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ELECTRON - PHONON INTERACTION IN A STRONGLY CORRELATED LOW DIMENSIONAL SYSTEM : A SLAVE BOSON APPROACH

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The electron - phonon interaction and the ensuing transition to the charge density wave (CDW) state is studied for a low dimensional strongly correlated metal. It was shown that in general the electron correlation tends to suppress the CDW state. This has been established by calculating the variation with electronic correlation of the Peierl's instability, the phase diagram, the CDW order parameter and the spectral density function of the collective modes.

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1 Introduction.

The discovery of high temperature superconductivity (SC) in different systems such as the cuprates, the bismathate and the alkali doped fullerenes has raised the issue regarding the mechanism of pairing. While in the cuprates the high transition temperatures (T_c) and the associated anomalous behaviour of their normal state properties has focussed attention on the study of strongly correlated systems [1], still the role of electron-phonon (EP) interaction in the pairing mechanism is under debate [2]. The bismathates on the other hand (also have relatively large superconducting transition temperature (T_c)), exhibit strong EP interaction which is believed [3] to be responsible for the SC. In the third category there are systems like the alkali doped fullerenes [4] and the organic superconductors [5] which exhibit properties indicating that both electron correlation and EP interaction are responsible for SC in these systems. Therefore a detailed analysis of the interplay between electron correlations and EP interaction is essential for a proper understanding of the phenomenon of high temperature superconductivity. There had been several attempts at such an analysis showing conflicting results ; Zielinski et al, [6] following a strong coupling theory arrived at the conclusion that there is an enhancement of T_c (EP coupling constant) around quarter filling of the band due to the presence of strong correlation. On the other hand Kim et al, [7] argue that the EP interaction strength decreases with Coulomb correlation, due to the suppression of charge fluctuation as one approaches the Metal-Insulator transition. More recently Kulic and Zeyher [8] carried out a more detailed calculation and find that the EP coupling constant is enhanced for small wave vectors and suppressed at large wave vectors in the limit of low dopant concentration (δ). While these studies focussed on how the EP coupling constant and hence T_c is effected by strong correlation, there have been others (Deeg et al, [9]), which primarily looked at the resulting phase diagram of the system due to the interplay between the strong correlation and the EP interaction. These later authors used Slave Boson method (and its generalization to the case of two sublattices) to treat the strong correlation effects and examine the stability of different magnetic phases vis-a-vis the charge density wave (CDW) state.

It is well known that a low dimensional paramagnetic metal undergoes a transition to the CDW state in the presence of EP interaction. The so called Peierl's instability is brought about by the softening of the phonon with the wave vector ($\vec{Q}$) corresponding to the nesting of the Fermi surface. The aim of the present paper is to investigate how this transition gets effected in the presence of electron-electron interaction. While it is expected that at half filling the strong correlation will tend to drive the system towards the Mott-Hubbard insulator, the EP interaction will tend to stabilise the Peierl's transition. Therefore it is interesting to investigate the nature of the interplay of the two interactions on these instabilities when there is a deviation from half filling of the band. In an attempt to answer this question we treat the correlation problem using the Slave Boson method within the saddle point approximation [10] and deduce an effective EP interaction in sec. 2. The phonon softening and the Peierl's instability in the presence of correlation as well as a detailed study of the effect of electron correlation on the CDW order parameter are also discussed. We conclude in sec. 3 by comparing our results with those of the earlier calculations.

2 The Slave Boson approach to electron-phonon interaction in a Correlated system :

The problem of strong electron correlation is best discussed in terms of the single band Hubbard model [11] described by the Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} \qquad (1)$$

where the first term is the usual tight binding Hamiltonian with the hopping integral t_{ij}, the second term denotes the intratomic Coulomb repulsion (U) between two electrons with opposite spin occupying the same site and the third term denotes the chemical potential (μ) which can take into account the deviation from half filling. In its ground state the system will tend to minimize the number of doubly occupied sites.

2.1 Slave Boson Formulation of the Correlated Problem :

One of the main obstacles encountered in obtaining a solution to the Hubbard model is keeping track of the occupancy of a site. It was shown by Kotliar and Ruckenstein [10] that by introducing four different auxilliary Boson fields corresponding to a site being empty, singly occupied with a up or down spin electron, or doubly occupied ; one can overcome this difficulty to some extent. Ofcourse these Boson fields are not completely independent but are constrained by the requirements that (i) the total

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probability of occupation of a site being unity must be conserved and (ii) the local charge at a site is also conserved. Thus the original fermion annihilation (creation) operator $c_{i,\sigma}$ ($c^\dagger_{i,\sigma}$) of equation (1) can be expressed in terms of these Slave Boson operators and the constraints are introduced into the problem through Lagrange multipliers. The prescription for the transformation of equation (1) in terms of the Boson operators, is given below :

$$n_{i\uparrow}n_{i\downarrow} \rightarrow d^\dagger_i d_i$$

$$n_{i\sigma} \rightarrow \tilde{n}_{i\sigma}$$

$$c^\dagger_{i\sigma}c_{j\sigma} \rightarrow z^\dagger_{i\sigma}\tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}z_{j\sigma}$$

where

$$z_{i\sigma} = (1 - d^\dagger_i d_i - p^\dagger_{i\sigma}p_{i\sigma})^{-1/2}(e^\dagger_i p_{i\sigma} + p^\dagger_{i-\sigma}d_i)(1 - e^\dagger_i e_i - p^\dagger_{i-\sigma}p_{i-\sigma})^{-1/2} \qquad (2)$$

the auxilliary Boson field operators $e^\dagger_i$, $p^\dagger_{i\sigma}$ and $d^\dagger_i$ respectively creat an empty, singly occupied (with spin σ) and doubly occupied site ; and $\tilde{c}^\dagger_{i\sigma}$ is the modified Fermion creation operator. The form of $z_{i\sigma}$ is so chosen as to reproduce the correct band structure in the absence of correlation. Furthermore the constraints mentioned above are given by

$$e^\dagger_i e_i + \sum_\sigma p^\dagger_{i\sigma}p_{i\sigma} + d^\dagger_i d_i = 1 \qquad (3)$$

and

$$p^\dagger_{i\sigma}p_{i\sigma} + d^\dagger_i d_i = \tilde{n}_{i\sigma} \qquad (4)$$

The values of the Boson field operators and the Lagrange multipliers are determined by minimizing the free energy of the system in the saddle point approximation, where all these operators are replaced by c-numbers. In this approximation the Hamiltonian of the system takes the simple form of an effective tight binding model with a modified hopping integral of the form $t_{ij} \rightarrow \tilde{q}t_{ij}$, where the correlation effects are built-in through the multiplicative factor $\tilde{q} = z^\dagger z$. It was shown [10] that in the weak correlation limit $\tilde{q} = (1 - u^2)$, (where $u = (U/U_c)$, U_c being the critical value of U where the system undergoes the Metal-Insulator transition) and the Brinkman-Rice result is reproduced. The generalization of this result to the case of strong correlation $U > U_c$ when there is deviation from half filling (dopant concentration $\delta \neq 0$) is due to Lavagna [10], who showed that for small values of δ, $\tilde{q} = 2\delta/\xi$, where $\xi = (1 - u^{-1})^{1/2}$. The weak and the strong correlation limits are also called the metallic and the doped regimes, due to the realization of the fact that in the later limit the conduction (in the Mott-Hubbard insulator) takes place only on doping. However in general $\tilde{q}$ is expressed in terms of the dopant concentration (δ) and the double occupancy parameter $x = (e + d)$, and is given by

$$\tilde{q} = \frac{(2x^2 - x^4 - \delta^2)}{(1 - \delta^2)} \qquad (5)$$

where x is determined by the equation

$$x^5 + x^4[u(1 - \delta^2) - 1] - u\delta^2(1 - \delta^2) = 0 \qquad (6)$$

In the tight binding picture the EP interaction arises from the dependence of the hopping integral (t_{ij}) on the separation between the sites ($\vec{R}_{ij}$). In the presence of small displacements of ($\vec{u}_i$) of the atom at the site i , t_{ij} can be expanded in a Taylor series and the leading term in the displacement will give rise to the EP interaction Hamiltonian.

However, it was argued earlier that in the presence of electron correlation which is treated within the Slave Boson - saddle point approximation the effective Hamiltonian involves a modified hopping integral with a multiplicative factor ($\tilde{q}t_{ij}$). Therefore the corresponding EP interaction Hamiltonian will be of the form

$$H_{e-p} = g\tilde{q}\sum_{\vec{k}\vec{q}\sigma} \tilde{c}^\dagger_{\vec{k}+\vec{q}\sigma}\tilde{c}_{\vec{k}\sigma}A_{\vec{q}} \qquad (7)$$

where $A_{\vec{q}} = (b_{\vec{q}} + b^\dagger_{-\vec{q}})$ is the q-th Fourier component of the atomic displacement $\vec{u}_i$; with $b_{\vec{q}}(b^\dagger_{\vec{q}})$ denoting the phonon annihilation(creation) operator ; and g is the coupling constant. It is clear from equation (7) that within this approximation scheme the entire effect of electron correlation is to modify the EP coupling constant by the multiplicative factor $\tilde{q}$. In the weak correlation limit, $\tilde{q}$ tends to zero as the intratomic correlation U approaches the critical value (U_c) for the Brinkman-Rice transition. Therefore the EP coupling will gradually decrease and vanish at the Metal-Insulator transition ; a result in agreement with Kim et al [7]. On the other hand in strong correlation limit or the doped regime, it follows from the approximate form of $\tilde{q}$ for small δ that asymptotically as $u \rightarrow \infty$, $\tilde{q} \rightarrow 2\delta$. This again amounts to a large reduction in the effective EP coupling constant due to strong correlation. However, for large dopant concentrations $\tilde{q}$ has to be calculated from equations (5) and (6) and the conclusions drawn above do not hold good as will be shown later.

2.2 Peierl's Transition in a Correlated system :

The lattice instability in low dimensional metals is usually driven by the softening of the phonon with wave vector $\vec{Q}$; which in turn is intimately connected with the nesting property of the Fermi surface : given by $\epsilon_{\vec{k}+\vec{Q}} = -\epsilon_{\vec{k}}$. In order to see how the Peierl's transition is effected by the electron correlation, the phonon self energy arising from the EP interaction has to be calculated, which is given by

$$\Pi(\vec{q},\omega) = 4\pi^2(g\tilde{q})^2\chi(\vec{q},\omega) \qquad (8)$$

where the density response function $\chi(\vec{q},\omega)$ has to be evaluated using the Slave Boson effective Hamiltonian. In the saddle point approximation the density response function is just the modified Lindhard function given by

$$\chi(\vec{q},\omega) = \sum_{\vec{k}} \frac{f(\tilde{q}\epsilon_{\vec{k}+\vec{q}}) - f(\tilde{q}\epsilon_{\vec{k}})}{[\omega - \tilde{q}(\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}})]} \qquad (9)$$

The renormalised frequency of the phonon with wave vector $\vec{Q}$ is determined by the static response function and is given by

$$\Omega_{\vec{Q}} = \begin{cases} \omega_{\vec{Q}}[1 + (4\pi g^2\tilde{q}^2/\omega_{\vec{Q}})\chi(\vec{Q})]^{1/2} \\ \omega_{\vec{Q}}[1 - \lambda\tilde{q}ln(\tilde{q}/\tilde{T})]^{1/2} \end{cases} \qquad (10)$$

where $\lambda = (4g^2N(0)/\omega_{\vec{Q}})$ is the dimensionless coupling constant, $N(0)$ being the density of states at the Fermi energy, $\omega_{\vec{Q}}$ is the phonon frequency in the absence of

the EP interaction and the effective temperature $\tilde{T} = (k_B T/1.13\epsilon_B)$, ϵ_B being some cut-off energy. It is evident from equation (10) that the effect of electron correlation modifies the EP coupling constant as well as the Peierl's transition temperature ($\tilde{T}_p$). The transition takes place at the temperature at which the soft mode frequency vanishes, i.e, $\Omega_{\tilde{Q}} = 0$, so that

$$\tilde{T}_p = \tilde{q}\exp[-1/\lambda\tilde{q}] \tag{11}$$

Since $\tilde{q}$ is a function of u and δ, equation (11) essentially gives the phase diagram for the CDW state in the ($u \sim \tilde{T}$) and ($\delta \sim \tilde{T}$) planes. Equation (10) gives the temperature dependence of the frequency of the phonon with wave vector $\tilde{Q}$. But to trace the behaviour of the giant Kohn-anomaly as a function of the correlation or the dopant concentration it is necessary to obtain the temperature dependence of the phonons around the wave vector $\tilde{Q}$. This can be achieved by substituting $\vec{Q} \to \vec{Q} + \vec{q}$ in equation (10) for $|\vec{q}| \ll |\vec{Q}|$. Thus $\Omega_{\tilde{Q}+\tilde{q}}$ can be calculated by expanding the electron energy $\epsilon_{\tilde{k}+\tilde{Q}+\tilde{q}}$ and the Fermi function $f(\epsilon_{\tilde{k}+\tilde{Q}+\tilde{q}})$ in a Taylor series for small $\vec{q}$; for the evaluation of the density response function. Following this proceedure the dispersion around the giant Kohn anomaly phonon (Ω_Q) is given by

$$\frac{\Omega_{\tilde{Q}+\tilde{q}}}{\omega_{\tilde{Q}}} = (1+r)[1 - \lambda\tilde{q}\{\int_0^{i/1.13\tilde{T}} dx \tanh(x/2)(x + c\tilde{q}r^2/\tilde{T})^{-1} - \frac{2r^2}{2r^2+1}\}]^{1/2} \tag{12}$$

where the variable $r = q/Q$ and the parameter $c = (2\epsilon_F/1.13\epsilon_B)$. The u and δ dependence of the results of these calculations will be presented in sec.3.

2.3 Effect of Correlation on the CDW State :

So far, our main concern was to see how the electron correlation effects the EP interaction as well as the ensuing lattice instability of the system in the metallic state. However, it is possible that the system under consideration being at low temperatures ($T < \tilde{T}_p$) is already in the CDW state driven by the EP interaction ; then it is relevant to enquire how the electron correlation effects the CDW state ? The CDW state or the accompanying periodic lattice distortion is characterised by the non-vanishing expectation value of the phonon amplitude corresponding to the particular value of the wave vector $\vec{q} = \tilde{Q}$, i.e, $< A_{\tilde{Q}} > \neq 0$. Therefore the EP interaction Hamiltonian within the mean field approximation corresponding to the CDW state can be written as

$$H_{\tilde{Q}} \approx g\tilde{q}\sum_{k\sigma} c^\dagger_{\tilde{k}+\tilde{Q}\sigma} c_{\tilde{k}\sigma} < A_{\tilde{Q}} > \tag{13}$$

In analysing the problem of electron correlation for the CDW state within the Slave Boson approximation, it is convenient to define the two component Nambu operators $\Psi^\dagger_{\tilde{k}\sigma} = \begin{pmatrix} c^\dagger_{\tilde{k}\sigma} & c^\dagger_{\tilde{k}+\tilde{Q}\sigma} \end{pmatrix}$ in terms of which the free energy of the system can be cast in a form analogous to that in the metallic state. On minimizing the free energy the quasi particle energy of the CDW state turns out to be

$$E_k = \tilde{q}[\epsilon_k^2 + g^2 < A_{\tilde{Q}} >^2]^{1/2} + \lambda_1 \tag{14}$$

where λ_1 is the Lagrange multiplier associated with the constraint responsible for the local charge conservation which acts as the chemical potential. This is expected because in the CDW state the energy spectrum develops a gap at the Fermi energy. The minimization of the free energy also relates the gap parameter to the modulated charge density of the system as

$$g < A_{\tilde{Q}} > = -\frac{2g^2\tilde{q}}{\omega_Q}\frac{1}{N}\sum_{\tilde{k}\sigma} < \Psi^\dagger_{\tilde{k}\sigma}\hat{\tau}_1\Psi_{\tilde{k}\sigma} > \tag{15}$$

where $\hat{\tau}_i$ ($i = 1,2,3$) is the Pauli matrix. Furthermore, in the CDW state the Brinkman-Rice parameter U_c, at which the metal is driven into the insulating state differs from its value in the paramagnetic state, and is given by

$$U_c = 8[-\frac{1}{N}\sum_{\tilde{k}\sigma}\epsilon_k < \Psi^\dagger_{\tilde{k}\sigma}\hat{\tau}_3\Psi_{\tilde{k}\sigma} > + \frac{1}{2\tilde{q}}\omega_Q < A_{\tilde{Q}} >^2] \tag{16}$$

The extra contribution to U_c comes essentially from the elastic energy due to the periodic lattice distortion accompanying the CDW formation. Apart from these differences all the other quantities such as the mean field values of the Bose operators and the dependence of the band renormalization factor $\tilde{q}$ on the double occupancy parameter x remains the same as in the paramagnetic metallic state. To see the dependence of the CDW order parameter on the electronic correlation it is necessary to evaluate the right hand side of equation (15) explicitly from the effective saddle point Hamiltonian, which in the weak coupling limit gives

$$\Delta \equiv g < A_{\tilde{Q}} > = 2\omega_c \exp[-1/\lambda\tilde{q}] \tag{17}$$

where λ is the dimensionless coupling constant in the CDW state, ω_c is the cut-off frequency which determines the range of energy around the Fermi level beyond which the nesting property is destroyed. It is worth mentioning that the CDW order parameter depends on U_c through $\tilde{q}$ while U_c depends on the order parameter as can be seen from equation (16) ; which calls for a self-consistent solution. However, the qualitative dependence of the order parameter on correlation follows from equation (17), i.e, as $U \to U_c$ in the metallic regime the order parameter vanishes. This is physically understandable in the sense that if the Mott-Hubbard insulating phase sets in there will be localization of the electrons which will inhibit the formation of the CDW state. On the other hand in the doped regime the CDW order parameter is expected to grow on increasing the dopant concentration ; which clearly follows from the dependence of $\tilde{q}$ on δ in the limit of small δ.

The robustness of the ordered ground state is usually tested by looking at the response of the system to small fluctuations. In the case of the CDW state it is well known [12] that fluctuations of the phase and the amplitude of the order parameter results in the appearence of the collective modes of the system. While the phase mode is the Goldstone mode arising from the breaking of the symmetry, the amplitude mode is a measure of the CDW order parameter (Δ), which has a frequency $\omega_{AM} = 2\Delta$ at zero wave vector. Therefore, it is worthwhile to investigate the effect of the electron correlation on the CDW-amplitude mode. The frequency of the amplitude mode and its spectral density function can be calculated from the amplitude response function ($\chi^a(\vec{q},\omega)$) calculated [13] within the random phase approximation (RPA).

$$\chi^a(\vec{q},\omega) = \sum_{\tilde{k},\tilde{k}',\sigma,\sigma'} \ll \Psi(t)^\dagger_{\tilde{k}\sigma}\hat{\tau}_1\Psi(t)_{\tilde{k}+\tilde{q}\sigma}; \Psi(0)^\dagger_{\tilde{k}'+\tilde{q}\sigma'}\hat{\tau}_1\Psi(0)_{\tilde{k}\sigma} \gg_\omega \tag{18}$$

$$\chi^{a}_{RPA}(\vec{q},\omega) = \frac{\chi^{0}(\vec{q},\omega)}{[1-(\lambda\vec{q}^{2}/N(0))\chi^{0}(\vec{q},\omega)]} \tag{19}$$

where $\chi^0(\vec{q},\omega)$ is the response function in the CDW-state in the presence of electron correlation which at zero temperature is given by

$$\chi^{0}(0,\omega) = -\frac{4}{\pi}\sum_{\vec{k}} \frac{\vec{q}^{2}\epsilon_{\vec{k}}^{2}}{E_k(\omega^2 - 4E_k^{2})} \tag{20}$$

While the frequency of the amplitude mode is given by the pole of $\chi^a_{RPA}(0,\omega)$, the imaginary part of $\chi^a_{RPA}(0,\omega)$ gives its spectral density function. The frequency of the amplitude mode turns out to be

$$\omega_{AM} = 2\tilde{q}\Delta \tag{21}$$

Since the band renormalization factor ($\tilde{q}$) decreases with increasing value of the intratomic Coulomb repulsion (U) the CDW-amplitude mode frequency will also decrease with increasing u. The spectral density function is expected to show a peaked structure around ω_{AM}; but the nature of this peak will change (as will be shown in the next section) with increasing u in a manner such that it will indicate the suppression of the CDW state.

3 Results and Disscussion :

In the theory presented in sec.2. we analysed the effect of electron correlation (u) on various facets of EP interaction such as the coupling constant (λ), the on set of Peierl's instability, the ($u \sim \tilde{T}$) phase diagram, the CDW order parameter and the collective modes of the CDW state. The electron correlation has been dealt with in the Slave Boson approach within the saddle point approximation. It was shown that predominantly the correlation effect enters the calculation through the band renormalization factor $\tilde{q}$, which also depends on the dopant concentration δ. This dependence of $\tilde{q}$ on u and δ in the limit of small dopant concentrations has been discussed in sec.2.1 for both the metallic and doped regimes. However for any value of δ between $0 < \delta < 1$, the general dependence of $\tilde{q}$ on u and δ is governed by equations (5) and (6) and the behaviour is shown in figures 1 and 2 respectively. It can be seen from fig.1. that $\tilde{q}$ drops rapidly from its value of unity at vanishing correlation to a small value at large u for small dopant concentrations. However, with increasing δ, the value of $\tilde{q}$ at large u takes higher values. On the other hand at a given value of u, $\tilde{q}$ increases with increasing δ and becomes $\tilde{q} = 1$, at $\delta = 1$ which corresponds to an empty band in the case of hole doping and a full band in the case of electron doping. This obviously is an artifact of the saddle point approximation, and hence this results make sense only for more than half filling of the lower Hubbard band, for the case of hole doping. This behaviour of $\tilde{q}$ will be reflected in all the other quantities that are going to be calculated. For example in the presence of correlation the EP coupling constant gets multiplied by $\tilde{q}$, so that in general the effective strength of interaction will be reduced. Moreover due to the depedence of $\tilde{q}$ on u and δ, the strength of the interaction will decrease with increasing u, but increase with increasing δ.

The Peierl's instability of the system is determined by the giant Kohn anomaly, whose variation with the electron correlation u and the dopant concentration δ are shown in figs. 3 and 4. In the absence of correlation there is a softening of the Qth phonon at a particular temperature for a given value of the EP coupling constant. On increasing the value of u, the Kohn anomaly is suppressed as can be seen from fig.3., indicating that correlation effect suppresses the Peierl's instability in the metallic regime. On the other hand in doped regime, the Kohn anomaly which is present at a given dopant concentration is again suppressed with decreasing δ ; as can be seen from fig.4. This is again an indication of the fact that while the system can not undergo the CDW transition in the Mott-Hubbard insulating state, as it is metallised by increasing δ it becomes again prone to the Peierl's instability. Similarly the phase diagram of the system can be studied from equation (11), which is shown in fig.5 for different dopant concentrations. It can be seen from the figure that at low dopant concentrations the CDW phase appears for $u < 1$, i.e, only in the metallic regime. But with increasing δ the CDW state persists even at much higher values of u, indicating that there can be a Peierl's instability even in the doped regime although the corresponding transition temperatures are much lower. Fig.6 shows the variation of the CDW-gap parameter with the electronic correlation for different values of δ. The gap decreases rapidly in the begining with increasing value of u, but then it slowly vanishes with increasing u. With increasing δ, the critical value of u (below which the CDW state exists) increases. But for a given value of δ the variation of the gap with u is continuous. These results are in contradiction with that of Deeg et al, [9] where they obtained a first order discontinuous transition with increasing u, and also a decrease in order parameter with increasing δ. However their calculation differs from the present report in the sense that beside the transition to the CDW state they also incorporate the possibility of transition from the paramagnetic metal to an antiferromagnetic state with increasing u. Furthermore in the present calculation the possibility of a reduction in the nesting of the Fermi surface with increasing δ has not been accounted for. These differences could be the cause for the discrepancies in the results of the two calculations. Finally the variation of the spectral density function for the CDW-amplitude mode on increasing the electron correlation in the metallic regime is shown in fig.7. It can be seen from the figure that for vanishing u the spectral density function has a well defined peak corresponding to the CDW-amplitude mode at a frequency slightly less than 2Δ followed by a broad asymmetrical hump. On increasing u this peak shifts to lower frequency while its width decreases, while the hump becomes more prominant with increasing strength. For even larger values of u the peak vanishes and the hump further gains in strength ; as the system approaches the Metal-Insulator transition. This clearly signifies the suppression of the CDW state as the system is driven towards the Mott-Hubbard insulator due to electronic correlation. On the other hand in the doped regime a similar behaviour of the spectral density function results on lowering the dopant concentration δ. At larger values of δ a well defined peak corresponding to the CDW-amplitude mode exists, which vanishes on going to smaller values of δ. This again is an indication of the fact that the CDW state is suppressed in the low dopant concentrations in the doped regime. This result is physically understandable in the sense that in the doped regime (i.e, $u > 1$) for $\delta = 0$, the system is a Mott insulator, hence there is no possibility for a transition to the CDW-state.

In concluding we summarize the main results of the present paper : The effect of electron correlation on EP interaction and the ensuing transition to the CDW state has been studied in detail. It was shown that in general electron correlation tends to suppress the CDW state. In doing so the correlation problem has been treated using the Slave Boson formalism within the saddle point approximation. It has been shown that its effect on the EP interaction and the phenomenon of the CDW formation is predominantly determined by the band renormalization factor $\tilde{q}$. This has been established by calculating explicitly the variation with the electronic correlation, of the Peierl's instability, the phase diagram, the CDW order parameter

and the spectral density function of the collective modes. However, it has to be realised that these results are within the mean field approximation, and are likely to be altered on including the effects of fluctuation. These effects are presently under investigation and will be reported elsewhere.

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FIGURE CAPTIONS

Fig.1. Variation of $\bar{q}$ with u for different values of δ.

Fig.2. Variation of $\bar{q}$ with δ for different values of u.

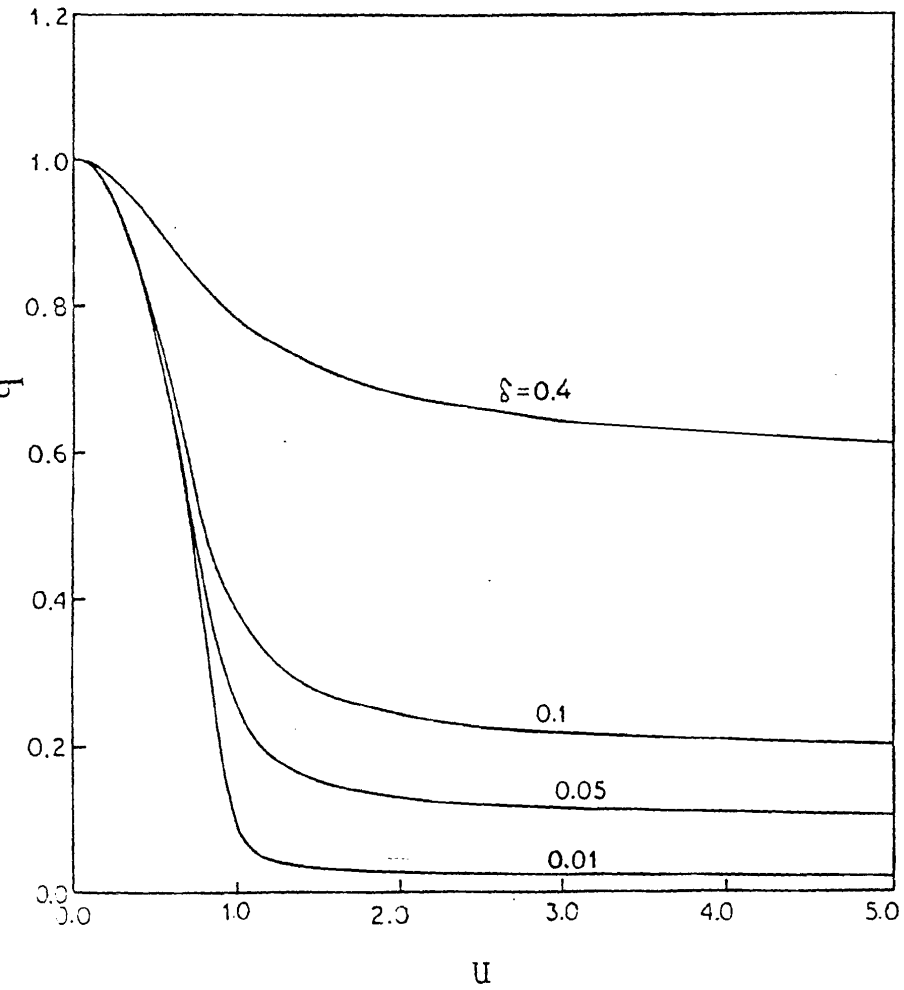
Fig.3. The dispersion of the giant Kohn anomaly phonon in the metallic regime for different values of u.

Fig.4. The dispersion of the giant Kohn anomaly phonon in the doped regime for different values of the dopant concentration δ.

Fig.5. The phase diagram for $\lambda = 0.2$.

Fig.6. The variation of the CDW gap with electron correlation for $\lambda = 0.2$.

Fig.7. Spectral density function for the CDW - amplitude mode as a function of reduced frequency (ω/Δ) for $\lambda = 0.94$ and for different values of u.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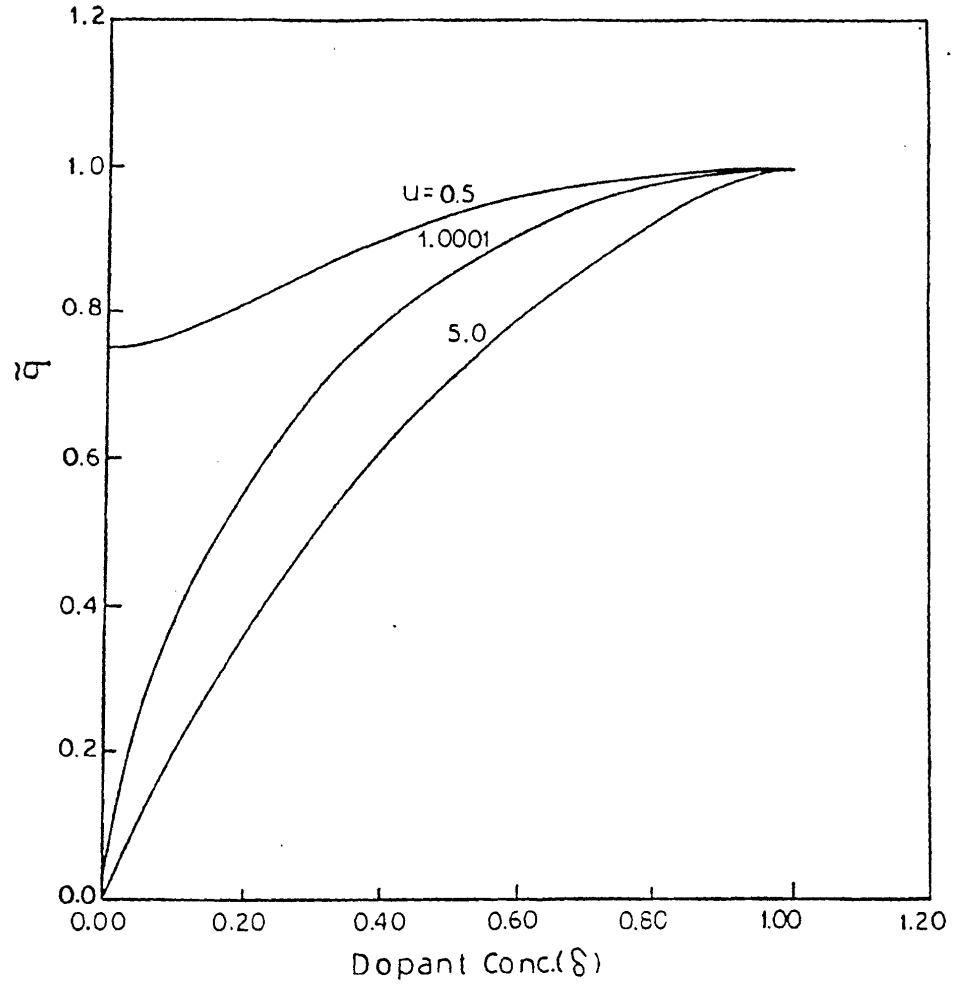
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Dopant Conc.(δ)
u=0.5
1.0001
5.0

Fig. 2

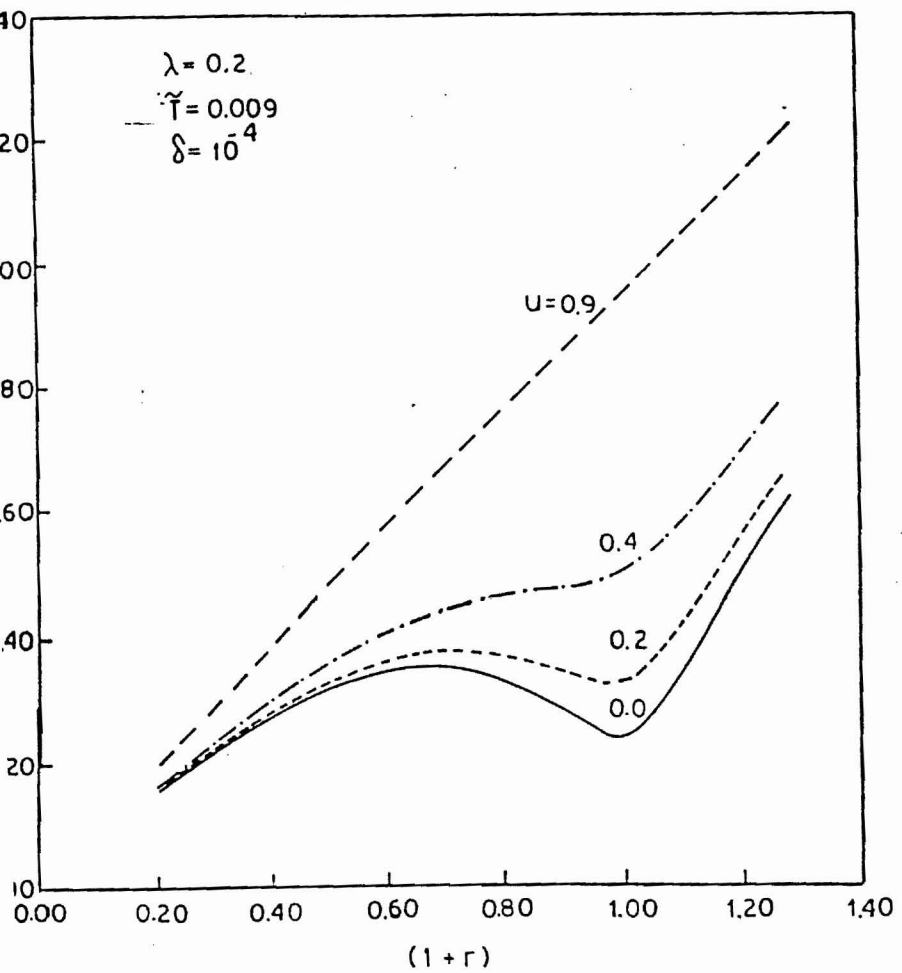
λ = 0.2
T̃ = 0.009
δ = 10⁻⁴
U = 0.9
0.4
0.2
0.0
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
(1 + r)

Fig. 3.

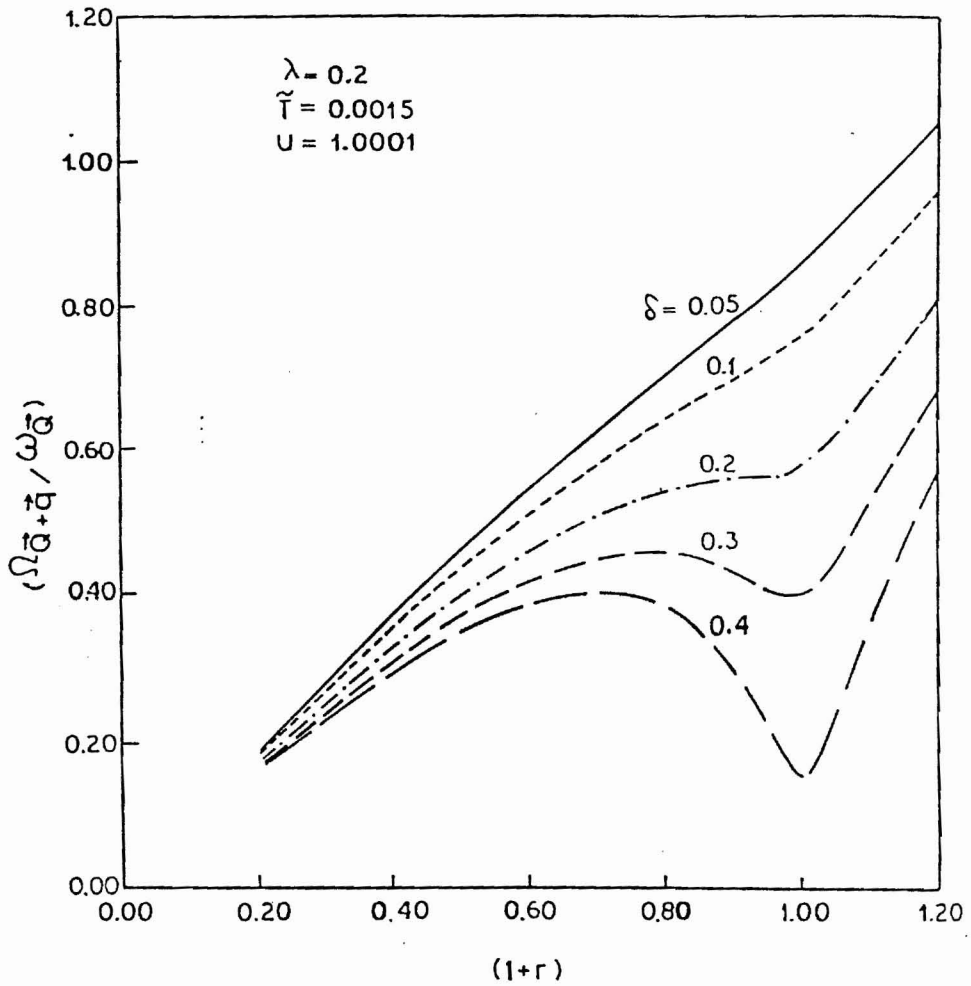
λ = 0.2
T̃ = 0.0015
U = 1.0001
δ = 0.05
0.1
0.2
0.3
0.4
$(\Omega_{\vec{Q}+\vec{q}} / \omega_{\vec{Q}})$
0.00
0.20
0.40
0.60
0.80
1.00
1.20
(1+r)

Fig. 4

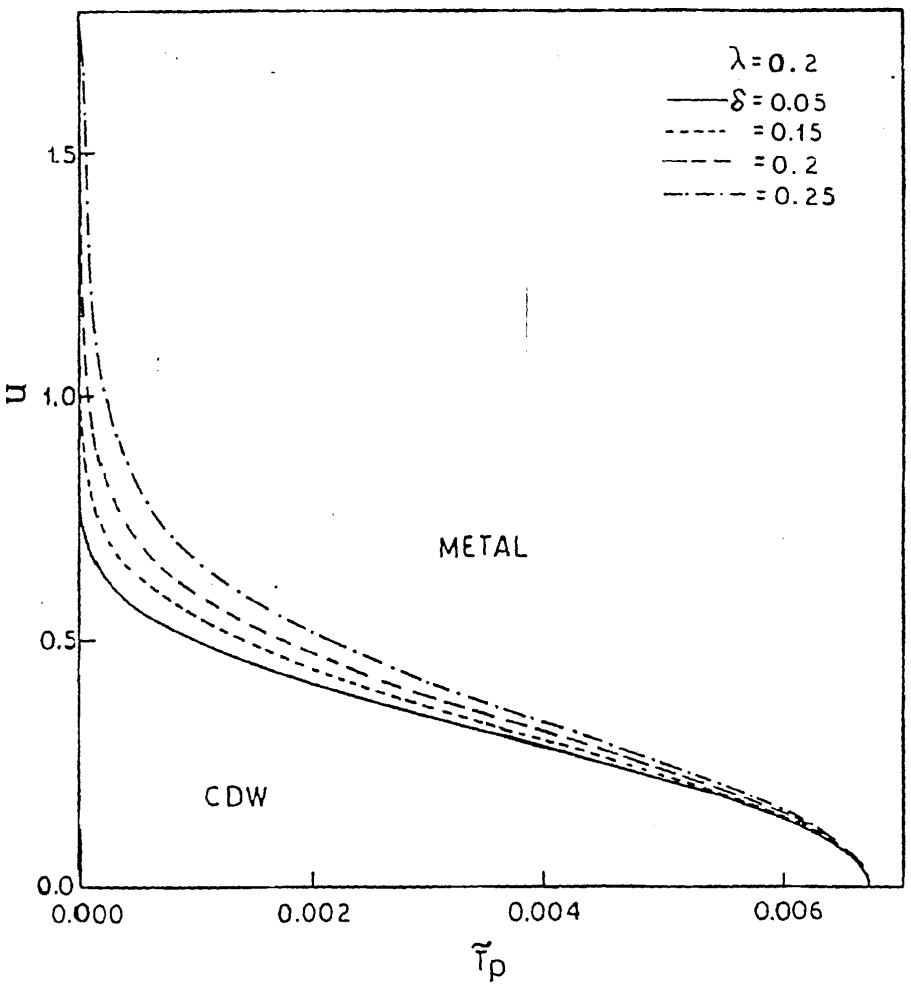
λ = 0.2
δ = 0.05
= 0.15
= 0.2
= 0.25
METAL
CDW
u
1.5
1.0
0.5
0.0
0.000
0.002
0.004
0.006
$\tilde{T}_p$

Fig 5.

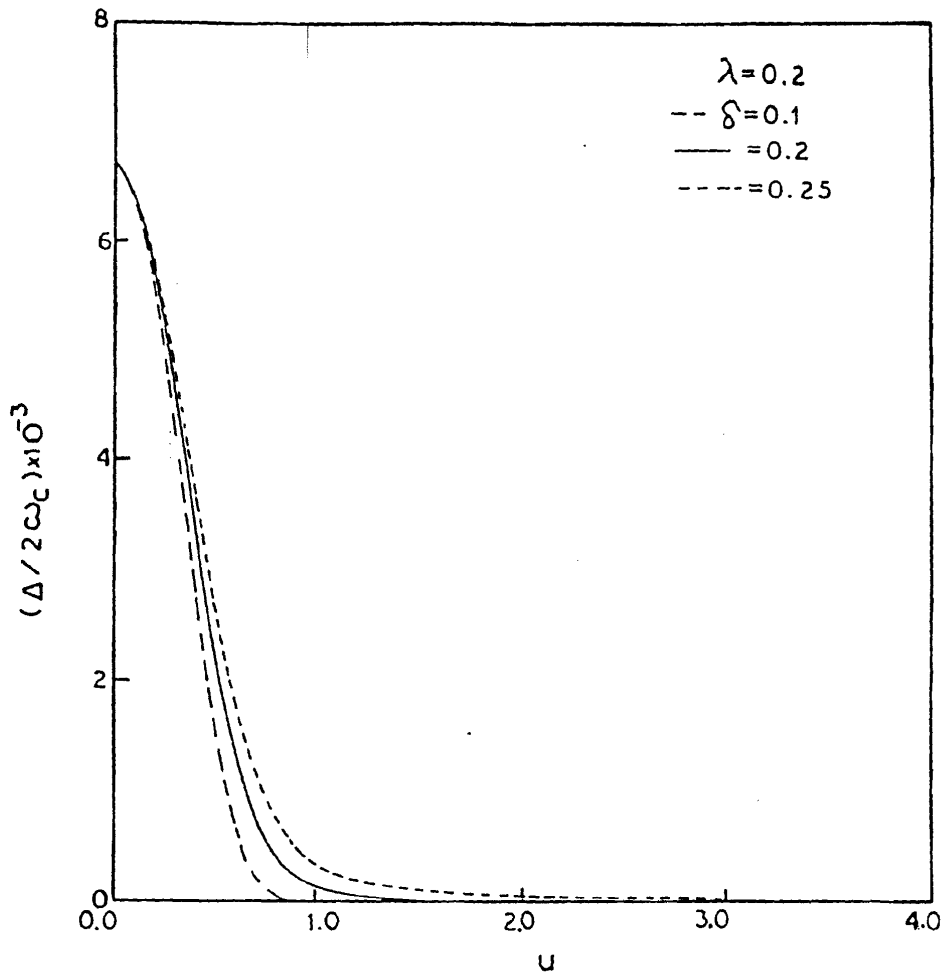
λ = 0.2
δ = 0.1
= 0.2
= 0.25
$(\Delta/2\omega_c)\times10^{-3}$
8
6
4
2
0
0.0
1.0
2.0
3.0
4.0
u

Fig. 6.

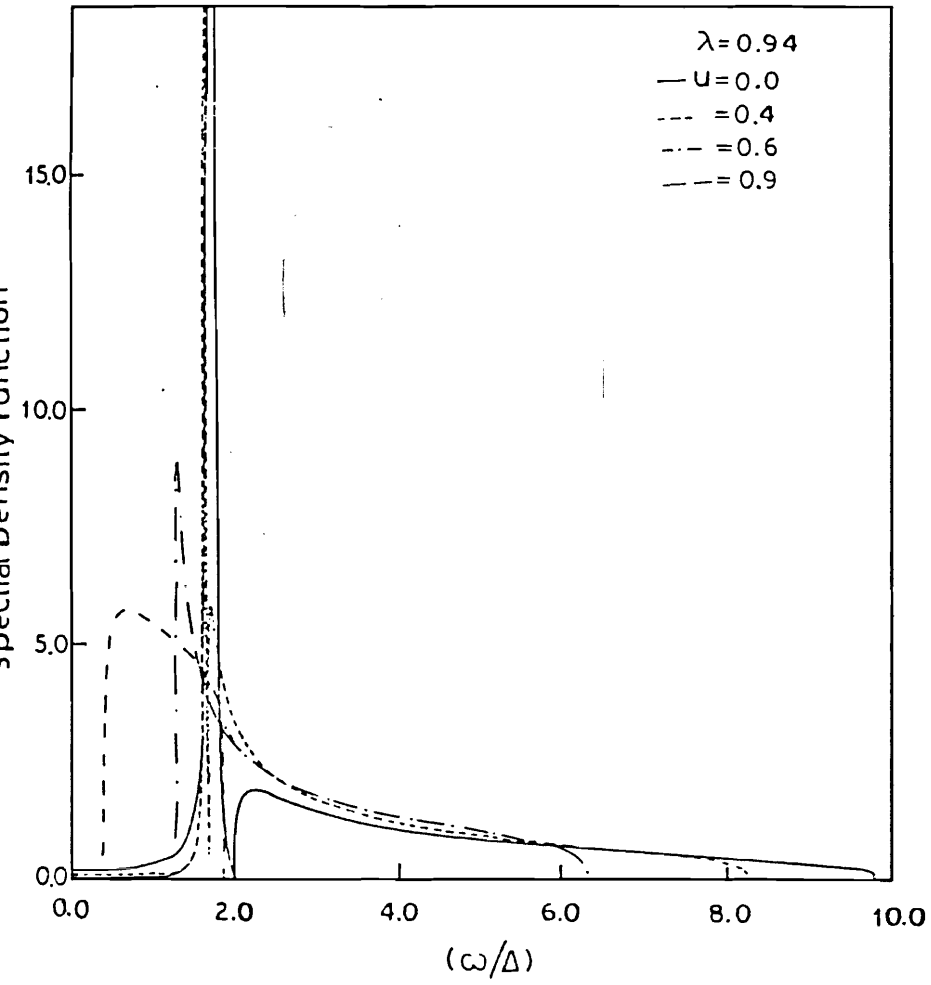

Fig 7