# Competition between Electron-Phonon Attraction and Weak Coulomb Repulsion

J. K. Freericks[1] and Mark Jarrell[2]
[1]*Department of Physics, Georgetown University, Washington, D.C. 20057-0995*
[2]*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221*
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The Holstein-Hubbard model is examined in the limit of infinite dimensions. Conventional wisdom states that charge-density-wave (CDW) order is more strongly affected by Coulomb repulsion than superconducting order (SC) because of the pseudopotential effect. We find that the CDW-SC phase boundary does move toward half filling as the Coulomb repulsion increases, but, surprisingly, the CDW transition temperature is initially more robust against Coulomb repulsion than the superconducting transition temperature. This puzzling feature is resolved by an analysis of weak-coupling perturbation theory.

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Interacting electronic systems with both electron-electron repulsion and phonon-mediated attractive interactions display a rich variety of ground states due to the competition between these interactions. In conventional low-temperature superconductors (SC), the electron-phonon interaction dominates over the Coulomb repulsion, since the latter is reduced from its bare values by the so-called pseudopotential effect [1,2]. The electron-phonon interaction is also believed to be responsible for charge-density-wave (CDW) order in weakly doped $BaBiO_3$. However, the Coulomb repulsion dominates over the electron-phonon interaction in the high-temperature superconducting cuprates, with commensurate spin-density-wave (SDW) order occurring in the (undoped) parent compounds.

Although the Coulomb interaction (in the form of the Hubbard model [3,4]) and the electron-phonon interaction (in the form of the Holstein model [5]) have both been extensively studied, there has been only limited work on the combined Holstein-Hubbard model [6] and only one exact theorem for the case of an attractive Coulomb interaction [7].

The conventional wisdom for the effect of the Coulomb interaction on a superconductor with strong electron-phonon interactions is that the Coulomb repulsion is *reduced* from its bare values. This is because the electron-phonon interaction is *retarded*, allowing the electrons to attract each other, through the exchange of a virtual phonon, without being at the same lattice site at the same time. A quantitative estimate for this so-called pseudopotential effect finds that the (dimensionless) Coulomb repulsion $\rho(\mu)U_C$ is reduced to

$$\rho(\mu)U_C^* := \frac{\rho(\mu)U_C}{1 + \rho(\mu)U_C \ln(W/2\omega_D)}, \qquad (1)$$

where $\rho(\mu)$ is the electronic density of states (DOS) for an electron (of one spin) at the Fermi energy, $U_C$ is the bare Coulomb repulsion, $W$ is the electronic bandwidth, and $\omega_D$ is the Debye frequency. There is, however, no pseudopotential effect for a CDW distortion, because retardation effects play a limited role in a *static* CDW, where the electrons remained paired at every other lattice site. Therefore, the conventional wisdom says that the Coulomb repulsion will reduce the transition temperatures for CDW order much more than for SC, and that the SC phase is thereby stabilized relative to the CDW phase.

The dynamical mean-field theory (MFT) [8] has been employed to exactly solve the Hubbard [9] and Holstein [10] models in infinite spatial dimensions using the quantum Monte Carlo (QMC) algorithm of Hirsch and Fye [11]. The dynamical MFT is a generalization of the Migdal-Eliashberg theory of superconductivity [12] that includes *all* effects of vertex corrections and nonconstant DOS.

The Holstein-Hubbard model,

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} + g\sum_i x_i(n_{i\uparrow} + n_{i\downarrow} - 1) + U_C \sum_i n_{i\uparrow}n_{i\downarrow} + \frac{1}{2}\sum_i\left(\frac{p_i^2}{M} + M\Omega^2 x_i^2\right), \qquad (2)$$

is written in standard notation: $c_{i\sigma}^\dagger$ is a creation operator for an electron localized at site $i$ with spin $\sigma$; $n_{i\sigma} := c_{i\sigma}^\dagger c_{i\sigma}$ is the corresponding number operator; $x_i$ is the phonon coordinate at site $i$; and $p_i$ is its momentum. The hopping integral is $t =: t^*/2\sqrt{d}$, the deformation potential is $g$, $U_C$ is the Coulomb repulsion, $\Omega$ is the phonon frequency, and $M = 1$ is the phonon mass. The scaled hopping integral $t^*$ determines the energy unit and is set equal to 1 ($t^* = 1$). The effective electron-electron attraction (due to phonon exchange) satisfies $U = -g^2/M\Omega^2$, and competes with the Coulomb repulsion $U_C > 0$.

The Holstein-Hubbard model is solved by QMC simulation. The QMC algorithm determines the local electronic Green's function $G(i\omega_n)$ at each fermionic Matsubara frequency $\omega_n := \pi T(2n + 1)$, by mapping the infinite-dimensional lattice to an impurity problem [3,13]. The Green's function satisfies

$$G(i\omega_n) = F_\infty[i\omega_n + \mu - \Sigma(i\omega_n)], \qquad (3)$$

with $\Sigma(i\omega_n)$ the electronic self-energy and $F_\infty(z) := \int dy\, \rho(y)/(z - y)$ the rescaled complementary error

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function of a complex argument [$\rho(y) := \exp(-y^2)/\sqrt{\pi}$ is the noninteracting DOS].

The momentum-dependent susceptibility $\chi(\mathbf{q}) = T\sum \tilde{\chi}_{mn}(\mathbf{q}) =: T\sum \tilde{\chi}(\mathbf{q}, i\omega_m, i\omega_n)$ (for CDW, SDW, or SC order) satisfies a Dyson equation

$$\tilde{\chi}_{mn}(\mathbf{q}) = \chi^0_m(\mathbf{q})\delta_{mn} - T\sum_p \chi^0_m(\mathbf{q})\Gamma_{mp}\tilde{\chi}_{pn}(\mathbf{q}) \quad (4)$$

for each ordering vector $\mathbf{q}$, with $\chi^0$ the relevant bare susceptibility, and $\Gamma_{mp}$ the local irreducible vertex function. The bare susceptibility for commensurate [$\mathbf{q} = \mathbf{Q} := (\pi, \pi, \pi, \ldots)$] CDW or SDW order is

$$\chi^0_n(\mathbf{Q}) := -\frac{G(i\omega_n)}{i\omega_n + \mu - \Sigma(i\omega_n)}, \quad (5)$$

with a more complicated form for incommensurate wave vectors [14]. On the other hand, the uniform bare susceptibility for SC order satisfies

$$\chi^{0'}_n(\mathbf{0}) := -\frac{\mathrm{Im}G(i\omega_n)}{\omega_n - \mathrm{Im}\Sigma(i\omega_n)}. \quad (6)$$

The irreducible vertex functions are extracted directly from the QMC data [5]. Figure 1 displays the lowest-order diagrammatic contributions to the vertex functions in the (a) CDW, (b) SC, and (c) SDW channels.

Transition temperatures are found by calculating the temperature where the susceptibility for each ordered phase diverges. The highest transition temperature $T_c$ determines the initial symmetry of the ordered phase.

The phase diagrams for the Holstein-Hubbard model, with $g = 0.5$, $\Omega = 0.5$, $U = -1.0$, and $U_C = 0.0, 0.25, 0.5, 0.75$, are displayed in Fig. 2. These phase diagrams are determined by QMC calculations and by a second-order iterated perturbation theory (IPT) [15] (there are no detectable phase transitions with the IPT for $U_C = 0.75$). The solid dots (lines) depict the commensurate CDW, the open dots (dotted lines) depict the incommensurate order, and the open triangles (dot-dashed lines) depict the SC phase for the QMC (IPT) calculations.

The QMC data display two types of notable behavior. First, there are no stable incommensurate phases when $U_C = 0$; the incommensurate phases become stable near

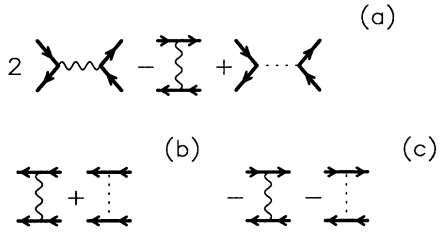


FIG. 1. Lowest-order contribution to the irreducible vertex function in the (a) charge-density-wave, (b) superconducting, and (c) spin-density-wave channels. The solid lines denote electron propagators, the wiggly lines denote phonon propagators, and the dotted lines denote the Coulomb repulsion.

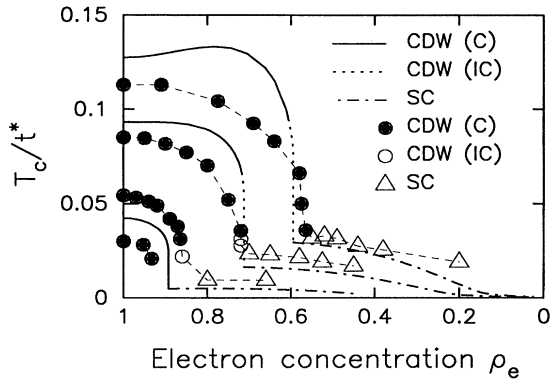


FIG. 2. Phase diagram for the Holstein-Hubbard model with $g = 0.5$, $\Omega = 0.5$, $U = -1.0$, and $U_C = 0.0, 0.25, 0.5$, and 0.75. The solid dots (lines) are for the commensurate CDW, the open dots (dotted lines) are for the incommensurate CDW, and the open triangles (dot-dashed lines) are for the SC as determined from a QMC (IPT) calculation. There are no transitions detected by the IPT for $U_C = 0.75$. The dashed line through the QMC points is a guide to the eye.

the CDW-SC phase boundary only for $U_C > 0$. The explanation for this is simple: if the SC phase was ignored, the CDW phase would suffer a commensurate-incommensurate phase transition as $T_c \to 0$ in a similar fashion to the repulsive Hubbard model [16]; however, for $\Omega = 0.5$, the SC transition temperature is greater than the highest incommensurate CDW transition temperature, precluding its appearance at $U_C = 0$. As $U_C$ increases, the SC $T_c$ drops below the maximal incommensurate CDW $T_c$, which allows the incommensurate order to occur (in the limit $\Omega \to 0$, incommensurate order will occur at $U_C = 0$ because the SC $T_c$ will be smaller than the maximal incommensurate $T_c$, whereas in the limit $\Omega \to \infty$ there is never any incommensurate order, since CDW phases occur only at half filling). Second, even though the region where the CDW phase is stable shrinks as $U_C$ is increased, the CDW transition temperature *is reduced by a smaller factor* than the SC transition temperature, in opposition to the conventional wisdom.

The IPT approximation is reasonably accurate for both the CDW and SC $T_c$'s and for the phase boundary between CDW and SC order. The approximate CDW transition temperature is again reduced by a smaller factor than the SC transition temperature as $U_C$ increases. Thus one can understand this effect by studying the weak-coupling formalism. The IPT errs only by predicting a large incommensurate CDW-ordered region at $U_C = 0$, which shrinks as $U_C$ increases, exactly opposite to what the QMC found, and it is unable to predict any finite $T_c$'s for $U_C = 0.75$.

The modification of the CDW transition temperature at half filling is plotted versus $U_C$ in Fig. 3. The CDW phase is followed for $0 < U_C < |U|$, since a SDW phase is expected to be the stable phase for $U_C > |U|$ at half filling

[6] (this can be seen at weak coupling by comparing the CDW vertex to the SDW vertex in a power series as shown in Fig. 1, indicating $\Gamma_{\rm SDW} > \Gamma_{\rm CDW}$ when $U_C > |U|$). $T_c(U_C)$ is smaller than $T_c(U_C = 0)$ in the weak-coupling regime ($g < 0.625$) and the curves are nearly linear in $U_C/|U|$, with a decreasing slope as $g$ increases. In the strong-coupling regime ($g = 1.0$), the Coulomb repulsion initially *enhances* the transition temperature (since it reduces the energy of the virtual state formed by breaking the bipolaron) before causing a reduction as $U_C \to |U|$.

Much of the unexpected and notable behavior found in the QMC and IPT results can be illustrated within an analytic approximation. A weak-coupling analysis of the CDW and SC transition temperatures is performed in the square-well approximation [where the soft cutoffs $\Omega^2/\{\Omega^2 + (\omega_m - \omega_n)^2\}$ are replaced by hard cutoffs $\theta(\omega_c - |\omega_m|)\theta(\omega_c - |\omega_n|)$] [17]. A first-order calculation is accurate only to the lowest order in $1/U$. Since this analysis is standard, we only summarize the main results here. Extensions of these results to include vertex corrections will be given elsewhere.

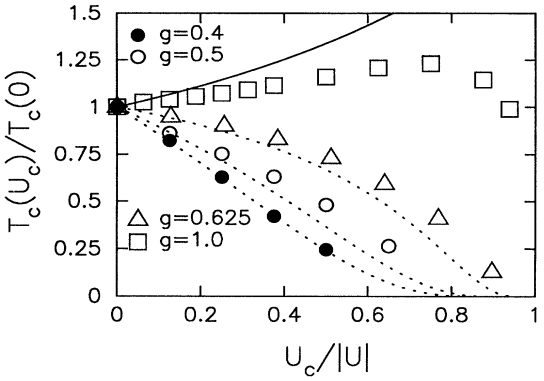


FIG. 3. Relative change in the CDW transition temperature at half filling due to Coulomb repulsion. Four different cases are shown: $g = 0.4$ (solid dots), $g = 0.5$ (open dots), $g = 0.625$ (open triangles), and $g = 1.0$ (open squares). The dotted lines are the weak-coupling approximations for $g = 0.4$, 0.5, and 0.625. The parameter $I$ is adjusted to produce the correct slope as $U_C \to 0$. The solid line is a fourth-order strong-coupling approximation for the $g = 1.0$ case.

In the SC channel, for small $U_C$ one finds [18]

$$\frac{T_c^{\rm SC}(U_C)}{T_c^{\rm SC}(0)} \approx \exp\left[-\frac{1}{\rho(\mu)|U| - \rho(\mu)U_C/[1 + \rho(\mu)U_C I]} + \frac{1}{\rho(\mu)|U|}\right] \approx \exp\left[-\frac{U_C/|U|}{\rho(\mu)|U|}\right], \tag{7}$$

for arbitrary filling, with

$$I := -\frac{T}{\rho(\mu)} \sum_{|\omega_n|>\omega_c} \frac{{\rm Im}F_\infty(i\omega_n + \mu)}{\omega_n} \approx \frac{2}{\pi}\int_0^\infty \frac{dy}{y}\frac{\rho(y+\mu) + \rho(y-\mu)}{2\rho(\mu)} \tan^{-1}\frac{y}{\omega_c}, \tag{8}$$

and $\omega_c$ is the cutoff frequency for the square well (the second line holds when $T_c \ll \omega_c$). In the limit $\omega_c \to 0$, one finds $I \to \ln(W/2\omega_c)$, as in the original work [1], but the above expression also holds for arbitrary electronic DOS [19].

Calculations in the CDW phase are more difficult. Restricting to the case of half filling ($\mu = 0$) and again for small $U_C$, one finds

$$\frac{T_c^{\rm CDW}(U_C)}{T_c^{\rm CDW}(0)} \approx \exp\left[-\frac{1}{\rho(0)[\{2 - \alpha(U_C)\}|U| - U_C]} + \frac{1}{\rho(0)\{2 - \alpha(0)\}|U|}\right] \approx \exp\left[-\frac{U_C/|U| + \alpha(U_C) - \alpha(0)}{\{2 - \alpha(0)\}^2\rho(0)|U|}\right], \tag{9}$$

with $\alpha(U_C)$ a parameter that measures the reduction of the direct electron-phonon attraction by the exchange diagrams in Fig. 1(a). This parameter satisfies $0 < \alpha < 1$ with $\alpha \to 0$ as $\Omega \to 0$ and $\alpha \to 1$ as $\Omega \to \infty$ [5]. An estimate for $\alpha$ (in the square-well approximation) yields

$$\alpha(U_C) \approx 1 - \frac{I\rho(0)(|U| - U_C)}{1 - I\rho(0)|U|}, \tag{10}$$

which does approach 1 as $\omega_c \to \infty$ ($I \to 0$) and 0 as $\omega_c \to 0$ [$I \to 1/\rho(0)(2|U| - U_C)$] [19]. Substituting Eq. (10) into Eq. (9) finally yields

$$\frac{T_c^{\rm CDW}(U_C)}{T_c^{\rm CDW}(0)} \approx \exp\left[-\frac{U_C}{|U|}\left(\frac{1}{\rho(0)|U|} - I\right)\right]. \tag{11}$$

The resolution of the puzzle of how $U_C$ affects $T_c$(CDW) vs $T_c$(SC) is seen by examining the small $U_C$ limits of Eqs. (7) and (9). The pseudopotential effect disappears in the SC channel as $U_C \to 0$, and the effect on $T_c$ is enhanced away from half filling since the DOS satisfies $\rho(\mu) < \rho(0)$. On the other hand, the effect of $U_C$ on the CDW transition temperature is further reduced by the parameter $I$ in Eq. (11). For these two reasons, $U_C$ initially reduces the SC $T_c$ more than it does the CDW $T_c$. Conventional wisdom, however, is restored when $\rho(\mu) \approx 1/\ln(W/2\omega_D)$ as the pseudopotential effect becomes operative.

Figure 3 shows the weak-coupling results (with the parameter $I$ fitted to the QMC data for small Coulomb repulsion). One can see the weak-coupling formalism is excellent for $g = 0.4$, but becomes less accurate as the coupling strength increases.

How is this analysis modified in the conventional limit of $\Omega \to 0$? Since $\alpha \to 0$ in this limit, the robustness of the CDW $T_c$ against $U_C$ actually *increases*. The

pseudopotential effect still vanishes for small Coulomb repulsion [$\rho(\mu)U_C \ll 1/\ln(W/2\omega_D)$], but the crossover value of $U_C$, where the conventional wisdom is restored, is also small, and $U_C$ does not lie in this small-Coulomb-repulsion regime for conventional materials.

The CDW phase becomes less robust against $U_C$ as the system is doped away from half filling. Here the conventional wisdom is also restored, and it explains why both the incommensurate CDW and the SC phases are stabilized relative to the commensurate CDW (in the sense that the CDW-SC phase boundary moves toward half filling and the incommensurate CDW phases become stable).

In the strong-coupling limit, where the electrons are paired into bipolarons at a temperature much higher than the transition temperature for the ordered phase, the initial effect of $U_C$ is to *enhance* the CDW $T_c$, because Coulomb repulsion *reduces* the bipolaron binding energy $E_b$, thereby increasing $T_c \propto 1/E_b$. The analysis for the pure electron-phonon case is easily modified by changing the energy of all intermediate states to take into account the Coulomb repulsion [20]. The CDW transition temperature at half filling becomes

$$\frac{T_c^{\mathrm{CDW}}(U_C)}{T_c^{\mathrm{CDW}}(0)} \approx \frac{1}{1 - U_C/|U|}\left[1 + \sum_{n=1}^{\infty} \frac{(-S)^n}{(1+S')(2+S')\cdots(n+S')}\right] \Bigg/ \left[1 + \sum_{n=1}^{\infty} \frac{(-S)^n}{(1+S)(2+S)\cdots(n+S)}\right] \tag{12}$$

to second order in $|U|$, with $S := |U|/\Omega$ and $S' := S - U_C/\Omega$. This analysis has been extended to fourth order and is plotted with the solid line in Fig. 3.

In conclusion, we have found that the conventional wisdom for how Coulomb repulsion affects the electron-phonon interaction is flawed in assuming the SC transition temperature is more robust than the CDW transition temperature, but is resolved by detailed analysis of the weak-coupling theory. The conventional wisdom is restored away from half filling since it predicts that the Coulomb repulsion moves the CDW-SC phase boundary toward half filling. The conventional wisdom is also restored as $U_C$ increases since the pseudopotential effect becomes active. What happens to the phase diagram for $U_C > |U|$? We conjecture that the CDW phase is taken over by the SDW phase at half filling, but do not know whether or not SC phases can remain stable away from half filling (due to the pseudopotential effect) or if paramagnetism prevails.

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