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Dynamical mean-field approximation for a two-component Fermi gas

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The properties of nonrelativistic two-component Fermi gas with attractive two-body contact interaction are studied within dynamical mean-field theory. To this end, the problem is approximated by the lattice Hubbard Hamiltonian. We have found that the low-density gas, corresponding to the limit of empty lattice, can be appropriately described in this theory. Moreover, we have also found that the main properties of the BCS-BEC transition are qualitatively captured as well.

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INTRODUCTION

Dynamic mean-field theory (DMFT), introduced over a decade ago by Georges and Kotliar,[1] has become an important tool for studying strongly correlated lattice fermion systems. In this theory, the lattice problem is mapped into a self-consistently embedded impurity problem.[2] This mapping becomes exact in the limit of infinite spatial dimensions $d\to\infty$ due to the localization of the self-energy $\Sigma(\boldsymbol{k},\omega)\to\Sigma(\omega)$.[3] For finite dimensions DMFT is no longer exact, yet can be regarded as a useful approximation in which a purely local self-energy is assumed.

In this work, we apply the DMFT to study the properties of dilute Fermi gas with attractive pair interaction. In such systems the effective range for two-body scattering is much smaller than the interparticle distance and therefore the interaction needs only to be characterized by its scattering length a_s and the system as a whole depends on the dimensionless parameter $\eta=a_s k_F$. It is well known that this simple model of low-density Fermi gas exhibits fascinating behavior.

In the weak-coupling limit the system is a BCS superconductor, which transforms smoothly into Bose-Einstein condensation of tightly bound pairs when the attraction between the fermions is increased. For small values of $|\eta|$ the system can be modeled effectively either through the BCS theory (η small and negative) or as an interacting gas of bound pairs (η small and positive). To study systems, such as dilute neutron gases or cold Fermi atoms tuned to be near a Fesbach resonance,[4] characterized by $|\eta|\geq 1$ one must rely on numerical simulations.[5,6] This regime is of special interest as in the limit $|\eta|\to\infty$ the system is expected to present universal behavior regardless of its constituents.

Applying the DMFT to study the properties of continuous Fermi gas, one can pursue two ways. Either formulate a continuum DMFT or, as done here, construct a lattice version of the problem and seek the continuum limit in the end. For finite gas densities the lattice filling vanishes in this limit.

THE LATTICE FORMULATION

To construct a lattice version of the continuum problem we represent the configuration space as an N^3 cubic lattice, where N is the number of sites in each space direction. The time direction is kept continuous. Next, we replace the position and momentum variables by the grid indices $\boldsymbol{x}\to\boldsymbol{n}$, $\boldsymbol{p}\to\frac{2\pi}{N}\boldsymbol{k}$, where $\boldsymbol{n},\boldsymbol{k}$ are integer vectors. The grid position and momentum are given by $a\boldsymbol{n}$ and $\boldsymbol{p}/a$, where a is the lattice spacing. The fermionic fields $\psi_\sigma(\boldsymbol{x})\to(a)^{-3/2}\psi_{\boldsymbol{n}\sigma}$ are discretized to obey the anticommutation relations $\{\psi_{\boldsymbol{n}\sigma},\psi^\dagger_{\boldsymbol{n}\sigma}\}=\delta_{\sigma\sigma'}\delta_{\boldsymbol{n},\boldsymbol{n}'}$. The continuum many-body Hamiltonian for dilute low energy Fermi gas is

$$H=-\frac{\hbar^2}{2m}\sum_\sigma\int d\boldsymbol{x}\,\psi^\dagger_\sigma(\boldsymbol{x})\nabla^2\psi_\sigma(\boldsymbol{x})+\frac{1}{2}V_0\sum_\sigma\int d\boldsymbol{x}\,\psi^\dagger_\sigma(\boldsymbol{x})\psi^\dagger_{-\sigma}(\boldsymbol{x})\psi_\sigma(\boldsymbol{x})\psi_{-\sigma}(\boldsymbol{x}). \tag{1}$$

The corresponding lattice theory is the Hubbard Hamiltonian

$$H=-\frac{\hbar^2}{2ma^2}\sum_\sigma\sum_{nn'}D_{nn'}\psi^\dagger_{n\sigma}\psi_{n'\sigma}+\frac{1}{2}\frac{V_0}{a^3}\sum_{\sigma n}\psi^\dagger_{n\sigma}\psi^\dagger_{n-\sigma}\psi_{n\sigma}\psi_{n-\sigma}, \tag{2}$$

where $(D\psi_\sigma)_n=\Sigma_i(\psi_{n+e_i,\sigma}-2\psi_{n,\sigma}+\psi_{n-e_i,\sigma})$. Here, e_j is a unit vector in the direction j. The spectra of the free lattice Hamiltonian is given by

$$\epsilon_p=\frac{\hbar^2}{ma^2}\Delta_p,\quad \Delta_p=2\sum_i\sin^2\frac{p_i}{2}. \tag{3}$$

In the following we shall use natural units setting $\hbar=m=1$. The strength of the two-body interaction is determined by the parameter V_0. This parameter can be related to the two-body scattering length a_s through summation of the ladder diagrams for two fermions interacting at zero energy, zero temperature, and zero chemical potential $\mu\to 0^-$,[7,8]

$$\frac{1}{4\pi a_s}=\frac{1}{V_0}+\frac{C}{2a}=\frac{1}{V_0}+\Lambda_K\frac{C}{4\pi}, \tag{4}$$

where

$$C=\int\frac{d\boldsymbol{p}}{(2\pi)^3}\frac{1}{\Delta_p}\approx 0.5048 \tag{5}$$

and $\Lambda_K=2\pi/a$ is the grid momentum cutoff. The integral in Eq. (5) is to be carried over the Brillouin zone $|p_i|\leq\pi$. Due to the finite lattice spacing, the two-body interaction acquires an effective range, given approximately by $r_{\text{eff}}\approx 4/\pi\Lambda_K$

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$=2a/\pi^2$.[9] When the magnitude of r_{eff} is comparable to the interparticle distance, the system becomes sensitive to the grid cutoff. A reliable description of the Fermi gas with contact interaction, can be obtained if $r_{\text{eff}}k_F \ll 1$. This criterion can be expressed as $\frac{2a}{\pi^2}\sqrt[3]{\frac{3\pi^2\langle n\rangle}{a^3}} \approx \frac{2}{\pi}\sqrt[3]{\langle n\rangle} \ll 1$, where $\langle n\rangle$ is the average lattice filling, i.e., the number of particles per site. Actual DMFT calculations with finite lattice filling of $0.1 \geq \langle n\rangle \geq 0.01$ (to be presented later), correspond to $0.3 \geq r_{\text{eff}}k_F \geq 0.14$.

Lattice fermions with attractive local interaction were studied within DMFT by several authors.[10,11] Keller *et al.*[10] have established the phase diagram of the system within the DMFT framework. As expected, at large temperature the system is a Fermi liquid that becomes a superconductor at a critical temperature T_c. Although the Fermi liquid is not the ground state of the system, Capone *et al.*[11] have found that in the weak-coupling regime, at zero temperature, a metastable metallic phase exists. This solution exists as long as the attraction is too weak for creating a two-fermion bound state. Once two-fermion bound states are formed the system undergoes a sharp transition into the real (pairing phase) ground state. In the current study we focus on the continuum limit, which for finite density $\rho=\langle n\rangle/a^3$ and fixed scattering length corresponds to $\langle n\rangle \to 0$, $|V_0| \to 0$ in the limit $a \to 0$. For simplicity we shall concentrate on the Fermi liquid state.

DMFT

A solution of the lattice Hamiltonian (2) can be sought for using a Monte Carlo simulation.[12] Such a direct attempt to solve the many-body problem usually involves heavy computational effort which increase tremendously with the grid size. The DMFT provides an alternative theoretical framework in which the solution is approximated by replacing the lattice Hamiltonian with an effective single-site impurity model. The quality of the approximation depends on the number of actual grid nodes in the impurity. The effective action in the lowest order approximation employed here,[2] is (no summation on the lattice index i)

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{i,\sigma}^\dagger(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_{i,\sigma}(\tau') - \frac{V_0}{a^3}\int_0^\beta d\tau c_{i\uparrow}^\dagger(\tau)c_{i\uparrow}(\tau)c_{i\downarrow}^\dagger(\tau)c_{i\downarrow}(\tau). \tag{6}$$

The corresponding impurity Green's function is given by

$$\mathcal{G}(\tau-\tau') = \langle Tc_{i,\sigma}c_{i,\sigma}^\dagger\rangle_{S_{\text{eff}}}. \tag{7}$$

The self-energy is deduced from

$$\Sigma(i\omega_n) = \mathcal{G}_0^{-1}(i\omega_n) - \mathcal{G}^{-1}(i\omega_n), \tag{8}$$

where $\omega_n=(2n+1)\pi/\beta$ are the Matsubara frequencies. The connection to the physical lattice is made through the self-consistency requirement that the impurity Green's function is equal to the local lattice Green's function

$$\mathcal{G}(\tau-\tau') = G_{ii}(\tau-\tau'), \tag{9}$$

where $G_{ii}=\Sigma_{\boldsymbol{k}}\frac{1}{i\omega_n+\mu-\epsilon_{\boldsymbol{k}}-\Sigma(i\omega_n)}$.

It can be proven that by using the DMFT equations (6)–(9), not only the free Fermi gas is recovered when the interaction is switched off, but also the first order perturbation theory.

SOLVING THE IMPURITY MODEL

Caffarel and Krauth[13] proposed to approximate the "free" impurity Green's function $\mathcal{G}_0$ in the following way:

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_p \frac{W_p^2}{i\omega_n - \tilde{\epsilon}_p}, \tag{10}$$

which corresponds to the Anderson Hamiltonian

$$\mathcal{H}_{\text{And}} = \sum_{p\geq 2,\sigma}\tilde{\epsilon}_p a_{p\sigma}^\dagger a_{p\sigma} + \sum_{p\geq 2,\sigma} W_p(a_{p\sigma}^\dagger c_\sigma + c_\sigma^\dagger a_{p\sigma}) + Un_\uparrow n_\downarrow, \tag{11}$$

with $U=V_0/a^3$. For small number of auxiliary fields $a_{p\sigma}$ this Hamiltonian can be solved using standard diagonalization methods, or for $T=0$ using the Lanczos method.[2]

EXTRACTING THE PHYSICS

Solving the DMFT equations yields the local approximation for the self-energy $\Sigma(\boldsymbol{k},i\omega_n)\approx\Sigma(i\omega_n)$, and correspondingly

$$G(\boldsymbol{k},i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma(i\omega_n)}. \tag{12}$$

Once G is known, the number of particles per site and the energy can be calculated through the Matsubara sums

$$\langle n\rangle = \frac{1}{\beta}\sum_{\sigma\boldsymbol{k}}\sum_{n=-\infty}^{\infty} e^{i0^+}G(\boldsymbol{k},i\omega_n) \tag{13}$$

$$\langle H\rangle = \frac{1}{2}\frac{1}{\beta}\sum_{\sigma\boldsymbol{k}}\sum_{n=-\infty}^{\infty} e^{i0^+}(i\omega_n+\epsilon_{\boldsymbol{k}}+\mu)G(\boldsymbol{k},i\omega_n). \tag{14}$$

The number of particles can also be calculated directly from the impurity action. If $\mathcal{G}=G_{ii}$ these two results should coincide. However, since at best $\mathcal{G}\approx G_{ii}$, these results do not always coincide, and in the following we shall use Eq. (13). Since direct evaluation of the Matsubara sums is impractical, we calculate $\langle n\rangle,\langle H\rangle$ in the following manner. We create a Pade approximation for Σ,

$$\Sigma^{\text{Pade}}(i\omega_n) = \frac{P(i\omega_n)}{Q(i\omega_n)} = \frac{\sum_0^m a_j(i\omega_n)^j}{\sum_0^m b_l(i\omega_n)^l}, \tag{15}$$

and use it to evaluate analytically the number of particles per site $\langle n\rangle_{\text{Pade}}$ and the energy $\langle H\rangle_{\text{Pade}}$, using $G^{\text{Pade}}=\frac{1}{i\omega_n+\mu-\epsilon_{\boldsymbol{k}}-\Sigma^{\text{Pade}}}$. Then for a limited range of low frequencies we calculate for the number of particles per site the difference

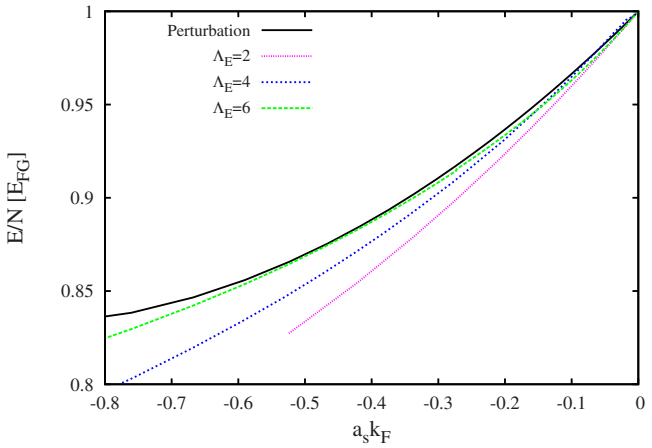

FIG. 1. (Color online) Energy per particle in the weak-coupling regime. A comparison between perturbation theory and DMFT for various energy cutoffs Λ_E.

$$\delta\langle n\rangle = \frac{1}{\beta}\sum_{\sigma \boldsymbol{k}} \sum_{n=-N}^{N} [G(\boldsymbol{k}, i\omega_n) - G^{\mathrm{Pade}}(\boldsymbol{k}, i\omega_n)], \tag{16}$$

and equivalently for the energy. Finally, $\langle n\rangle = \langle n\rangle_{\mathrm{Pade}} + \delta\langle n\rangle$ and $\langle H\rangle = \langle H\rangle_{\mathrm{Pade}} + \delta\langle H\rangle$. The order of the polynomials P, Q must be equal since in the limit $\omega \to \infty$, $G \to 1/\omega$. Using the standard contour integration one gets

$$\sum_{n=-\infty}^{\infty} \frac{e^{i0^+}}{i\omega_n + \mu - \epsilon - P/Q} = \sum_{p=1}^{n+1} \mathrm{Residue}\left(\frac{Q(\omega)}{R(\omega)}\right)_{\omega=\omega_p} \frac{\beta}{e^{\beta\omega_p} + 1}, \tag{17}$$

where $R(\omega) = (\omega + \mu - \epsilon)Q(\omega) - P(\omega)$ and ω_p are its roots.

RESULTS

In the following we shall only consider the zero temperature case. The impurity problem was solved using the Caffarel-Krauth method[13] with $n_s = 8$ fermion fields. In the weak-coupling regime the energy per particle is given to second order by[14] $E/N = E_{\mathrm{FG}}(1 + \frac{10}{9\pi} k_F a_s + \frac{4(11-2\log 2)}{21\pi^2}(k_F a_s)^2 + \cdots)$, where $E_{\mathrm{FG}} = 0.6\epsilon_F$ is the energy per particle for free Fermi Gas. In Fig. 1 we present a comparison between this result and the DMFT calculations performed with $\mu = 0.1$ and different energy cutoffs $\Lambda_E = \Lambda_K^2/2$. The DMFT results have been normalized to 1 at $a_s = 0$ to account for the grid dispersion relations. It can be seen that with increasing cutoff the DMFT approach the perturbation theory.

In the unitary limit $a_s \to \infty$, Chen and Kaplan[8] used a mean-field approach to find a first-order phase transition between a low-density phase with $\langle n\rangle \approx 0$ and a high-density phase with lattice filling $\langle n\rangle = O(1)$. Using the slave-boson mean-field theory[15] we have confirmed this observation. For the metallic phase no such phase transition is observed in the DMFT approach, below the two-body threshold. In Figs. 2 and 3, the density and energy per particle around the unitarity limit are presented for different cutoffs. For properly renormalized theory one would expect the density and energy to be invariant to the cutoff value, given that Λ_E is large enough. From the figures it is evident that where as in the weak-coupling regime one gets a cutoff invariant result, around the $a_s \to \infty$ limit there is a strong cutoff dependence. By inspecting Fig. 2 it is clear that the x axis should be rescaled in order to get a cutoff independent result. Modifying Eq. (4) in the following way,

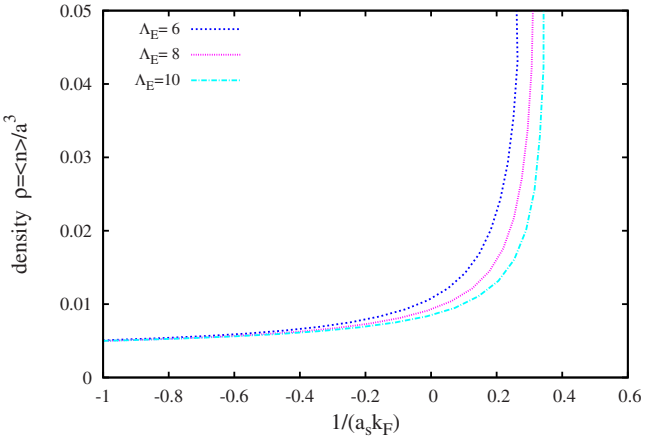

FIG. 2. (Color online) The density as a function of the dimensionless parameter $1/(a_s k_F)$, for various energy cutoffs and $\mu = 0.1$.

$$\frac{1}{4\pi a_s} = \frac{1}{V_0} + \Lambda_K \frac{C + \delta C}{4\pi}, \tag{18}$$

we found that $\delta C = -0.09$ leads to cutoff independent results, i.e., it leads to the desired continuum limit. The resulting density and energy per particle are presented in Figs. 4 and 5, where it can be seen that the cutoff dependence has disappeared. At this point we cannot justify the value of δC, although one can speculate that it is a result of the diagrams neglected in the DMFT.

In the theory of unitary Fermi gas it is customary to define the parameter ξ as the ratio between the energy per particle at unitarity to that of a free Fermi gas. As can be seen in Fig. 5,

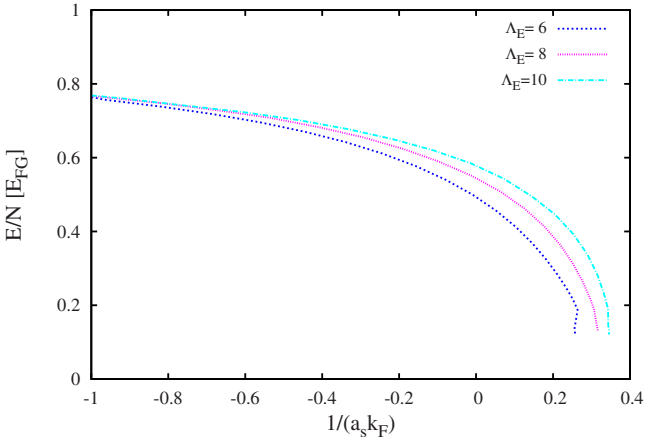

FIG. 3. (Color online) Energy per particle as a function of the dimensionless parameter $1/(a_s k_F)$, for various energy cutoffs and $\mu = 0.1$.

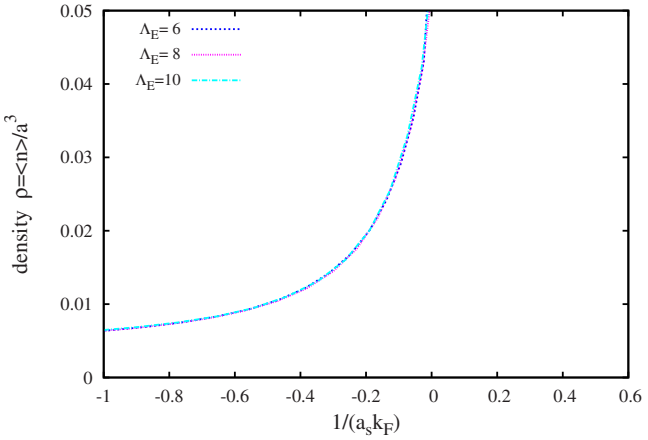

FIG. 4. (Color online) Same as Fig. 2. The scattering length is deduced from Eq. (18).

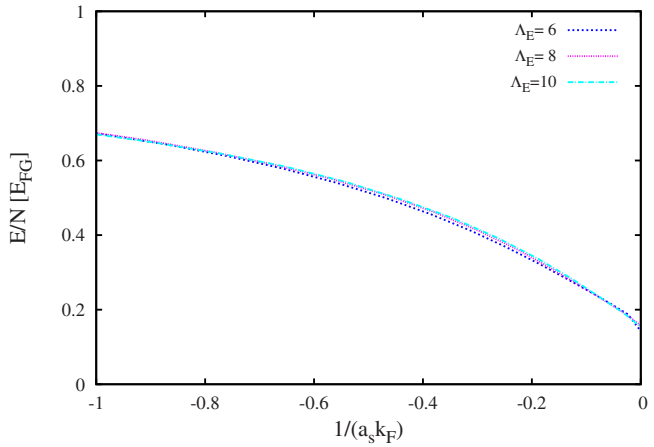

FIG. 5. (Color online) Same as Fig. 3. The scattering length is deduced from Eq. (18).

DMFT produces the general qualitative behavior expected in the BCS-BEC transition. Using Eq. (18), DMFT predicts that $\xi \approx 0.15$, to be compared with $\xi = 0.44 \pm 0.01$ obtained by[5,16] using the fixed-node diffusion Monte Carlo method.

CONCLUSIONS

In applying the DMFT to study Fermi gas we have found that (i) The Fermi gas is described accurately in the weak-coupling regime. (ii) For the metallic phase, DMFT presents no first-order phase transition in the strong-coupling regime below the two-body threshold. Therefore the continuum limit can be realized, predicting the existence of a metastable mettalic phase below the two-body threshold. (iii) The general behavior of attractive Fermi gas is qualitatively captured. We also found that the procedure introduced in Ref. 17 to relate the scattering length to V_0 does not lead to cutoff independent results around the unitarity limit. With an *ad hoc* modification of this procedure the energy and density become cutoff independent. The single site DMFT that we have used here can be further improved using larger clusters. It can also be extended to study the superconducting ground state properties of the system. It is expected that with such improvements the parameter ξ will approach the Monte Carlo value.[5,6]

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