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 $Z=\mathrm{Tr}\ \exp(-\beta H)$ for the interacting MC model can be written as :

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

(received December 31, 1989)

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 $p=\pm$ 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 $q\simeq 0$ 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 $p=\pm$ 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:

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

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:

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

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 $\ell=\ell n(E_F/\bar{T}_{MF})$ [1a]:

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

leading to the power law decay

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

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

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

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

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

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 $\bar{T}_{MF}$ 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 $\langle\bar{\delta}\rangle(\omega_o)/\langle\bar{\delta}\rangle(0)$ is equal to $\langle\bar{T}\rangle_{MF}/\langle\bar{T}\rangle^{o}_{MF}$. 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.

Acknowledgements

The authors would like to thank S. Barisic for useful remarks concerning the limitations of the present approach in the non adiabatic limit. Discussions with Dr J. Voit and Prof. A. Bjelis are also greatly acknowledged.

References

1 a) C. Bourbonnais, L. G. Caron, J. Physique 50, 2751(1989); Synthetic Metals A27, 27(1988); b) H. Zheng, D. Feinberg and M. Avignon, Phys. Rev. B39, 940(1989) and this conference; c) S. Aubry and P. Quemerais, preprint and this conference.

2 J. E. Hirsch and E. Fradkin, Phys. Rev. B27, 1680(1983).

3 S. Barisic, Mol. Cryst. Liq. Cryst. 119, 413(1985).

4 Y. A. Bychov, L. P. Gor'kov and I. E. Dzyaloshinskii, Sov. Phys. JETP 23, 489(1989).

5 L. G. Caron and C. Bourbonnais, Phys. Rev. B27, 4302(1984).