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Local approximation to the spinless Falicov-Kimball model

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The local approximation is applied to the spinless Falicov-Kimball model in one and two dimensions. The local approximation may be viewed as a zeroth-order expansion in $1/d$ that is exact in the weak-coupling limit. The local approximation rapidly becomes inaccurate as a function of interaction strength in one dimension, but is accurate in two dimensions. This result indicates that the $1/d$ expansion converges rapidly for the Falicov-Kimball model in $d \geq 2$ and that exact solutions of many-body problems in infinite dimensions are quantitatively relevant for physical dimensions.

I. INTRODUCTION

Mathematical models that describe strong electron-electron correlations are difficult to solve exactly. Approximation methods based upon weak- or strong-coupling expansions tend to have limited regions of validity. It is therefore important to study approximation techniques that are valid over the entire range of parameter space. One such approximation is the so-called local approximation.[1] In the local approximation, both the self-energy and the irreducible vertex functions are approximated by time-dependent functionals that are local in space (have no momentum dependence). The local approximation becomes exact as the number of spatial dimensions becomes infinite[2] and can be viewed as the zeroth term in an expansion in powers of $1/d$. The spatial dimensionality enters in both the noninteracting density of states and in the noninteracting (momentum-dependent) susceptibilities (see below), which guarantees that the local approximation will become exact in the weak-coupling limit. Here the local approximation is applied to the simplest many-body problem, the spinless Falicov-Kimball model.[3]

The spinless Falicov-Kimball model has received a lot of interest recently because it can be solved exactly in the infinite-dimensional limit[4-10] and rigorous results can be proven in special cases.[11-17] The spinless Falicov-Kimball model describes the order-disorder transitions of an annealed binary alloy in which itinerant electrons interact locally with static ions. Its Hamiltonian is

$$H=-\frac{t^*}{2\sqrt{d}}\sum_{\langle j,k\rangle}(c_j^\dagger c_k+c_k^\dagger c_j)+U\sum_{j=1}^{N}c_j^\dagger c_j W_j -\mu\sum_{j=1}^{N}c_j^\dagger c_j+E\sum_{j=1}^{N}W_j\ , \quad (1)$$

where $c_j^\dagger$ (c_j) is the creation (destruction) operator for a spinless electron located at site j, and W_j is a classical variable that assumes the value 1 (0) if site j is occupied by an ion of type A (B). The difference in on-site energies between the A ion and the B ion is denoted U, and the chemical potentials for electrons and A ions are represented by μ and ($-E$), respectively. The electrons hop between nearest neighbors on a hypercubic lattice of dimension d with t^* being the rescaled hopping integral (all energies are measured in units of t^*). The thermodynamic limit is taken where the number of lattice sites approaches infinity ($N\rightarrow\infty$) but the electron concentration ($\rho_e=\sum_{j=1}^{N}\langle c_j^\dagger c_j\rangle/N$) and the A-ion concentration ($\rho_i=\sum_{j=1}^{N}W_j/N$) remain constant. The symmetric 50%-50% binary-alloy problem ($\rho_i=\frac{1}{2}$) is the only case considered in this contribution.

The spinless Falicov-Kimball model displays numerous ordered phases including both commensurate and incommensurate order and segregation. At half-filling ($\rho_e=\frac{1}{2}$), the system always orders in a chessboard phase at a low enough temperature[11,12] where the A ions occupy one of the two sublattices of the bipartite lattice and the B ions occupy the other sublattice. When the electron density is low, or the interaction strength is large, the system segregates[13-16] so that all of the A ions and B ions cluster among themselves, separating into two pure phases. In between these two extreme cases there is a rich phase diagram that contains commensurate and incommensurate ordered phases that change both continuously and discontinuously with electron concentration.

In Sec. II the formalism of the local approximation is described and is applied to the spinless Falicov-Kimball model in one and two dimensions. Section III presents the conclusions.

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II. FORMALISM OF THE LOCAL APPROXIMATION

The Falicov-Kimball model is analyzed by determining the local Green's function, which may be represented in terms of a momentum- and frequency-dependent self-energy $\Sigma(\mathbf{k},\omega)$,

$$G(\omega)=\sum_{\mathbf{k}} G(\mathbf{k},\omega) = \sum_{\mathbf{k}} [\omega+\mu-\epsilon(\mathbf{k})-\Sigma(\mathbf{k},\omega)]^{-1} . \tag{2}$$

Here $\epsilon(\mathbf{k})=-\sum_{j=1}^{d}\cos(\mathbf{k}_j)/\sqrt{d}$ is the band structure of a hypercubic lattice in d dimensions and the momentum summation extends over the entire Brillouin zone. The local approximation replaces the momentum-dependent self-energy $\Sigma(\mathbf{k},\omega)$ by a momentum-independent self-energy $\Sigma^{\rm loc}(\omega)$.

The local problem retains a time dependence that mimics the hopping of an electron onto the local site at a time τ and off the local site at a time τ'. The time-dependent problem can be solved to find the self-energy as a functional of the Green's function.[4] The result is

$$\Sigma_n^{\rm loc}[G]=\frac{U}{2}-\frac{1}{2G_n}[1\pm\sqrt{1+U^2G_n^2}] \tag{3}$$

for the 50%-50% binary alloy, where the n subscript denotes evaluation of the Green's function or self-energy at the nth Matsubara frequency $[\omega=i\omega_n\equiv i(2n+1)\pi T]$. The self-consistency relation for the Green's function (2) then becomes

$$G_n=F_d(i\omega_n+\mu-\Sigma^{\rm loc}[G]) \tag{4}$$

in the local approximation, where $F_d(z)$ is the Hilbert transform of the noninteracting density of states in d dimensions, $F_d(z)\equiv\int dy\,\rho_d(y)/(z-y)$ with

$$\rho_1(y)=\frac{1}{\pi}\frac{1}{\sqrt{1-y^2}},\quad \rho_2(y)=\frac{\sqrt{2}}{\pi^2}K(\sqrt{1-y^2/2}) , \tag{5}$$

in one and two dimensions. Here $K(z)$ is the complete elliptic integral of the first kind.

At high temperatures the ions are uniformly distributed throughout the lattice and there is no long-range order. As the temperature is lowered, a second-order phase transition to a state with a modulated charge-density distribution occurs when the susceptibility (at the relevant ordering wave vector) diverges. The static charge-density-wave susceptibility is defined by a density-density correlation function

$$\chi(\mathbf{q},T)\equiv-\frac{1}{N}\sum_{\mathbf{R}_j-\mathbf{R}_k} e^{i\mathbf{q}\cdot(\mathbf{R}_j-\mathbf{R}_k)} \times\int_0^{\beta}d\tau\langle T_\tau c_j^{\dagger}(\tau)c_j(\tau)c_k^{\dagger}(0)c_k(0)\rangle , \tag{6}$$

at each ordering wave vector $\mathbf{q}$. After some tedious algebra,[4] one finds that the transition temperature (in the local approximation) $T_c(\mathbf{q})$ satisfies

$$1=\frac{U^2}{4}\sum_{n=-\infty}^{\infty}\frac{\eta_n(\mathbf{q})}{\left[(i\omega_n+\mu^*-\lambda_n)^2-\frac{U^2}{4}\right][(i\omega_n+\mu^*-\lambda_n)\{1+2G_n\eta_n(\mathbf{q})\}-\eta_n(\mathbf{q})]} , \tag{7}$$

where $\mu^*=\mu-U/2$,

$$\eta_n(\mathbf{q})\equiv-\frac{G_n}{\tilde{\chi}_n^0(\mathbf{q})}-\frac{1}{G_n},\quad \lambda_n\equiv i\omega_n+\mu-G_n^{-1} , \tag{8}$$

and

$$\tilde{\chi}_n^0(\mathbf{q})\equiv-\frac{1}{N}\sum_{\mathbf{q}}G_n(\mathbf{k}+\mathbf{q})G_n(\mathbf{k}) \tag{9}$$

is the "bare" susceptibility.

The local approximation becomes *exact* in the weak-coupling limit because it employs the full momentum dependence of the noninteracting susceptibility $\tilde{\chi}_n^0(\mathbf{q})$. If the local approximation also becomes exact in the strong-coupling limit ($U\to\infty$), then one might expect the local approximation to be a quantitatively accurate approximation for all values of U. In fact, this appears to be true for the spinless Falicov-Kimball model in $d\geq 2$ (see below).

The ordering wave vector $\mathbf{q}$ can be described by a "direction" in reciprocal space and a "magnitude"

$$X(\mathbf{q})=\frac{1}{d}\sum_{i=1}^{d}\cos\mathbf{q}_i . \tag{10}$$

This parametrization is useful because in the infinite-dimensional limit, all wave-vector dependence is contained in the scalar X. For example, the chessboard phase corresponds to $X=-1$ and the segregated phase to $X=1$.

The zero-temperature phase diagram for $d\geq 2$ is expected to separate into two distinct regions:[10] In the weak-coupling regime, the system lies in the segregated phase for a range of electron concentrations from zero up to some finite concentration $\rho_c^{\rm seg}(U)$ that is a function of the interaction strength. As the electron concentration is increased above this critical concentration, the system orders in various long-period (commensurate and incommensurate) phases until the electron concentration is increased to an upper critical concentration $\rho_c^{\rm cb}(U)$ where the system orders into the chessboard phase. The critical concentration for segregation $\rho_c^{\rm seg}(U)$ remains finite in the limit as $U\to 0$. In the strong-coupling regime the lower and upper critical concentrations are equal $[\rho_c^{\rm seg}(U)=\rho_c^{\rm cb}(U)]$ and the system changes directly from the segregated phase to the chessboard phase without any long-period phases intervening. The system also tends toward segregation in the strong-coupling limit $[\rho_c^{\text{seg}}(U\to\infty)\to\frac{1}{2}]$. The one-dimensional phase diagram is a singular limit of the phase diagram for higher dimensions.[10,13] It always lies in the weak-coupling regime with $\rho_c^{\text{cb}}(U)=\frac{1}{2}$ for all U. The system segregates as $U\to\infty$ but not as $U\to 0$ $[\rho_c^{\text{seg}}(U\to\infty)\to\frac{1}{2}$, $\rho_c^{\text{seg}}(U\to 0)\to 0]$.

The phase diagram may be found in the local approximation by determining the critical electron concentrations where the transition temperature $T_c(\mathbf{q})$ is no longer a maximum at $X(\mathbf{q})=\pm 1$. The sign of the directional derivative of $T_c(\mathbf{q})$ in the direction $\mathbf{e}$ satisfies

$$\text{sgn}\,\mathbf{e}\cdot\nabla_{\mathbf{q}}T_c(\mathbf{q})=\text{sgn}\sum_{n=-\infty}^{\infty}\frac{(i\omega_n+\mu^*-\lambda_n)\mathbf{e}\cdot\nabla_{\mathbf{q}}\eta_n(\mathbf{q})}{\left[(i\omega_n+\mu^*-\lambda_n)^2-\dfrac{U^2}{4}\right][(i\omega_n+\mu^*-\lambda_n)\{1+2G_n\eta_n(\mathbf{q})\}-\eta_n(\mathbf{q})]^2} \tag{11}$$

at each ordering wave vector $\mathbf{q}$. In one dimension, it is easy to calculate both the upper and lower critical concentrations and the contours where the value of X remains constant as a function of ρ_e and U. In two dimensions, the upper and lower critical concentrations are also easily determined, but the contours of constant X require complicated two-dimensional momentum summations and have not been calculated here. In the strong-coupling regime, the critical electron concentration is found by determining where the transition temperatures for the chessboard phase and the segregated phase are equal $[T_c(X=1)=T_c(X=-1)]$. This latter phase line can be compared with the exact solution at $T=0$ determined by calculating the ground-state energies of the chessboard and segregated phases as a function of electron concentration.

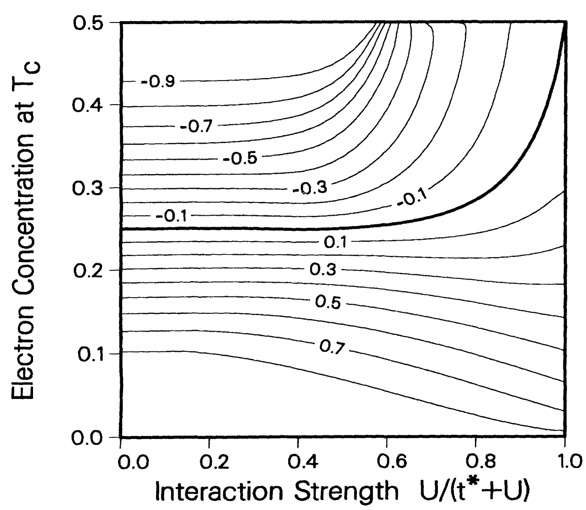

FIG. 1. Schematic "phase diagram" for the local approximation to the spinless Falicov-Kimball model in one dimension. The horizontal axis plots the interaction strength $U/(U+t^*)$ and the vertical axis plots the electron concentration at T_c. The contours displaying the constant values of $X(\mathbf{q})$ are depicted by solid lines. Note that the chessboard phase becomes unstable (at half-filling) at $U=1.35t^*$ and that the segregated phase is not present.

The schematic "phase diagram" for the one-dimensional spinless Falicov-Kimball model in the local approximation is depicted in Fig. 1. The electron concentration is determined at the relevant critical temperature, which can be viewed as an approximation[18] for the electron concentration at $T=0$, and therefore the "phase diagram" calculated in this manner is an approximation to the zero-temperature phase diagram. The "phase diagram" has qualitatively incorrect features in the large U limit. The chessboard phase becomes unstable at half-filling for $U\geq 1.35$ and the segregated phase is never stable. Only the contour with $X=0$ displays the correct qualitative behavior. Clearly, the local approximation is

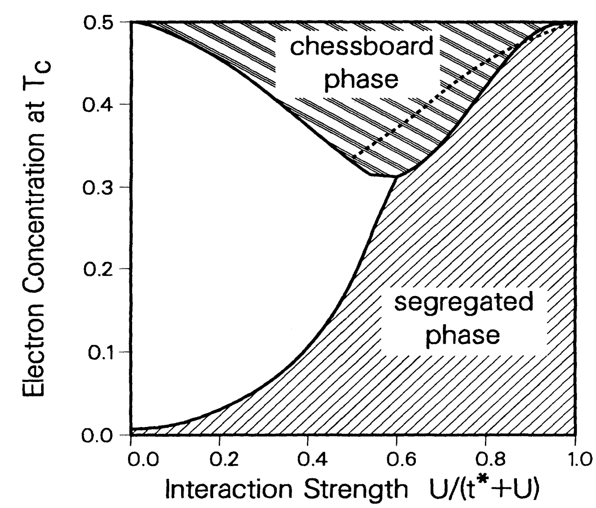

FIG. 2. Schematic "phase diagram" for the local approximation to the spinless Falicov-Kimball model in two dimensions. The bold right cross-hatched region is the region where the chessboard phase ($X=-1$) is stable, the light left cross-hatched region is the region where the segregated phase ($X=1$) is stable, and the white region is the region where the ground state possesses incommensurate long-range order ($-1<X<1$). The exact solution (at $T=0$) for the transition from the chessboard phase to the segregated phase is depicted by the dashed line. Note that the local approximation has the qualitatively correct features as $U\to 0$ and $U\to\infty$ and produces agreement with the exact solution at about the 10% level.

poor for the one-dimensional system.

The schematic "phase diagram" for the two-dimensional spinless Falicov-Kimball model in the local approximation is depicted in Fig. 2. The "phase diagram" is very close to the infinite-dimensional phase diagram[10] with the exception that the segregated phase is less stable, as expected. Comparison with the exact solution in the strong-coupling regime (dashed line) shows quantitative agreement at about the 10% level. Because the local approximation is qualitatively correct in the limit $U \rightarrow \infty$ in two dimensions, one expects the disagreement with the exact solution to be greatest at intermediate coupling strengths ($U \approx t^*$). It appears that the local approximation is quite accurate in two dimensions, indicating that a $1/d$ expansion should converge rapidly for $d \geq 2$ for the Falicov-Kimball model.

III. CONCLUSION

In conclusion, the local approximation to the spinless Falicov-Kimball model has qualitatively incorrect features in one dimension, but is both qualitatively and quantitatively accurate in two dimensions. This implies that infinite-dimensional solutions are relevant for the physical dimensions of $d=2$ and $d=3$, and a $1/d$ expansion will converge rapidly for $d \geq 2$. What is expected for other many-body problems? The local approximation is a time-dependent mean-field theory that will, in general, display finite transition temperatures. The spinless Falicov-Kimball model also has finite transition temperatures for $d \geq 2$ which provides a possible explanation for the accuracy of the local approximation in $d \geq 2$. We are therefore left with the conjecture that the local approximation will be qualitatively accurate for any many-body theory that possesses finite transition temperatures (such as the three-dimensional Hubbard model). It would be interesting to test this conjecture against exact solutions found with quantum Monte Carlo simulations. Furthermore, for the same reason, we conjecture that the local approximation will always be inaccurate in one dimension.

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[18]If the temperature dependence of the electron concentration can be neglected as the temperature is reduced from T_c to zero, the schematic "phase diagram" calculated in the fashion described in the text will be a good approximation to the zero-temperature phase diagram.