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The electron-phonon problem in infinite dimensions

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ABSTRACT: Monte Carlo simulations are performed to examine superconductivity and charge-density-wave fluctuations in the infinite-dimensional electron-phonon problem. The maximum charge-density-wave transition temperature is an order of magnitude smaller than the effective electronic bandwidth and is virtually independent of the phonon frequency. The maximum superconducting transition temperature depends strongly on phonon frequency and is bounded by the maximum charge-density-wave transition temperature. The crossover from weak to strong coupling is illustrated by the evolution of an effective phonon potential that develops a double-well structure as the electron-phonon interaction increases.

Revised version

Migdal and Eliashberg pioneered the study of the electron-phonon problem in the limit where the phonon energy scale is much smaller than the electronic energy scale [1] . Their theory predicts that the transition temperature in the superconducting (SC) channel will increase without an upper bound as the electron-phonon interaction strength increases [2]. A strong-coupling expansion, however, predicts that the system has a transition temperature that decreases as the electron-phonon interaction strength increases and that the charge-density-wave (CDW) channel is favored over the SC channel [3]. As a result, one would like to know if there is a maximum transition temperature, what parameters set the scale for this transition temperature, and what is the character of the ordered state (SC or CDW)?

Monte Carlo (MC) simulations are employed to bridge the gap between weak-coupling and strong-coupling expansions. Previous work has concentrated on one-dimension where it was found that the system always dimerized into a CDW-Peierls state at half-filling [4], and on two-dimensions where it was found that the CDW state was unstable with respect to electron concentration and the system superconducted when doped sufficiently far away from half-filling [5]. Here we will explore the electron-phonon problem in infinite dimensions.

The limit of infinite dimensions is expected to be relevant to models in three (or possibly two) dimensions. In the case of the Hubbard model, the infinite-dimensional solution [6,7] displays all of the qualitative physics of the three-dimensional model (commensurate and incommensurate antiferromagnetism, crossover between metallic and insulating behavior, etc.). The Néel temperature at half-filling in infinite dimensions is *quantitatively* close to the transition temperature in three dimensions [8]. Thus we expect that the electron-phonon problem in infinite dimensions should also capture the relevant physics of its three-dimensional counterpart.

The electron-phonon model chosen here is the Holstein model [9], in which the conduction

electrons interact with local phonon modes:

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle j,k\rangle\sigma} (c^\dagger_{j\sigma} c_{k\sigma} + c^\dagger_{k\sigma} c_{j\sigma}) + \sum_j (g x_j - \mu)(n_{j\uparrow} + n_{j\downarrow}) + \frac{1}{2} M\Omega^2 \sum_j x_j^2 + \frac{1}{2M} \sum_j p_j^2 \quad (1)$$

where $c^\dagger_{j\sigma}$ ($c_{j\sigma}$) creates (destroys) an electron at site j with spin σ, $n_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$ is the electron number operator, and x_j (p_j) is the phonon coordinate (momentum) at site j. The hopping matrix elements span the nearest neighbors of a hypercubic lattice in d-dimensions and the rescaled matrix element t^* sets the energy scale (all energies are measured in units of t^*). The local phonon has a mass M and a frequency Ω associated with it; the combination $\kappa \equiv M\Omega^2$ is the spring constant. The electron-phonon coupling constant is an energy per unit length and is denoted by g. A useful combination of fundamental parameters is the bipolaron binding energy $U \equiv -g^2/M\Omega^2 = -g^2/\kappa$, which determines the energy scale for the effective electron-electron interaction. Once the energy scale is set by t^* and the electron filling is determined by the chemical potential μ, three additional parameters remain: the coupling strength g; the mass M; and the spring constant κ. Here we fix the mass ($M = 1$) and use $|U|$ and Ω as free parameters.

In infinite dimensions ($d \to \infty$) the hopping from one lattice site to its nearest neighbor is scaled to zero [see Eq. (1)] in such a fashion that the free-electron kinetic energy remains finite while the self energy for the single-particle Green's function and the irreducible vertex functions have no momentum dependence and are functionals of the local Green's function [10,11]. The many-body problem is solved by mapping it onto an auxiliary impurity problem [12,13] in a time-dependent field (that mimics the hopping of an electron onto a site at time τ and off the site at a time τ'). The effective action for the impurity problem is [14]

$$\begin{aligned} S_{eff.} = &\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \sum_\sigma \int_0^\beta d\tau [g x(\tau) - \mu] c^\dagger_\sigma(\tau) c_\sigma(\tau) \\ &+ \frac{1}{2} M \int_0^\beta d\tau [\Omega^2 x^2(\tau) + \dot{x}^2(\tau)] \end{aligned} \quad (2)$$

where G_0^{-1} is the "bare" Green's function that contains *all of the dynamical information of the other sites of the lattice*. The interacting Green's function is determined by

$$G_n^{-1} \equiv G^{-1}(i\omega_n) = G_0^{-1}(i\omega_n) - \Sigma(i\omega_n), \tag{3}$$

at each Matsubara frequency $\omega_n = (2n+1)\pi T$. The impurity problem is mapped onto the infinite-dimensional lattice by self-consistently equating the impurity Green's function with the local Green's function of the lattice

$$G_{jj}(i\omega_n) = \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy \frac{\exp(-y^2)}{i\omega_n + \mu - \Sigma_n - y} \quad . \tag{4}$$

The dynamics of the impurity problem is identical to the dynamics of the Anderson impurity model [11–14,6] and may be solved by using the quantum MC algorithm of Hirsch and Fye [15]. Since the bare Green's function G_0^{-1} in Eq. (2) is not *a priori* known, the MC algorithm must be iterated to determine a self-consistent solution for the Green's function of the infinite-dimensional lattice. The procedure [6] is to begin with a bare Green's function G_0^{-1}, use the quantum MC algorithm to determine the self energy Σ, calculate the lattice Green's function from Eq. (4), and determine a new bare Green's function from Eq. (3). This process is iterated until convergence is reached. A variety of two particle properties may also be calculated in the quantum MC approach [16] since the irreducible vertex function is also local. In particular, the static susceptibilities for both the CDW and SC response were determined. The corresponding transition temperatures were calculated by determining the temperature at which the relevant susceptibility diverged (further details on the MC technique are presented elsewhere [6,17]). The results of the MC simulation are compared to various approximation techniques below.

In the limit $|U| << t^*$ a weak-coupling conserving Hartree-Fock approximation [18] should describe the Holstein model well. The electronic self energy is represented by

$$\Sigma_n = -UT \sum_m G_0(i\omega_m) \frac{\Omega^2}{\Omega^2 + (\omega_m - \omega_n)^2} \quad , \tag{5}$$

to lowest order. The full Green's function G is determined self-consistently from the self energy Σ and the bare Green's function G_0 by the same procedure outlined above for the MC calculation. At half-filling the system always orders in a CDW state. The transition temperature is determined by solving the Bethe-Salpeter equation in the traditional manner [19] with the following irreducible vertex function

$$\Gamma_{mn}^{CDW} = U\left[2 - \frac{\Omega^2}{\Omega^2 + (\omega_m - \omega_n)^2}\right] \quad . \tag{6}$$

In the opposite limit of strong coupling ($|U| >> t^*$), the electrons pair into bipolarons and the Holstein Hamiltonian can be mapped onto an anisotropic (XXZ) Heisenberg antiferromagnet in a uniform external field [3,20]. In infinite dimensions the mean-field theory for the spin-$\frac{1}{2}$ anisotropic Heisenberg antiferromagnet is exact and at half-filling the system orders in a CDW state with a transition temperature [3,4]

$$T_c(CDW) = \frac{|t^*|^2}{2|U|}\left[1 + \sum_{n=1}^{\infty} \frac{(-S)^n}{(1+S)(2+S)\cdots(n+S)}\right]. \tag{7}$$

Here the polaron band-narrowing parameter S is defined to be $S \equiv |U|/\Omega$.

The results for these approximation schemes are compared to the MC results in Fig. 1 for an intermediate value of the phonon frequency ($\Omega/t^* = 0.5$). As the phonon frequency varies, the height of the peak remains essentially the same, but the critical value of g (where the maximum CDW transition temperature is attained) changes.

In order to shed some light on the transition from weak to strong coupling the MC simulations were sampled to determine a time-averaged effective phonon potential. The probability $P(x)$ that the phonon coordinate $x(\tau_\ell)$ lies in the interval from x to $x+\delta x$ was calculated for each time slice τ_ℓ and averaged over all time slices. An effective phonon potential $V_{eff.}(x)$ was then extracted from the probability distribution $P(x) \propto \exp[-\beta V_{eff.}(x)]$ [21]. This effective potential is plotted in Fig. 2 for four different values of the electron-phonon coupling strength at a temperature $T = 1/7$. In the case of weak coupling ($g = 0.325$), the potential

appears harmonic. The potential flattens when $U \approx t^*$ ($g = 0.5$) and as g increases further, a double-well structure develops [22]. The barrier height grows linearly with g as does the separation of the minima. The peak of the $T_c(g)$ curve for the CDW transition (see Fig. 1) is reached at the point where the barrier height is on the order of T_c ($g = 0.625$). Beyond this point ($g = 1.0$) the system enters the strong-coupling regime and T_c decreases.

In the region where the double-well potential has developed, the phonon coordinate tunnels between the wells and the tunneling rate decreases as the temperature is lowered below the barrier height. At this point the system may be considered to be a random mixture of empty sites and bipolarons that fluctuates in time. Tunneling through the barrier produces correlations between the empty-sites and the bipolarons resulting in a condensed CDW phase. However as the barrier height increases, the transition temperature drops because the tunneling is suppressed. The transition temperature reaches its maximum at the point where the barrier height is equal in magnitude to T_c.

As the system is doped away from half-filling there is a competition between CDW order and superconductivity . The CDW susceptibility is calculated at all momenta $\mathbf{q}$ in the Brillouin zone and found to either diverge at the "antiferromagnetic" point or not to diverge at all (there is no evidence for incommensurate order in $d = \infty$[17]). Figure 3 displays the results for the transition temperature of the Holstein model with $\Omega/t^* = 0.5$ as a function of electron concentration at three different values of the electron-phonon coupling ($g = 0.4$, $g = 0.5$, and $g = 0.625$). In the weak-coupling regime ($g = 0.4$), the transition from CDW order to SC order occurs at $n_c = 0.84$, and the SC transition temperature is about a factor of four smaller than the CDW transition temperature at half-filling. As the coupling strength is increased ($g = 0.5$), the superconducting transition temperature does increase, but the critical electron filling has decreased to $n_c = 0.52$. As the interaction strength is increased further ($g = 0.625$), the maximum superconducting transition temperature decreases because the critical electron density where SC onsets has been pushed out too far [23]. For

fixed electron-phonon interaction strength g, the critical electron concentration $n_c(g,\Omega)$ is an increasing function of the phonon frequency approaching 1 as the frequency becomes infinite (since the Holstein model maps onto an attractive Hubbard model as $\Omega \to \infty$) and approaching 0 as the frequency vanishes (since a static phonon field cannot support superconductivity). Therefore, the maximum SC transition temperature depends strongly upon phonon frequency, and is always bounded from above by the CDW transition temperature at half-filling.

In conclusion, the electron-phonon problem (Holstein model) has been examined in the limit of large spatial dimensions including the first exact treatment of the crossover from weak to strong coupling. The maximum CDW transition temperature is set by the electronic energy scale, and is virtually *independent* of the phonon frequency. Its magnitude is on the order of $0.15t^*$ and occurs at half-filling when the polaron binding energy $|U|$ is on the order of the bandwidth t^*. The maximum SC transition temperature, on the other hand, is very strongly dependent upon the phonon frequency (as evidenced by the frequency dependence of the SC-CDW phase boundary in Fig. 3). In the case considered here ($\Omega/t^* = 0.5$), the maximum SC transition temperature appears to be a factor of five smaller than the maximum CDW transition temperature $T_c(SC) \leq 0.035t^*$. The crossover from a weak-coupling picture to a strong-coupling picture is illustrated with an effective phonon potential that continuously changes from a (harmonic) single well to a (anharmonic) double well.

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23. It is possible that as the temperature is reduced below the critical temperature for CDW order another transition from CDW order to SC order occurs as seen in Ref. 3. Monte Carlo simulations would need to be run in the ordered CDW phase to detect such a secondary transition.

FIGURE CAPTIONS

Figure 1. T_c for the commensurate CDW transition at half-filling in the Holstein model (with $\Omega/t^* = 0.5$) plotted against g. The CHF approximation (dashed line) and strong-coupling theory (solid line) are compared to the MC results (solid dots). The size of the plotting symbols is chosen to roughly correspond to the combined statistical and systematic error.

Figure 2. Effective phonon potential for the Holstein model at half-filling (with $\Omega/t^* = 0.5$ and $\beta = 7$) plotted versus the renormalized coordinate $x^* = -xM\Omega^2/2g$. Four values of g are included: $g = 0.325$ (dotted line); $g = 0.5$ (dashed line); $g = 0.625$ (solid line); and $g = 1.0$ (chain-dashed line).

Figure 3. T_c versus electron concentration in the Holstein model for $\Omega/t^* = 0.5$. Three values of g are shown: $g = 0.4$ (dotted line); $g = 0.5$ (dashed line); and $g = 0.625$ (solid line). The solid dots represent CDW order and the open diamonds represent SC order. The size of the plotting symbols is chosen to roughly correspond to the combined statistical and systematic error.