Electron–phonon interaction for adiabatic anharmonic phonons

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Abstract

A model with Holstein-like electron–phonon coupling is studied in the limit of adiabatic phonons. The phonon distribution is anharmonic with two degenerate maxima. This model can be related to fermions in a correlated binary alloy and describes microscopic phase separation. We discuss the weak and strong electron–phonon coupling limits and present a qualitative phase diagram. In terms of the phononic displacements it consists of a homogeneous, an alternating, and a disordered phase. There is a first-order phase transition between the homogeneous and the alternating phases, and a second-order phase transition between the alternating and the disordered phases. The opening of a gap inside the disordered phase is treated using dynamical mean-field theory.

1. Introduction

Adiabatic (or static) phonons have been discussed in the literature by many authors [1–4]. They can be considered as a first step towards a full treatment of the electron–phonon interaction in a many-body system. The latter is plagued by a number of difficulties like the unrestricted number of phonons at each lattice site. These problems are partially avoided by taking the adiabatic limit, where the phonons are described with classical degrees of freedom.

In general, the electron–phonon interaction can be successfully treated in a self-consistent perturbation theory, as long as the corresponding coupling is small. This approach is known as the Migdal–Eliashberg theory [5, 6]. At strong coupling, however, this theory experiences problems known as the breakdown of the Migdal–Eliashberg theory. In the case of the Holstein model it was argued by Benedetti and Zeyher that this breakdown at large electron–phonon coupling is associated with the appearance of an effective double-well potential for the atomic positions [7]. It is conceivable that the appearance of a degeneracy in the atomic positions is a source of problems in a perturbative approach like that of Migdal and Eliashberg.

The aim of this work is to discuss the physics of anharmonic adiabatic phonons with two degenerate maxima of the distribution at each lattice site in terms of a simple model. We ignore

the electronic spin which is of no interest in our study and concentrate only on the scattering of spinless fermions. Our discussion includes the derivation of an effective Ising spin model, where the spins represent the degenerate maxima of the distribution, and the application of the dynamical mean-field theory, which corresponds to the infinite-dimensional limit of the model. Our anharmonic model can also be considered as the strong coupling regime of the adiabatic Holstein model.

The paper is organized as follows. The model is discussed in section 2 and an effective distribution of the adiabatic phonons is derived in section 3. In the limit of discrete phonon degrees of freedom (correlated binary alloy) this is related to a distribution of Ising spins (section 3.1). The latter is studied in the weak (section 4.1) and strong coupling (section 4.2) limits. In section 5 we apply the dynamical mean-field approach to our model. Finally, the results of the two approaches are discussed in section 6.

2. The model for adiabatic phonons

The Holstein-like model with spinless fermions coupled to adiabatic anharmonic phonons is defined by the Hamiltonian H_{f} and the thermal phonon distribution P_0 at inverse temperature β:

$$H_{\mathrm{f}} = -\bar{t}\sum_{\langle r,r'\rangle} c_r^{\dagger}c_{r'} - \sum_r (\mu - g x_r)c_r^{\dagger}c_r, \qquad P_0(x_r) \propto \exp[-\beta U(x_r^2-1)^2]. \tag{1}$$

$c_r^{\dagger}$ (c_r) are the fermionic creation (annihilation) operators and the real variable x_r represents the phonon degrees of freedom. The latter describes the displacements of the atoms at sites r, assuming that it is thermally distributed according to P_0. The fermions feel the displaced atom as a one-body potential $-gx_r$. For harmonic phonons we have a Gaussian distribution

$$P_h(x_r) \propto \exp(-\beta x_r^2), \tag{2}$$

instead of P_0, with $x_r = 0$ as the position with maximal weight. The anharmonic distribution P_0, on the other hand, has two degenerate positions with maximal weight, namely $x_r = \pm 1$. The coupling to the fermions, however, can break this degeneracy, leading to homogeneous and inhomogeneous equilibrium distributions of the atomic positions on the lattice.

Although the model defined in equation (1) looks like a model for Anderson localization this is not a correct interpretation. The reason is that a model for Anderson localization requires the averaging of the Green function with respect to P_0. This is not the case for the adiabatic phonons: a grand-canonical ensemble of spinless fermions, coupled to adiabatic phonons, is defined by the partition function

$$Z = \mathrm{Tr}\ \mathrm{e}^{-\beta H} = \int \mathrm{Tr}_{\mathrm{f}}\ \mathrm{e}^{-\beta H_{\mathrm{f}}} \prod_r P_0(x_r)\,\mathrm{d}x_r \tag{3}$$

which represents an *annealed* average of the fermionic system. The fermionic Green function then reads in the temperature formalism

$$G_{r,t;r',0} = \frac{1}{Z}\mathrm{Tr}\big[\mathrm{e}^{-(\beta-t)H}c_r\mathrm{e}^{-tH}c_{r'}^{\dagger}\big] = \frac{1}{Z}\int \mathrm{Tr}_{\mathrm{f}}\big[\mathrm{e}^{-(\beta-t)H_{\mathrm{f}}}c_r\mathrm{e}^{-tH_{\mathrm{f}}}c_{r'}^{\dagger}\big]\prod_r P_0(x_r)\,\mathrm{d}x_r. \tag{4}$$

The anharmonicity is related to previous studies where an effective anharmonic (double-well) potential for the electrons was found [7]. Here the main idea is that the tunnelling of the fermions is much faster than the motion of the atoms between the two maxima of the distribution. Therefore, the dynamics of the phonons is negligible and adiabatic phonons can serve as phononic degrees of freedom.

3. Effective phonon distribution

The trace with respect to the fermions can be performed in equations (3) and (4), since the fermions do not interact directly in the Hamiltonian H_{f} [8]. This gives the determinant of an $N \times N$ matrix, averaged with respect to the distribution P_0, such that the partition function reads [9]

$$Z = \int \det\left[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-gx)}\right] \prod_r P_0(x_r)\,\mathrm{d}x_r.$$

N is the number of lattice sites and $\hat{t}$ is the hopping matrix. The integrand of Z is a positive expression and can be considered as an effective distribution of the adiabatic phonons that replaces P_0:

$$P(\{x_r\}) = \frac{1}{Z}\det\left[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-gx)}\right] \prod_r P_0(x_r). \tag{5}$$

3.1. Ising spin representation

For the evaluation of the effective phonon distribution given in equation (5) we consider the limiting case $U \gg 1$. Then the distribution P_0 selects

$$x_r \to S_r = \pm 1,$$

where S_r is formally an Ising spin which describes discrete displacements of the atoms. This case can be considered as a correlated binary alloy (CBA), where the correlations are mediated by the fermions through the determinant in equation (5). The partition function is now a sum with respect to Ising spins:

$$Z = \sum_{\{S_r=\pm 1\}} Z(\{S_r\}) \qquad \text{with } Z(\{S_r\}) = \det\left[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-gS)}\right].$$

Then the fermionic Green function is a resolvent, averaged with respect to the effective phonon distribution [9]:

$$\langle(\mathrm{i}\omega + \mu + \hat{t} - gS)^{-1}\rangle_{\mathrm{Ising}},$$

where $\langle\cdots\rangle_{\mathrm{Ising}}$ is the CBA distribution

$$P(\{S_r\}) = \frac{\det[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-gS)}]}{\sum_{\{S_r\}} \det[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-gS)}]}. \tag{6}$$

It should be noted that the CBA distribution is not Z_2 invariant, i.e. not invariant under a global flip of the spins or the coupling constant g, in contrast to the distribution P_0.

4. Approximations of the CBA distribution

The effective phonon distribution given in equation (6) can describe different types of order of the displacements of the atoms, depending on the inverse temperature β. At high temperatures we expect a paramagnetic (disordered) distribution, and at low temperatures some kind of order. Some insight can be obtained by evaluating the distribution in the asymptotic regimes of weak as well as strong coupling. More details of the calculations are given in the appendix. For further simplification of the results we restrict our interest to the low temperature regime, i.e. to $\beta \sim \infty$.

4.1. Weak coupling limit

The weak coupling limit is obtained from an expansion for small values of g. According to the appendix the regime describes an uncorrelated binary alloy with the distribution

$$P_{\mathrm{w}}(\{S_r\}) = \prod_r \frac{\mathrm{e}^{-\beta g h S_r}}{\sum_{S_r=\pm 1} \mathrm{e}^{-\beta g h S_r}}, \qquad \text{with } h = \int \Theta(\mu + \epsilon(k)) \frac{\mathrm{d}^d k}{(2\pi)^d}, \tag{7}$$

where $\epsilon(k)$ is the dispersion of the tunnelling term $\hat{t}$. Thus the fermions create a homogeneous magnetic field gh for the Ising spins with $0 \leqslant h \leqslant 1$. This favours the atomic position $x_r = -1$:

$$\langle S \rangle = -\tanh(\beta g h).$$

For a low fermion density (i.e. for $\mu + \epsilon(k) < 0$) there is no magnetic field ($h = 0$). Then the Ising spins are paramagnetic (disordered without correlations).

4.2. Strong coupling limit

The strong coupling regime enables us to apply an expansion in terms of the fermion hopping. As shown in the appendix we can write for the effective phonon distribution

$$P_{\mathrm{s}} \propto \prod_r \left[1 + \mathrm{e}^{\beta(\mu - g S_r)}\right] \exp\left\{\sum_{r,r'} [E_1(S_r + S_{r'}) + E_2 S_r S_{r'}]\right\}$$

with coefficients

$$E_1 = \hat{t}_{rr'}\hat{t}_{r'r}\frac{\beta^2}{8}\left[\frac{\mathrm{e}^{\beta\mu-\beta g}}{(1+\mathrm{e}^{\beta\mu-\beta g})^2} - \frac{\mathrm{e}^{\beta\mu+\beta g}}{(1+\mathrm{e}^{\beta\mu+\beta g})^2}\right] \quad \text{and}$$

$$E_2 = \hat{t}_{rr'}\hat{t}_{r'r}\left\{\frac{\beta^2}{8}\left[\frac{\mathrm{e}^{\beta\mu-\beta g}}{(1+\mathrm{e}^{\beta\mu-\beta g})^2} + \frac{\mathrm{e}^{\beta\mu+\beta g}}{(1+\mathrm{e}^{\beta\mu+\beta g})^2}\right] - \frac{\beta}{4g}\frac{\mathrm{e}^{\beta\mu}\sinh(\beta g)}{1+\mathrm{e}^{2\beta\mu}+2\mathrm{e}^{\beta\mu}\cosh(\beta g)}\right\}.$$

This gives in the low temperature regime ($\beta \sim \infty$):

$$E_1 \sim 0, \qquad E_2 \sim \begin{cases} -\dfrac{\beta}{4g}\hat{t}_{rr'}\hat{t}_{r'r} & \text{for } -g < \mu < g \\ 0 & \text{otherwise} \end{cases}$$

and for the distribution density

$$P_{\mathrm{s}} \sim \begin{cases} 1 & \text{for } \mu < -g \\ \exp\left\{-\beta\left[\displaystyle\sum_r (\mu+g)S_r/2 + \bar{t}^2 \sum_{\langle r,r'\rangle} S_r S_{r'}/4g\right]\right\} & \text{for } -g < \mu < g \\ \exp\left(-\beta g \displaystyle\sum_r S_r\right) & \text{for } g < \mu. \end{cases} \tag{8}$$

In terms of the Ising spins there is a paramagnetic phase for $\mu < -g$. For $-g < \mu < g$ the competition of the magnetic field term and the antiferromagnetic spin–spin interaction leads to a first-order phase transition between ferromagnetic and antiferromagnetic states, at least for low temperatures. A simple mean-field approximation reveals that the Ising ground state is an antiferromagnet for $\mu < \mathrm{d}\bar{t}^2/g - g$ and a ferromagnet for $\mu > \mathrm{d}\bar{t}^2/g - g$. Finally, for $\mu > g$ there is always a ferromagnetic state with $\langle S \rangle < 0$. These three phases are shown in the low temperature $\mu - g$ phase diagram in figure 1.

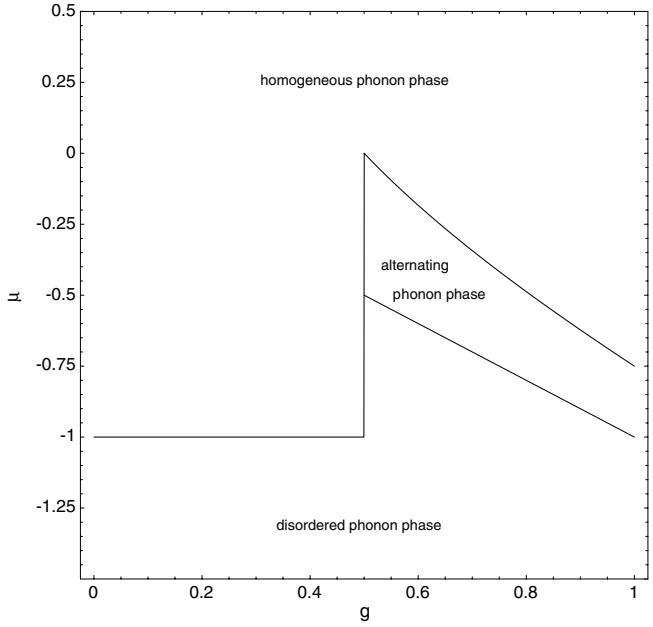

Figure 1. Mean-field $T = 0$ phase diagram. Thermal fluctuations are likely to create a disordered phase for small values of g and any value of μ.

5. The DMFT equations

The spectral density of the itinerant fermions can be evaluated conveniently using the dynamical mean-field theory (DMFT), originally developed for the Hubbard model [4, 10, 11]. The main idea of the DMFT is the infinite-dimensional limit of the system. This limit is characterized by a simplified scattering process in comparison with the situation in a finite-dimensional system: the scattering of the *same* pair of fermions is very unlikely due to the large phase space. In the case of our adiabatic phonon system it is very unlikely that a fermion scatters with the *same* phonon more than once. This enables us to consider only the effective scattering on a single site. A consequence is that the effective correlation between the phonons, discussed in the weak and strong coupling regimes, is excluded in the DMFT [13].

Formally, the Green function reads

$$G_n = \int \frac{\rho(\epsilon)}{\mathrm{i}\omega_n + \mu - \Sigma_n - \epsilon}\,\mathrm{d}\epsilon \tag{9}$$

with ω_n the Matsubara frequency and ρ the density of states of free fermions on the lattice. Moreover, the Green function can also be written as [4]

$$G_n = \frac{w_0}{G_n^{-1} + \Sigma_n + g} + \frac{1 - w_0}{G_n^{-1} + \Sigma_n - g}. \tag{10}$$

Equation (10) yields the self-consistent equation for the self-energy Σ_n:

$$\Sigma_n = -\frac{1}{2G_n} \pm \frac{1}{2}\sqrt{G_n^{-2} + 4g^2 + 4g(1 - 2w_0)G_n^{-1}}, \tag{11}$$

where the coefficient w_0 depends on the self-energy and G_n as

$$w_0 = \left(1 + \mathrm{e}^{-\beta g} \prod_{n=-\infty}^{\infty} \frac{\Sigma_n + G_n^{-1} + g}{\Sigma_n + G_n^{-1} - g}\right)^{-1}.$$

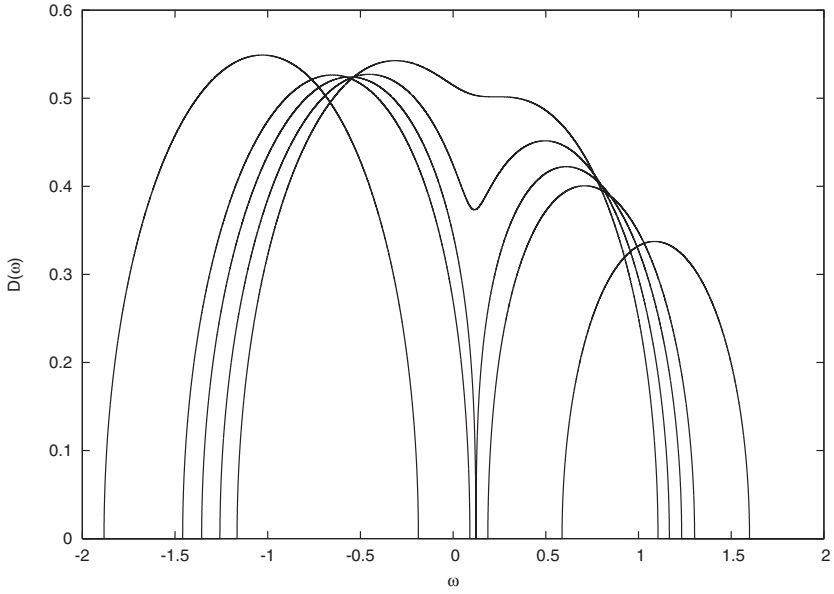

Figure 2. Density of states for varying coupling strengths ($g = 0.3$, 0.4, 0.5, 0.6, and 1.0) for $T = 1$, $\mu = 0$, and $\bar{t} = 0.5$. Increasing electron–phonon coupling favours the gap formation.

From these three equations the self-energy Σ_n and the Green function G_n can be determined numerically [4].

For a special form of the density of states ρ the integral in equation (9) can be evaluated explicitly. This simplifies the numerical effort of solving the equations substantially. An example is the case of a semicircular density of states $\rho(\epsilon) = \sqrt{4\bar{t}^2 - \epsilon}/2\pi\bar{t}^2$ which gives [12]

$$G_n = \frac{1}{2\bar{t}^2}\left(\zeta_n - \mathrm{sgn}(\mathrm{Re}\,\zeta_n)\sqrt{\zeta_n^2 - 4\bar{t}^2}\right) \tag{12}$$

with $\zeta_n = \mathrm{i}\omega_n + \mu - \Sigma_n$. w_0 is determined numerically using equations (11) and (12). Substituting $\Sigma_n = \mathrm{i}\omega_n + \mu - G_n^{-1} - \bar{t}^2 G_n$ in equation (10) yields a cubic equation for the Green function [14]:

$$\bar{t}^4 G_n^3 - 2\eta\bar{t}^2 G_n^2 + (\eta^2 + \bar{t}^2 - g^2)G_n - [\eta + g(1 - 2w_0)] = 0 \tag{13}$$

with $\eta = \mathrm{i}\omega_n + \mu$. Analytic continuation ($\mathrm{i}\omega_n \to \omega + \mathrm{i}0^+$, $G_n \to G(\omega)$) and the condition $\mathrm{Im}\,G(\omega) < 0$ leads to the fermionic density of states $D(\omega) = -\mathrm{Im}\,G(\omega)/\pi$. Our results are shown in figure 2.

6. Discussion of the results

The phase diagram of our model is complex and has been studied by two different mean-field approaches, a classical one for the Ising spin representation (i.e. the CBA) and the DMFT. It consists of paramagnetic, ferromagnetic, and antiferromagnetic phases in terms of the Ising spins (cf equation (8)). The latter correspond to displacement configurations of the adiabatic phonons: disordered phonons (or phonon liquid) and homogeneous and alternating (charge-ordered) phases. There are phase transitions between these phases. According to our mean-field calculations, a first-order transition appears between the metallic homogeneous

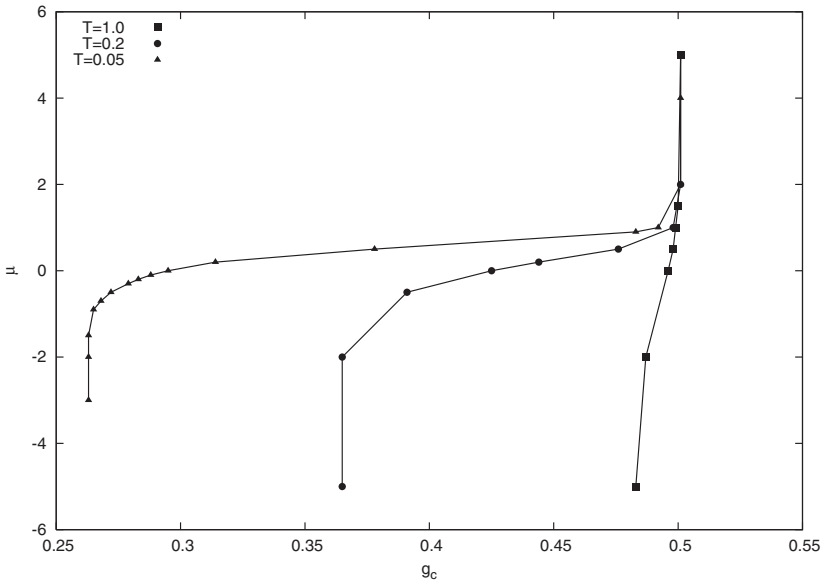

Figure 3. Chemical potential versus the critical value of the electron–phonon coupling g_c plotted for $\bar{t} = 0.5$ and several temperatures $T = 0.05$, 0.2, and 1.0 (from left to right). The lines are guides to the eyes.

and the insulating alternating phases. The transition between the disordered and insulating alternating phases is second order. The disordered phase is most likely also insulating due to Anderson localization of the fermions. The weak coupling behaviour of equation (7) indicates a disordered phase for $\mu < -2\,\mathrm{d}\bar{t}$ and a homogeneous phase for $\mu > -2\,\mathrm{d}\bar{t}$. These results are summarized in the qualitative phase diagram of figure 1.

Our DMFT results do not agree very well with the picture obtained from the CBA. This might be a consequence of the fact that the DMFT is a local approach, at least in the version discussed in this paper [13]. There is a critical coupling g_c that indicates the opening of a gap for $g > g_c$. In our model g_c changes with μ and T (see figure 3). Large positive values for μ imply $g_c \approx 0.5$ for the hopping rate $\bar{t} = 0.5$. Decreasing μ results in a reduced value of g_c. The lower the temperature the lower the value of g_c. Lower temperatures favour the insulating phase.

The gap opening at g_c cannot be directly linked to a characteristic change of the ordering of the adiabatic phonons, at least not in the regime of strong coupling and/or high temperatures. The anharmonicity plays a crucial role here because it can open a gap of width $2g$ already in the absence of tunnelling. This can be compared with the situation of harmonic phonons: in equation (1) we replace the distribution P_0 by the harmonic distribution in (2) and study the strong coupling regime. The treatment of the determinant of equation (5) in strong coupling does not depend on the type of the random variable x_r. Thus we obtain the distribution for x_r as given in equation (8), except for an extra factor $P_h(x_r)$. In contrast to the distribution of the Ising spins, this distribution has only disordered or homogeneously ordered phases for x_r and no staggered order, implying the absence of a gap. It remains an open question whether or not the gap opening and the order of the adiabatic anharmonic phonons are related in general. This can be compared with the metal–insulator transition of the Hubbard model inside a paramagnetic phase [10, 11]. It might be that the gap opening in both cases does not require any additional

change of order in the models. A common feature of these models is the appearance of two eigenstates which are separated by the interaction energy if electronic tunnelling is absent. This is fundamental also for the gap formation in the system with electronic tunnelling. Such a separation of electronic state does not exist for adiabatic *harmonic* phonons. A remaining puzzle is that the strong coupling result in equation (8) is an antiferromagnetic Ising model that provides a metallic homogeneous or a gapped alternating phase, whereas the DMFT result indicates only a gap in the disordered phase.

The experimental relevance of our results can be linked to the complex structures observed in manganites and related materials [15, 16]. It is believed that the interesting properties of these materials (like the colossal magnetoresistance, or CMR) are caused by a frozen mixture of ferromagnetic metallic and antiferromagnetic (or charge-ordered) insulating clusters. The typical size of these clusters is of the order of ten to a hundred nanometres. This has been understood as electronic phase separation due to the proximity to a first-order phase transition. Although our model contains far fewer degrees of freedom than a realistic description of manganites, the phenomenon of self-organized phase separation due to frozen metallic (i.e. homogeneously ordered) and insulating (i.e. staggered) clusters and a first-order phase transition between the homogeneously ordered and the staggered phases is also essential in our theory in terms of the correlated binary alloy.

7. Conclusions

Anharmonic phonons were studied in the adiabatic limit of the Holstein model. We applied two different approaches to study the effect of the electron–phonon coupling; one is based on a correlated binary alloy (represented by Ising spins), and the other one on the dynamical mean-field theory. These approaches cover different regions of the phase diagram. In terms of the phonons the correlated binary alloy reveals a homogeneous, an alternating (or charge-density wave), and a disordered phase. In terms of the fermions there is a metallic state in the homogeneous phonon phase, and insulating states in the alternating phonon phase (with a gap) and in the disordered phonon phase (without gap). The dynamical mean-field theory, on the other hand, indicates a gapped insulating state inside the disordered phase.

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Appendix. Effective Ising models

The determinant in equation (6)

$$P = \frac{1}{Z}\det\left[\mathbf{1} + \mathrm{e}^{\beta(\mu+\hat{t}-\Delta g S)}\right] \tag{A.1}$$

is expanded in powers of g (weak coupling regime) or in powers of the tunnelling rate $\bar{t}$ (strong coupling regime).

In the weak coupling regime we can expand the argument of the exponential function in powers of g. This gives in leading order

$$P \approx \exp\left\{-\beta g \,\mathrm{Tr}\left[G_0 \mathrm{e}^{\beta(\mu+\hat{t})} S\right]\right\}\Big/ N_{\mathrm{w}} = \exp\left\{-\beta g \sum_r \left[G_0 \mathrm{e}^{\beta(\mu+\hat{t})}\right]_{rr} S_r\right\}\Big/ N_{\mathrm{w}}$$

with $G_0 = (\mathbf{1}+\mathrm{e}^{\beta(\mu+\hat{t})})^{-1}$ and the normalization N_w. $[G_0\mathrm{e}^{\beta(\mu+\hat{t})}]_{rr}$ can be evaluated by Fourier transformation ($\hat{t} \to \epsilon$) as

$$\left[G_0\mathrm{e}^{\beta(\mu+\hat{t})}\right]_{rr} = \int \left[1+\mathrm{e}^{-\beta(\mu+\epsilon(k))}\right]^{-1} \frac{\mathrm{d}^d k}{(2\pi)^d}.$$

In the limit $\beta \to \infty$ the integrand becomes the Heaviside step function $\Theta(\mu+\epsilon(k))$.

The expansion of the expression in equation (A.1) in powers of $\hat{t}$ can be applied in the strong coupling regime:

$$\exp\left\{\mathrm{Tr}\left[\ln\left(\mathbf{1}+\mathrm{e}^{\beta(\mu+\hat{t}-gS)}\right)\right]\right\} \approx \det\left(G_1^{-1}\right)\exp[\mathrm{Tr}(G_1 D) - \tfrac{1}{2}\,\mathrm{Tr}(G_1 D G_1 D)]$$

$$\text{with} \quad G_1^{-1} = \mathbf{1}+\mathrm{e}^{\beta(\mu-gS)} \text{ and } D = \mathrm{e}^{\beta(\mu\hat{t}+gS)} - \mathrm{e}^{\beta(\mu-gS)}.$$

A lengthy but straightforward calculation gives with $A_r = \mu - gS_r$ the relation

$$\mathrm{Tr}(G_1 D) - \frac{1}{2}\,\mathrm{Tr}(G_1 D G_1 D) \approx \frac{\beta}{2}\sum_{r,r'} \frac{\mathrm{e}^{\beta A_r} - \mathrm{e}^{\beta A_{r'}}}{A_r - A_{r'}} \frac{\hat{t}_{rr'}\hat{t}_{r'r}}{(1+\mathrm{e}^{\beta A_r})(1+\mathrm{e}^{\beta A_{r'}})}$$

Since there are only values $S_r = -1, 1$, the term

$$E(S_r, S_{r'}) = \frac{\mathrm{e}^{\beta A_r} - \mathrm{e}^{\beta A_{r'}}}{A_r - A_{r'}} \frac{\hat{t}_{rr'}\hat{t}_{r'r}}{(1+\mathrm{e}^{\beta A_r})(1+\mathrm{e}^{\beta A_{r'}})}$$

can also be expressed as a quadratic form with respect to the Ising spins:

$$E(S_r, S_{r'}) = E_0 + E_1(S_r + S_{r'}) + E_2 S_r S_{r'}$$

with

$$E_0 = \tfrac{1}{4}\,[E(1,1) + E(-1,-1) + 2E(1,-1)]$$

$$= \hat{t}_{rr'}\hat{t}_{r'r}\left\{\frac{\beta^2}{8}\left[\frac{\mathrm{e}^{\beta\mu-\beta g}}{(1+\mathrm{e}^{\beta\mu-\beta g})^2} + \frac{\mathrm{e}^{\beta\mu+\beta g}}{(1+\mathrm{e}^{\beta\mu+\beta g})^2}\right] + \frac{\beta}{4g}\frac{\mathrm{e}^{\beta\mu}\sinh(\beta g)}{1+\mathrm{e}^{2\beta\mu}+2\mathrm{e}^{\beta\mu}\cosh(\beta g)}\right\},$$

$$E_2 = \tfrac{1}{4}\,[E(1,1) + E(-1,-1) - 2E(1,-1)]$$

$$= \hat{t}_{rr'}\hat{t}_{r'r}\left\{\frac{\beta^2}{8}\left[\frac{\mathrm{e}^{\beta\mu-\beta g}}{(1+\mathrm{e}^{\beta\mu-\beta g})^2} + \frac{\mathrm{e}^{\beta\mu+\beta g}}{(1+\mathrm{e}^{\beta\mu+\beta g})^2}\right] - \frac{\beta}{4g}\frac{\mathrm{e}^{\beta\mu}\sinh(\beta g)}{1+\mathrm{e}^{2\beta\mu}+2\mathrm{e}^{\beta\mu}\cosh(\beta g)}\right\},$$

and

$$E_1 = \frac{1}{4}[E(1,1) - E(-1,-1)] = \hat{t}_{rr'}\hat{t}_{r'r}\frac{\beta^2}{8}\left[\frac{\mathrm{e}^{\beta\mu-\beta g}}{(1+\mathrm{e}^{\beta\mu-\beta g})^2} - \frac{\mathrm{e}^{\beta\mu+\beta g}}{(1+\mathrm{e}^{\beta\mu+\beta g})^2}\right].$$

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