# Weak-coupling expansions for the attractive Holstein and Hubbard models

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Weak-coupling expansions (conserving approximations) are carried out for the attractive Holstein and Hubbard models (on an infinite-dimensional hypercubic lattice) that include all band-structure and vertex correction effects. Quantum fluctuations are found to renormalize transition temperatures by factors of order unity, but may be incorporated into the superconducting channel of Migdal-Eliashberg theory by renormalizing the phonon frequency and the interaction strength.

Interacting electron-phonon systems sustain both charge-density-wave (CDW) and superconducting (SC) order. Migdal[1] and Eliashberg[2] showed that a self-consistent theory for the electron-phonon problem can be constructed that neglects so-called vertex corrections (Migdal's theorem) in the limit were the phonon frequency is small compared to the Fermi energy. Numerical calculations of SC transition temperatures based upon experimentally extracted (interacting) electron-phonon spectral densities[3] soon followed. The Migdal-Eliashberg (ME) theory is successful for predicting transition temperatures (and other materials properties) of virtually all low-temperature superconductors.[4,5]

However, ME theory assumes that the electronic bandwidth is infinite, and that vertex corrections may be completely ignored. Although the former can be handled by simple modifications of the basic theory,[4,6] the latter require complicated extensions of the ME framework. Grabowski and Sham[7] carried out such an analysis for the interacting electron gas and found that vertex corrections strongly suppressed $T_c$ for plasma frequencies larger than 10% of the Fermi energy. Van Dongen[8] analyzed the Hubbard model (which can be viewed as the infinite-frequency limit of an electron-phonon model) and showed that quantum fluctuations (vertex corrections) reduced Hartree-Fock transition temperatures by more than a factor of 3.

In this contribution, ME theory is extended to include vertex corrections and produce weak-coupling expansions for $T_c$ that are accurate for the entire range of phonon frequencies (Coulomb repulsion effects are neglected here). Comparison of these weak-coupling expansions are made to quantum Monte Carlo simulations over a wide range of parameter space. Effects due to vertex corrections are strong when expressed in terms of the bare microscopic parameters, but can be incorporated into the ME theory (to lowest order) by renormalizing these parameters.

The electron-phonon Hamiltonian chosen here is that of the Holstein model[9] in which conduction electrons interact with localized (Einstein) phonons:

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

where $c_{j\sigma}^\dagger$ ($c_{j\sigma}$) creates (destroys) an electron at site $j$ with spin $\sigma$, $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$ is the electron number operator, and $x_j$ ($p_j$) is the phonon coordinate (momentum) at site $j$. The hopping matrix elements connect the nearest neighbors of a hypercubic lattice in $d$ dimensions and for concreteness the infinite-dimensional limit ($d\to\infty$) of Metzner and Vollhardt[10] is taken ($1/d$ corrections should be less than 5% in three dimensions[8]). The unit of energy is chosen to be the rescaled matrix element $t^*$. The phonon has a mass $M$ (chosen to be $M=1$), a frequency $\Omega$, and a spring constant $\kappa \equiv M\Omega^2$ associated with it. The electron-phonon coupling constant is denoted by $g$; the effective electron-electron interaction strength is then the bipolaron binding energy

$$U \equiv -\frac{g^2}{M\Omega^2} = -\frac{g^2}{\kappa} \,. \quad (2)$$

In the limit where $\kappa$ remains finite and $\Omega$ is large compared to the bandwidth ($\Omega\to\infty, U=$ finite), the Holstein model maps onto the attractive Hubbard model[11]

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle j,k\rangle\sigma} (c_{j\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{j\sigma}) + U\sum_j n_{j\uparrow}n_{j\downarrow} \,, \quad (3)$$

with $U$ defined by Eq. (2).

Our weak-coupling expansions are based upon the conserving approximations of Baym and Kadanoff:[12] The free energy $\Phi$ is expanded to a given order in the interaction strength; the self-energy $\Sigma(i\omega_n)$ is determined by functional differentiation $\Sigma(i\omega_n) = \delta\Phi/\delta G(i\omega_n)$ at each Matsubara frequency $\omega_n \equiv (2n+1)\pi T$; and the irreducible vertex functions $\Gamma(i\omega_m, i\omega_n)$ (in the relevant channels) are determined by a second functional differentiation. The free energy must be expanded to order $U^2$ in order to determine the correct transition temperature in the limit $|U|\to 0$.[8] The necessary diagrams for the free energy in the Holstein model are presented in Fig. 1. Note that conventional ME theory is identical to a first-order (Hartree-Fock) conserving approximation for the SC channel (with the exception that the phonon propagator is dressed), but is quite different in the CDW channel, because exchange diagrams are important even at the Hartree-Fock level.[12]

The many-body problem in infinite dimensions maps onto a self-consistently embedded Anderson impurity

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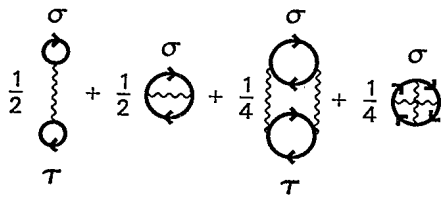


FIG. 1. First- and second-order contributions to the free energy in a conserving approximation for the Holstein model. The solid lines are dressed electronic Green's functions and the wiggly lines are phonon propagators. The spin indices $\sigma$ and $\tau$ are summed over.

problem because the self-energy has no momentum dependence.[13,14] The self-consistent embedding of the impurity problem is solved by iteration:[14] The self-energy is calculated from the dressed (local) Green's functions by a conserving approximation for the impurity problem $\Sigma[G]$ and the new (local) Green's function is determined by the embedding

$$G(i\omega_n) = \int_{-\infty}^{\infty} dy \frac{\rho(y)}{i\omega_n + \mu - \Sigma_n[G] - y} \equiv F_\infty(i\omega_n + \mu - \Sigma_n[G]) \,, \tag{4}$$

with $\rho(y) \equiv \exp(-y^2)/\sqrt{\pi}$ the bare density of states in infinite dimensions.

To illustrate the connection between the microscopic parameters of the Holstein model and the renormalized parameters of the ME theory, the SC transition temperature is calculated in a square-well approximation at half-filling. The transition temperature is assumed to satisfy $T_c << \min(\Omega, t^*)$. In this case, the electron self-energy becomes[12] (to lowest order in $U$)

$$\Sigma(i\omega_n) \equiv i\omega_n Z(i\omega_n),$$
$$Z(i\omega_n) = 1 - U\int_{0^-}^{\infty} dy\rho(y)\frac{\Omega}{\omega_n^2 + (\Omega+y)^2} \,, \tag{5}$$

and the irreducible vertex function in the SC channel satisfies[12] (to second order in $U$)

$$\Gamma_{SC}(i\omega_m, i\omega_n) = UT\left\{\theta(\omega_c - |\omega_m|)\theta(\omega_c - |\omega_n|)\left[1 + \frac{2U}{\pi}\int_0^\infty dy F_\infty^2(iy)\frac{y^2}{\Omega^2+y^2}\right] - \frac{U}{\pi}\int_0^\infty dy F_\infty^2(iy)\frac{\Omega^4}{(\Omega^2+y^2)^2}\right\} \tag{6}$$

in the square-well approximation[4] with $\omega_c$ the cutoff frequency. The transition temperature is determined in the standard fashion,[3–5]

$$T_c/t^* = \exp\left[-\frac{1}{|U|\rho(0)}\right]\exp\left[-\frac{2}{\sqrt{\pi}}\int_0^\infty dy F_\infty^2(iy)\right]\exp\left[-\int_0^\infty dy\frac{\rho(y)}{\rho(0)}\frac{\Omega}{(\Omega+y)^2}\right] \times\left\{0.85\exp\left[-\frac{2}{\pi}\int_0^\infty\frac{dy}{y}\frac{\rho(y)}{\rho(0)}\tan^{-1}\frac{y}{\omega_c}\right]\right\}\exp\left[\frac{2}{\sqrt{\pi}}\int_0^\infty dy F_\infty^2(iy)\frac{\Omega^2}{\Omega^2+y^2}\left\{1+\frac{1}{2}\frac{\Omega^2}{\Omega^2+y^2}\right\}\right] \,, \tag{7}$$

including all nonvanishing factors in the limit $|U| \to 0$. The first factor is the contribution to lowest order in $|U|$. The remaining terms are constant factors arising from the following four sources (in order of appearance): the phonon self-energy contributions, the electronic self-energy contributions, the finite bandwidth contributions, and the vertex corrections. The phonon self-energy term (equal to $\exp[2.493]$ in infinite dimensions) is normally incorporated into the dressed phonon propagator in ME theory $\lambda \equiv |U|\rho(0)/[1 - 2.493|U|\rho(0)]$. The electron self-energy term approaches $e^{-1}$ as $\Omega \to 0$ and $e^0$ as $\Omega \to \infty$. The finite-bandwidth term should be proportional to $\Omega$ if the phonon frequency is much smaller than the electronic energy scale, but should be replaced by the electronic energy scale when the phonon frequency becomes the largest energy scale. For concreteness, the cutoff frequency is chosen to be $\omega_c = 0.6\Omega$, so that this factor approaches the correct limits of $0.69\Omega$ as $\Omega \to 0$ (Ref. 5) and 0.85 as $\Omega \to \infty$ (Ref. 8). Finally, the fifth term contains the vertex corrections which vanish as $\Omega \to 0$ (Ref. 1) and approach $\exp[-3.739]$ as $\Omega \to \infty$.[8] The above equation for $T_c$ has the correct limits as $\Omega \to 0$ $[T_c = 0.69\Omega\exp\{-(1+\lambda)/\lambda\}]$ and as $\Omega \to \infty$ $[T_c = 0.24\exp\{-1/|U|\rho(0)\}]$. The coefficient of $\exp[-1/|U|\rho(0)]$ in Eq. (7) is plotted in Fig. 2. Note that the maximum occurs at $\Omega \approx 0.8t^*$ (approximately 20% of the effective bandwidth), but the transition temperature is weakly dependent upon $\Omega$ for larger

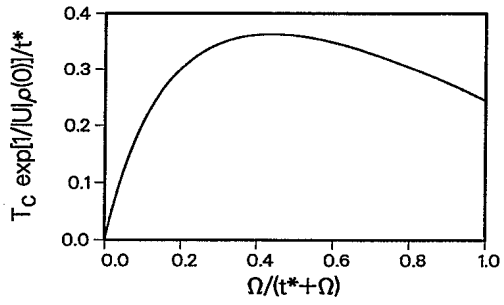


FIG. 2. Constant factor in the analytic formula for the superconducting transition temperature in Eq. (7) plotted as a function of phonon frequency. Note that the constant term has a maximum at $\Omega \approx 0.8t^*$.

values. The ME form for the transition temperature, $T_c = 1.14\omega_c \exp[-(1+\lambda)/\lambda]$, can be fit to the above form in Eq. (7) by renormalizing the electron-phonon interaction $\lambda$ and the cutoff frequency $\omega_c$ [since the contributions from second-order terms (phonon self-energy and vertex corrections) simply modify the prefactor of the $T_c$ formula], explaining its robustness for real materials calculations.

In order to make comparisons with the quantum Monte Carlo calculations,[15] the self-consistent perturbation theory is solved numerically. An energy cutoff employing 256 positive Matsubara frequencies is used, and the self-consistent equations are iterated until the largest deviation of each $G(i\omega_n)$ is less than one part in $10^8$. At half-filling the instability always lies in the CDW channel. The effective electronic bandwidth in infinite dimensions is of order $4t^*$ and the phonon frequency is chosen to be approximately one-eighth of this electronic bandwidth ($\Omega = 0.5t^*$) as in the quantum Monte Carlo simulations.

Both the first-order and second-order conserving approximations are compared to the quantum Monte Carlo data in Fig. 3. The transition temperature determined in the second-order approximation is found to be renormalized (by more than a factor of 2 at low temperatures) from the transition temperature calculated in the first-order approximation. The second-order conserving approximation deviates[16] from the Monte Carlo results when $g$ is greater than $0.4t^*$. Furthermore, the turnover of the transition temperature curve as $g$ increases is not reproduced by these finite-order conserving approximations. Probably an infinite-order summation scheme (such as the fluctuation-exchange approximation[12]) will be required to properly account for this turnover.

In the high-frequency limit ($\Omega \to \infty$), the Holstein model maps onto an attractive Hubbard model. In this limit many "direct" diagrams cancel against "exchange" diagrams (there is no interaction between electrons with the same spin) and the perturbation theory is easier to control. Quantum Monte Carlo simulations have already been performed,[14] and weak-coupling expansions through second order (for transition temperatures) have also been investigated with different techniques.[8,17]

The relevant diagrams for the free energy of the Hubbard model through third order are depicted in Fig. 4.

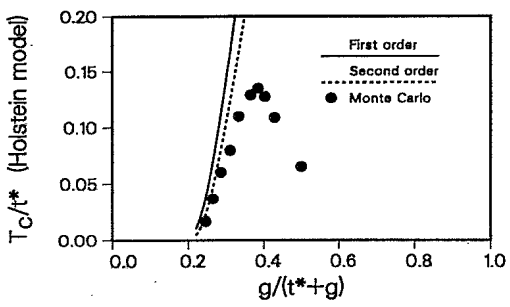


FIG. 3. Charge-density-wave transition temperature for the Holstein model at half-filling with $\Omega = 0.5t^*$ plotted against the electron-phonon interaction $g$. The first-order (solid line), second-order (dashed line), and quantum Monte Carlo results (Ref. 15) (solid dots) are included.

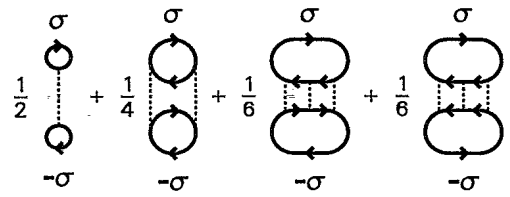


FIG. 4. First- through third-order contributions to the free energy in a conserving approximation for the Hubbard model (the dashed line is the electron-electron interaction $U$). The spin index $\sigma$ is summed over.

The transition temperature in the CDW channel is plotted in Fig. 5 for the first through third-order approximations and for the quantum Monte Carlo simulations. Note that the agreement with the Monte Carlo data is excellent and that the weak-coupling expansions appear to have an alternating character for the Hubbard model with odd orders overestimating $T_c$ and even orders underestimating $T_c$.

Weak-coupling conserving approximations (that are valid for all values of the phonon frequency) have been carried out for the Holstein (and Hubbard) model at half-filling. Calculations must be performed to second order in the effective electron-electron interaction in order to produce the correct limiting behavior as $U \to 0$. Comparison was made with quantum Monte Carlo simulations and excellent agreement was found for weak coupling.

Migdal's theorem states that, in the small-frequency limit, transition temperatures may be determined with a first-order approximation (using a dressed phonon propagator) because the vertex corrections vary as $\Omega/t^*$. This result is easily seen in our framework, but the corrections to $T_c$ due to a nonvanishing phonon frequency can be large (when expressed in terms of the bare parameters). Migdal-Eliashberg theory is, however, quite robust, and the effects of a finite band-structure and vertex corrections (to lowest order) can be incorporated by renormalizing the phonon frequency and the interaction strength (in the superconducting channel).

Extensions of these results off of half-filling, comparison with other techniques such as the fluctuation-

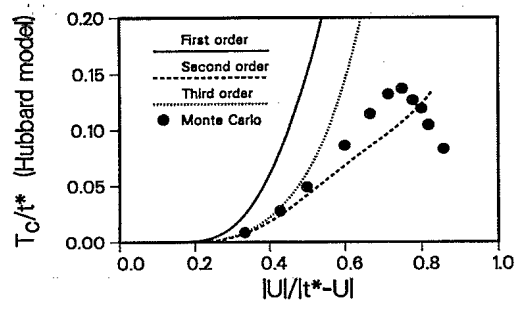


FIG. 5. Charge-density-wave (and superconducting) transition temperature for the Hubbard model at half-filling plotted against the interaction strength $|U|$. The first-order (solid line), second-order (dashed line), third-order (dotted line), and quantum Monte Carlo results (Ref. 14) (solid dots) are included.

exchange approximation[12] or the iterated perturbation theory,[13] and an investigation of Coulomb effects will be presented elsewhere.

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