta S[\phi]+\delta S[\psi^*,\psi]+\delta S_\lambda[\psi^*,\psi,\phi]\Big\}.\qquad(2)$$

Successive integrations of fermion degrees will then lead to the renormalization of each term of the full action. Furthermore the partial trace operation will generate for $\delta S[\phi]$ an infinite series of *new* phonons terms to all order in perturbation theory. Focusing on the phonon part of the action we get at the step ℓ and up to fourth order in ϕ's:

$$S[\phi]=-M\sum_{q,\omega}\Big[\omega_m^2+\omega_o^2(1+2\lambda^2K^{-1}\chi[\ell(q,\omega_m,T)])\Big]|\phi(q,\omega_m)|^2-T/L\sum_{(q,\omega)}\Big\{B_4[\{q,\omega\},\ell]\times$$
$$\times\ \phi(q_1+2k_F,\omega_{m1})\phi^*(q_2+2k_F,\omega_{m2})\phi(q_3+2k_F,\omega_{m3})\phi^*(q_4+2k_F,\omega_{m4})+B'_4[\{q,\omega\},\ell]\times$$
$$\times\ \phi(q_1+2k_F,\omega_{m1})\phi^*(q_2+2k_F,\omega_{m2})\phi(q_3,\omega_{m3})\phi^*(q_4,\omega_{m4})\Big\}+\ldots\qquad(3)$$

bubble insertion which has the power law singularity $\chi(\ell)= -(2\pi t)^{-1}[e^{\gamma\ell}-1]$ at $v_F q = \omega_m = 0$, with the exponent $\gamma = g_2/2\pi t$ in first order of the RG. The quartic terms in (3) correspond to the mode mode coupling of the ϕ's through fourth order fermion loops (B_4 and B'_4). Quantum lattice degrees of freedom are present through the Matsubara frequencies of the phonon field. The phonon softening at $\omega_m=0$ leading to the Peierls instability will then be affected by these quantum effects. In a one-loop scheme where for these quartic terms, an integration over two external phonon lines at $\omega_m \neq 0$ is performed and the softening condition for the Peierls instability reads at $\ell=\ln(E_F/\overline{T}_{MF})$ [1a]:

$$1 - \lambda^2(2\pi K\gamma t)^{-1}\left[(E_F/\overline{T}_{MF})^{\gamma} - 1\right] + A(\lambda,\omega_o) = 0$$

leading to the power law decay

$$\overline{T}_{MF} = \overline{T}^{o}_{MF} \Big/ \left[1+A(\lambda,\omega_o)[1+\lambda^2(2\pi K t\gamma)^{-1}]^{-1}\right]^{1/\gamma} \qquad (4)$$

Therefore the renormalized mean field (MF) Peierls temperature $\overline{T}_{MF}$ is depressed compared to the adiabatic result $\overline{T}^{o}_{MF} = E_F \overline{\lambda}^{2/\gamma}/[1+\overline{\lambda}^2]^{1/\gamma}$ when $\omega_o=0 (A=0)$ and where $\overline{\lambda}^2=\lambda^2/2\pi K\gamma t$. At finite ω_o quantum anharmonic terms contribute to $A(\lambda,\omega_o)$ which is found to be:

$$A(\lambda,\omega_o) = C\lambda^4\overline{T}^{o}_{MF}(32\pi K^2 t^3)\left\{3/2(1+\gamma)^{-1}\left[(E_F/\overline{T}^{o}_{MF})^{\gamma}-1\right] + (2+\gamma)^{-1}\left[(E_F/\overline{T}^{o}_{MF})^{2+\gamma}-1\right]\right\}$$
$$\times[\overline{\beta}^{o}_{MF}\omega_o/2 \coth(\overline{\beta}^{o}_{MF}\omega_o/2) - 1]. \quad (C=7\zeta(3)/2\pi^2) \qquad (5)$$

Here the fourth order fermion loops and theirs vertex parts are evaluated at $\overline{\ell}^{o}_{MF}=\ln(E_F/\overline{T}^{o}_{MF})$. In the non interacting limit $\gamma \to 0$, the MF temperature profile with ω_o reduces to [1a]:

$$T_{MF}=T^{o}_{MF} \exp\left\{-C(\lambda/\sqrt{Kt})^2 T^{o}_{MF}/8t \left[(E_F/T^{o}_{MF})^2-1\right][\beta^{o}_{MF}\omega_o/2 \coth(\beta^{o}_{MF}\omega_o/2)-1]\right\} \qquad (6)$$

which now decreases exponentially. Here $T^{o}_{MF}= E_F\exp(-2\pi Kt/\lambda^2)$. In 1-D systems there is no long range order at finite temperature but $\overline{T}_{MF}$ and T_{MF} still remain as characteristic energies for the true Peierls gap Δ at T=0K which in turn, is proportional to the ground state $2k_F$ dimerization δ. It follows that the ratio $^{(}\overline{\delta}^{)}(\omega_o)/^{(}\overline{\delta}^{)}(0)$ is equal to $^{(}\overline{T}^{)}_{MF}/^{(}\overline{T}^{)o}_{MF}$. The above results could then be compared [1a] to the Monte Carlo simulations of Hirsh and Fradkin [2] performed in non-interacting case. It was found that the depression of the dimerization with ω_o is very fast in agreement with the exponential decrease of (5). Numerical simulations however, indicate that there is a large but finite phonon frequency above which there is no dimerized ground state. Here in the non-adiabatic limit, the $2k_F$ electron-hole bubble in presence of absorption and emission of virtual phonons [eq.(5)] can no longer be evaluated by taking the adiabatic limit for the fourth order fermion loops B_4 and B'_4. Actually, whenever the well known non adiabatic condition $2\pi T^o_{MF} \gg \omega_o$ [3] is satisfied one should recover the complete interference between the Peierls and the Cooper channels of correlations [4] which in the present case is known [5] to destroy completely the Peierls gap.

CONCLUSION

In conclusion, we have applied a Kadanoff-Wilson type of renormalization group approach to a functional-integral formulation of the 1-D Molecular Crystal model. For the spinless half-filled band case with and without electron-electron interaction, a one-loop scheme approximation for the quantum part of the mode-mode phonon coupling term allows to follow continuously the suppression of the Peierls order paramater with the phonon frequency up to the non-adiabatic domain. In the non-interacting case, the ground state dimerization is found to be exponentially suppressed, a result which is compatible with the Monte Carlo simulations. The inclusion of electron-electron interaction is straightforward and the decay of the dimerization with frequency is found to be power law like with a non-universal exponent. Generalizations of the approach to electrons with spins and for non-half-filled band case are also straightforward.

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