Local phonon mode in a fermionic bath, and its relation to Kondo effect

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(Dated: November 14, 2006)

We have studied the interplay of a local phonon mode embedded in a metallic host using Abelian bosonization. The phonon frequency softens, which takes place in two steps: first, their frequency starts softening, and acquires finite lifetime. Then oscillations disappear from the response, and two distinct, finite dampings characterize them. Due to phonons, the electrons experience an attractive, dynamic interaction. As a result, the electronic charge response enhances similarly to the spin response in the Kondo model. Thus the chance of charge-Kondo effect emerges.

PACS numbers: 73.23-b,73.63-b,72.10.Fk

Single impurity models have a long history[1], and our understanding has profited a lot from different reliable techniques. Numerical renormalization group, conformal field theory, Nozières' Fermi liquid description, Bethe ansatz solution and bosonization completed each other, and highlighted different aspects of the same problem. In many cases, the latter, being nonperturbative and analytic, was able to provide us with a transparent picture of the underlying physics[2]. Its appeal is due the elegance of analytic solution, being able to treat dynamic quantities as well (correlation functions), and the simplicity of the picture emerging from it.

Beyond electron-electron interaction, which is a basic ingredient in Kondo type models, another source of correlation is represented by phonons[3–8]. They play a prominent role in explaining the conventional s-wave BCS superconductivity and the charge density wave formation in low dimensional systems. Their general feature is the generated dynamic interaction between the electrons, which, in essence, is attractive for small energy transfers.

In many strongly correlated systems, such as heavy fermions or valence fluctuation systems, lattice vibrations are known to couple strongly to electrons. Quantum dots, especially the ones based on single molecules (C_{60} for example[9]), also possess vibrational degrees of freedom, which will react to the electron transfer through them[10]. Therefore the properties of impurity models dominated by phonons are challenging. The applied methods should be able to treat dynamical properties, which rules out techniques as the Bethe ansatz.

Several theoretical investigation focused on electron transport in the presence of electron-phonon interacion based on the numerical renormalization group[4,5] and the non-equilibrium Keldysh formalism[7,8]. These works reported about the softening of the local phonon mode, and the enhancement of the charge susceptibility. These phenomena point toward the realization of the charge-Kondo effect, caused by the degeneracy of zero and doubly occupied electron states. In the present work, using abelian bosonization, for the first time to our knowledge to attack the local electron-phonon problem, we can not only confirm the prediction of previous works, but also study analytically the specific heat, the phonon Green's function, the charge susceptibility and especially the local density of states. We follow the softening of phonons from weak to strong coupling, and connect the present problem with the underscreened Kondo model in magnetic field.

We consider spinless fermions interacting with a single, dispersionless Einstein phonon mode, mainly at zero temperature. Coupling to acoustic phonons would also be a fruitful proposition, but the essence of physics is readily captured by the simplest model. When the coupling of the electron density to the phonon displacement field is isotropic, the model can be mapped onto a single branch of chiral fermion interacting with a single Einstein phonon only at the origin, and is suitable for Abelian bosonization.

In the Hamiltonian language, the model is given by:

$$H = -iv \int_{-L/2}^{L/2} dx \Psi^+(x)\partial_x \Psi(x) + gQ\rho(0) + \frac{P^2}{2m} + \frac{m\omega_0^2}{2}Q^2, \tag{1}$$

and only the radial motion of the particles is accounted for by chiral (right moving) fermion field[11], $\rho(x) =: \Psi^+(x)\Psi(x) :$ is the electron density, L is the length of the system, v is the Fermi velocity, g describes the local electron-phonon coupling, m and ω_0 are the phononic mass and frequency, respectively, Q and P are the phonon displacement field and momentum conjugate to it. In spirit, this model is similar to the underscreened Kondo model in a magnetic field (which quenches the remaining degrees of freedom) with phonons replacing the impurity spin, since the phonon displacement field (Q) can take any real values, while the electron density trying to compensate it, is bounded. The underscreened Kondo model in a magnetic field is governed by a Fermi liquid fixed point. We speculate that the model under study produces similar behaviour. When the magnetic field is switched off, the underscreened Kondo model shows singular Fermi liquid behaviour[12], whose analogue in the present case occurs at $g \to \infty$. Since the charge degrees of freedom are coupled to the local bosons, the possibility of observing the "underscreened" charge-Kondo effect opens[3]. The model can

be bosonized via[13,14] $\Psi(x) = \exp\left(i\sqrt{4\pi}\Phi(x)\right)/\sqrt{2\pi\alpha}$ to lead

$$H = v \int_{-L/2}^{L/2} dx(\partial_x\Phi(x))^2 - \frac{g}{\sqrt{\pi}} Q\partial_x\Phi(0) + \frac{P^2}{2m} + \frac{1}{2}m\omega_0^2 Q^2. \tag{2}$$

To determine the dynamics of our system, we start with the evaluation of the Green's function of the phonon displacement field, defined by $D_Q(\tau) = \langle T_\tau Q(\tau)Q(0)\rangle$, whose Matsubara form can easily be calculated using the standard diagrammatic technique as

$$D_Q(i\omega_m) = \frac{1}{m}\frac{1}{\omega_m^2 + \omega_0^2 - 2\rho g^2\chi(\omega_m)/m}, \tag{3}$$

where $\rho = 1/2\pi v$, ω_m is the bosonic Matsubara frequency and

$$\chi(\omega_m) = \sum_{q>0} \frac{(vq)^2}{\omega_m^2 + (vq)^2} \tag{4}$$

is the local susceptibility of the fermions without the phonons. After analytic continuation to real frequencies, it is given by $\chi(\omega \ll W) \approx \rho(W + i\pi\omega/2)$ for small frequencies, W is the cutoff or bandwidth, and the obtained formula holds regardless to the chosen cutoff procedure. The dynamics of the phonons can be inferred by investigating the pole structure of Eq. (3). The excitations energies become complex (i.e. finite lifetime or damping of phonon excitations) in the presence of finite coupling to the electrons, and are given by

$$\omega_{p\pm} = -i\Gamma \pm \sqrt{\omega_0^2 - \Gamma^2 - 4\Gamma W/\pi} \tag{5}$$

with $\Gamma = \pi(g\rho)^2/2m$. Below $\Gamma < \Gamma_1 = -2W/\pi + \sqrt{4W^2/\pi^2 + \omega_0^2}$, the square root in Eq. (5) is real, hence the displacements reach their equilibrium in an oscillatory fashion within a time characterized by $-1/\mathrm{Im}\omega_p$. For higher frequencies, the phonon mode is completely softened, $\mathrm{Re}\omega_p = 0$ (the square root becomes imaginary), the excitations have two different finite lifetimes or dampings determined from Eq. (5) between $\Gamma_1 < \Gamma < \Gamma_2 = \pi\omega_0^2/4W$. In this range, phonons can be excited with zero energy, and all the displacements are relaxed to equilibrium without oscillations. This relaxation slows down close to Γ_2. This region is very narrow, because for realistic values, $\omega_0 \ll W$, it shrinks as $\sim \omega_0^4/W^3$. For higher values of Γ, our approach breaks down, it signals lattice distortion with $\langle Q\rangle \neq 0$, as is indicated by the complete softening of the phonon mode. However, such a phenomenon is impossible in zero dimensional systems, and we ascribe it to bosonization. The explicit functional form of physical quantities on model parameters obtained by bosonization can deviate from the exact one. The phase shifts in impurity problems[15], the correlation exponents in Luttinger liquids determined via bosonization are only correct in the weak coupling limit[2]. This and the previous argumentation suggests, that in reality, Γ_2 should only be reached for $g \to \infty$, but the complete softening predicted at Γ_1 would take place at a finite value of g, and $\Gamma \sim g^2$ only at small g. The general behaviour of the eigenfrequencies is sketched in Fig. 1. The phonon density of states contains two Lorentzians with resonance widths -Im$\omega_{p\pm}$, located at Re$\omega_{p\pm}$. With increasing Γ, they become centered around the origin, and close to Γ_2, the one determined by ω_{p+} tends to $\delta(\omega)$. This is reminiscent to what happens in the channel anisotropic two channel Kondo model[16].

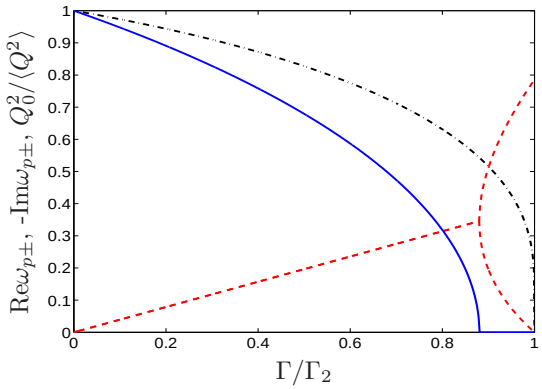

FIG. 1: (Color online) The real (blue solid line) and imaginary (red dashed line) part of the phonon excitation energies, and the inverse of the mean square value of the displacement field (black dashed-dotted line) are visualized as a function of the electron-phonon coupling for $W/\omega_0 = 2$.

The mean value of the displacement field is zero. The mean square value of the displacement field is calculated from Eq. (3) at $T = 0$ as

$$\langle Q^2\rangle = \lim_{T\to 0} T\sum_m D_Q(\omega_m) = Q_0^2 \frac{2i\omega_0}{\pi(\omega_{p+} - \omega_{p-})} \ln\frac{\omega_{p-}}{\omega_{p+}}, \tag{6}$$

where $Q_0^2 = 1/2m\omega_0$ is the value for $g = 0$. It is plotted in Fig. 1. As Γ passes through Γ_2, it diverges, indicating the change in the $\langle Q\rangle = 0$ relation. This is traced back to the transition to the phonon distorted state at $g = \infty$, as discussed below Eq. (5).

In a linear harmonic oscillator, the ground state wave function is a gaussian. It is natural to ask, to what extent this picture holds in the case of finite electron-phonon coupling. The probability distribution of the oscillator coordinator or displacement reads as

$$|\Psi_{osc}(x)|^2 = \langle\delta(Q-x)\rangle = \lim_{a\to 0}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\langle\exp(ik(Q-x)-ak)\rangle. \tag{7}$$

In the second step, a useful representation of the Dirac-delta function was inserted. Since the Hamiltonian is quadratic, or the corresponding action is gaussian for the phonons after integrating out the fermions, the expectation value of the exponent can be calculated following

Ref. 14, which leads to

$$|\Psi_{osc}(x)|^2 = \frac{1}{\sqrt{2\pi\langle Q^2\rangle}} \exp\left(-\frac{x^2}{2\langle Q^2\rangle}\right). \quad (8)$$

The ground state wave function remains gaussian, but the variance ($\langle Q^2\rangle$) increases monotonically with g. The region where the phonons are mainly restricted to, is wider than without electron-phonon coupling. This further corroborates the picture emerging from the previous studies.

The phonon contribution to the free energy can be calculated by using Pauli's trick of integrating over the coupling constant. After some algebra, one arrives at

$$\Omega = \Omega_0 + \int \frac{dx}{2\pi} b(x) \tan^{-1}\left(\frac{2\Gamma x}{x^2 - \omega_0^2(1-(\Gamma/\Gamma_2))}\right), \quad (9)$$

where Ω_0 is the free energy in the absence of coupling between the electrons and phonon, $b(x)$ is the Bose distribution function, and the integral should be limited to the bandwidth, but this can be sent to infinity when obtaining quantities by differentiating Ω[16]. One has to carefully chose the appropriate phase angle of the $\tan^{-1}$ function. This expression is similar to the free energy of the two channel Kondo model in a magnetic field ($\sim \omega_0\sqrt{1-(\Gamma/\Gamma_2)}$ here) along the Emery-Kivelson line[17], after replacing the Bose distribution function with the Fermi one. However, our "magnetic field" cannot be switched off, hence the entropy is zero at $T = 0$, similarly to the underscreened Kondo model[18]. The specific heat can be calculated by $C(T) = -1/T(\partial^2\Omega/\partial T^2)$. Its low temperature behaviour due to phonons reads as

$$C_p(T) = \frac{\pi T}{6v}\frac{\Gamma}{\Gamma_2 - \Gamma}, \quad (10)$$

which sharpens when Γ_2 is approached. The exponential freezing-out of the Einstein phonon changes to a linear T dependence, and adds to the Sommerfeld coefficient of the conduction electrons, and enhances it. Had we chosen acoustic phonons, their T^3 specific heat would also be overwhelmed at low temperatures. At higher temperatures, a broad bump shows up in the specific heat as a function of temperature due to the presence of g. This can serve as an identifier of the local electron-phonon interaction, and is shown in Fig. 2.

The phonons are expected to have a profound impact on the electronic properties. Had we integrated them out, we would have arrived to a local dynamic electron-electron interaction, attractive at low energies and repulsive for higher ones. Static interactions already modify significantly the electronic response, as was demonstrated in the Wolff model[19–21]. In the followings we are going to see the effect of dynamic one explicitly on the electron system.

The electric charge is defined through $\rho(x) = \partial_x\Phi(x)/\sqrt{\pi}$. The local charge correlation function is evaluated from Eq. (2) using the diagrammatic technique,

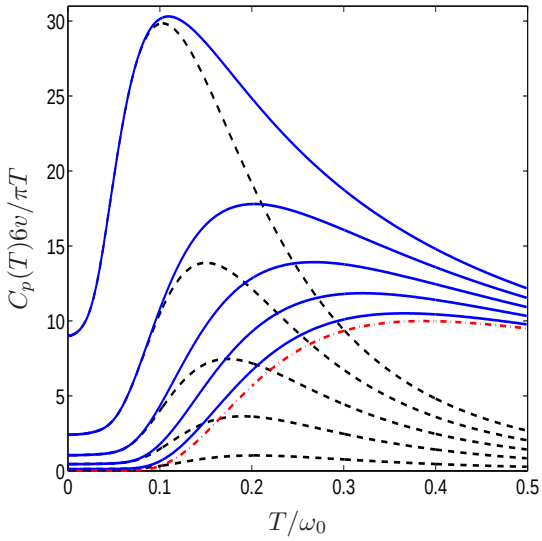

FIG. 2: (Color online) The total (blue solid line) phonon specific heat contribution for different values of the coupling constant $\Gamma/\Gamma_2 = 0.1$, 0.3, 0.5, 0.7 and 0.9, $W/\omega_0 = 10$ from bottom to top. The red dashed dotted line shows the pure phononic $\Gamma = 0$ specific heat, while the black dashed curves stands for their difference due to the finite coupling g. Note the sharpening of the broad bump at low T as Γ increases.

and along the real frequency axis it reads as

$$\chi_{charge}(\omega) = \frac{2\rho\chi(\omega)}{1 + \frac{2g^2\rho}{m(\omega^2 - \omega_0^2)}\chi(\omega)}. \quad (11)$$

This is the standard result in the random-phase-approximation, which turns out to be the exact one in the present case. Most of the many body contributions are canceled by the Ward identity, which relates the vertex function and the electron propagator. This could be expected from the fact that the model is solvable by bosonization. The very same phenomenon revealed itself during the study of the Wolff impurity model[20,22]. The dynamic nature of the phonons is observable in the denominator of Eq. (11). In the static limit, the effective interaction between the electrons is attractive, and changes to repulsive for frequencies exceeding the phonon energy ω_0. The static limit of the charge susceptibility simplifies to $\chi_{charge}(0) = 2\rho^2 W/(1-(\Gamma/\Gamma_2))$. In accordance with Eq. (5), this also predicts the transition to the distorted phase, which would be accompanied by the rearrangement of the charges as well. This signals that our model is on the brink of charge Kondo effect.

Since we work with spinless electrons, the single particle Green's function can be evaluated, unlike in the SU(N) Wolff model[19,21] or the two channel Kondo model[17]. There, such a calculation would involve formally $\sqrt{\Psi(x)}$, which is difficult to work with. The local

retarded Green's function is defined as

$$G_R(t) = -i\Theta(t)\langle\{\Psi(t),\Psi^+(0)\}\rangle = -i\Theta(t)\frac{\exp(-4\pi\langle\Phi^2\rangle)}{2\pi\alpha}\times \\ \times\left[\exp(4\pi\langle\Phi(t)\Phi(0)\rangle)+\exp(4\pi\langle\Phi(0)\Phi(t)\rangle)\right], \quad (12)$$

where in the second step we made use of the gaussian nature of the action and used the usual tricks of operator manipulation[13,14]. The task is to evaluate the correlator $C(t) = \langle\Phi(t)\Phi(0)\rangle$, its counterpart follows from time reversal symmetry as $\langle\Phi(0)\Phi(t)\rangle = C(-t)$. Given the fact that the bosonized Hamiltonian (Eq. (2)) is quadratic, we can evaluate this expectation value at bosonic Matsubara frequencies, then by transforming it to imaginary times, finally we can read off $C(t)$ after careful analytic continuation to real times. First we find for the Matsubara form that

$$C(\omega_m) = \frac{1}{4|\omega_m|} - \frac{m}{2}\Gamma D_Q(\omega_m). \quad (13)$$

Here the first term is responsible for the $1/\tau$ decay of fermionic correlations. Fortunately, the second expression, accounting for the phonon contribution, is separated from the first one, and does not require ultraviolet regularization unlike the first one, where the large ω_m part need to be cut off to avoid divergences. Its Fourier transform with respect to ω_m yields to the imaginary time ordered expression for the correlator, from which the desired relation can be obtained as

$$C(t) - C(0) = \frac{1}{4\pi}\ln\left(\frac{\alpha}{\alpha+ivt}\right) - \frac{m}{2}\Gamma(D_Q(t) - \langle Q^2\rangle), \quad (14)$$

where the equal time correlator need to be subtracted to regularize the first term on the right hand side and

$$D_Q(t) = \frac{2i}{m\pi(\omega_{p+}-\omega_{p-})}\left(f(\omega_{p+}t) - f(\omega_{p-}t)\right) \quad (15)$$

with

$$f(x) = -\sin(x)\mathrm{Si}(x) - \frac{\pi}{2}\sin(x) - \cos(x)\mathrm{Ci}(-x), \quad (16)$$

where $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$ are the sine and cosine integrals. At large times, its decay is characterized by the damping, $\mathrm{Im}\omega_{p\pm}$, and the frequency of oscillations by $\mathrm{Re}\omega_{p\pm}$. By plugging this formula to $G_R(t)$, we evaluate the retarded single particle Green's function. The local density of states follows as

$$\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{\infty} dt\exp(i\omega t)G_R(t), \quad (17)$$

and its change is denoted by $\Delta\rho(\omega) = \rho(\omega) - \rho_0$, ρ_0 is the dispersionless density of states in the pure system. It is shown in Fig. 3. The change in the residual density of states, $\Delta\rho(0)$ is positive for all values of Γ, and diverges at Γ_2 in agreement with other quantities[4]. Similar phenomenon occurs in the underscreened Kondo model with the offset of magnetic field[12]. The significant increase in $\Delta\rho(0)$ should be detected in point contact spectroscopy or by scanning tunneling microscopy experiments in bulk materials. For small values of Γ, a steplike drop occurs with increasing frequency close to $\omega = \mathrm{Re}\omega_{p\pm}0$, which smoothens as the electron-phonon coupling increases. As a function of increasing frequency, damped oscillations are exhibited in the density of states. First it even "undershoots" its pure value around $\omega = -\omega_{p+}\omega_{p-}$, and can severely suppress the density of states, but never produces negative values ($\rho(\omega) > 0$ always). Then "overshooting" occurs before reaching zero, similarly to Friedel oscillations, but as a function of energy and not of spatial coordinate. These features are different from that induced by a non-magnetic impurity or by a magnetic one, and the reason is the effective, dynamically attractive interaction generated by the phonons.

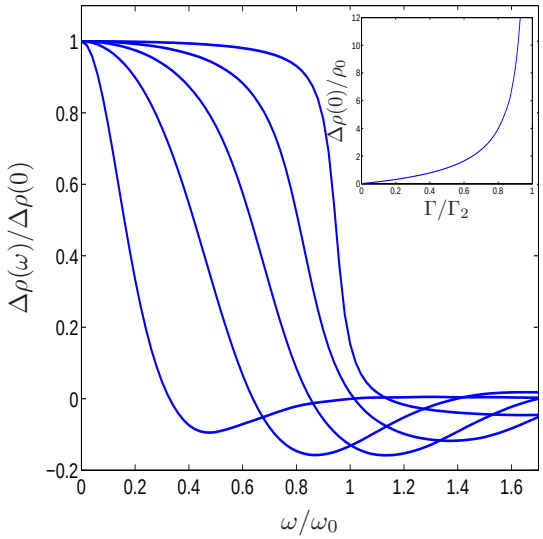

FIG. 3: The change of the local electron density of states at the impurity site is shown for $W/\omega_0 = 2$ for Γ/Γ_2=0.1, 0.3, 0.5, 0.7 and 0.9 from right to left. At the last value, the resonance frequency of the phonon is purely imaginary. The inset visualizes the change in the residual density of states, which diverges at $\Gamma = \Gamma_2$.

In conclusion, we have studied a model of spinless fermions interacting with an Einstein phonon using Abelian bosonization. With increasing coupling, the phonon mode softens, and at $g \to \infty$, distortion occurs. The present model resembles closely to the underscreened Kondo model in magnetic field. Especially, the singular Fermi liquid behaviour[12] of the latter in zero magnetic field corresponds to the $g \to \infty$ limit of the former. Closed expression is derived for the local electronic density of states, which diverges at the critical coupling, in accordance with the singular Fermi liquid picture. This should be observable in point contact spectroscopy, or on a molecule trapped near a tunnel junction, and influence the current-voltage characteristic as well.

We thank P. Fazekas and P. S. Cornaglia for useful

discussions.

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