CHIN. PHYS. LETT. Vol. 35, No. 11 (2018) 110301

Properties of One-Dimensional Highly Polarized Fermi Gases *

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(Received 8 May 2018)

Using both the exact Bethe ansatz method and the variational method, we study properties of the one-dimensional Fermi polaron. We focus on the binding energy, effective mass, momentum distributions, Tan contact and correlation functions. As the attraction increases, the impurity is more tightly bound and correlated with the surrounding particles, and the size of formed polaron decreases. In addition, compared with the Bethe ansatz method, the variational method is totally qualified to study the one-dimensional Fermi polaron. The intrinsic reason is that the number of particle-hole excitations in a Fermi sea, caused by a single impurity, is always rather small. The variational method can be well extended to other impurity systems.

PACS: 03.75.Ss, 67.85.Lm, 05.30.Fk DOI: 10.1088/0256-307X/35/11/110301

Due to the high tunability, the ultracold Fermi gas has been used as a versatile platform to explore various many-body phenomena.[1−5] In particular, recent experimental observations of Fermi polarons in two- and three-dimensional ultracold atoms[6−9] provide insightful understanding of the quasiparticle physics in many-body systems,[10] and make the impurity system and the associated concept of polarons attract much attention.[11−15] The Fermi polaron is a dressed impurity immersed in a Fermi sea, and undergoes a polaron-molecule transition in two and three dimensions as the attraction increases. In addition to the Fermi polaron, the concept has been extended to bosonic systems,[16−20] and even the impurity system with repulsive interactions.[21] The polaron not only has its own physical uniqueness, but also is the first step towards the multi-impurity system and even the imbalanced mixture.[22]

Theoretically, researchers are mainly using variational methods, including mean field theory, to study the polaron.[23,24] These methods are perturbative, based on the number of particle-hole excitations in the major component.[15,25] However, in one dimension (1D) the Fermi polaron can be exactly studied by the Bethe ansatz (BA) method.[26−30] It is a special case of the 1D spin-1/2 δ-function interacting Fermi gases, whose properties with arbitrary spin population imbalance were exactly studied by Yang[31] and Gaudin.[32] The BA method can be used to test the quality of other methods.

In this Letter, we utilize both the variational method and the exact BA method to study properties of the 1D Fermi polaron. Comparisons between the results obtained by these two methods are made. Although the binding energy and effective mass have been studied in Ref. [25], here we further calculate momentum distributions, Tan contact and correlation functions for different attractions. In particular, we extract the Tan contact from several aspects. The Tan contact measures the probability of finding two particles at the same place. It is highly related to the thermodynamics, the asymptotic behavior of the momentum distribution tail, and the local density-density correlation function.[33−35] It is a key property of many-body systems. The Tan contact for the 1D Fermi polaron has been calculated by the T-matrix method,[36] here we further focus on testing the quality of the variational method. Compared with the exact BA method, the variational method gives quite good results, especially the Tan contact. The variational method is totally qualified to study the 1D Fermi polaron, and could give reasonable good results for other impurity systems.

We consider a 1D highly polarized two-component fermionic system with a single spin-$\downarrow$ fermion in a spin-$\uparrow$ Fermi sea. The corresponding Hamiltonian can be written as

$$H = \sum_{k\sigma} \epsilon(k,\sigma) c^{\dagger}_{k\sigma} c_{k\sigma} + g \sum_{kk'q} c^{\dagger}_{k\uparrow} c^{\dagger}_{k'\downarrow} c_{q\downarrow} c_{k+k'-q,\uparrow}, \tag{1}$$

with $\epsilon(k,\sigma) = k^2_{\sigma}/2$ ($\hbar = 1$). The masses of fermions are the same, and are used as the unit of mass, $c^{\dagger}_{k\sigma}$ ($c_{k\sigma}$) is the creation (annihilation) operator of a fermion with momentum k and spin σ. The density for spin-$\uparrow$ fermion is denoted as $n_{\uparrow} = k_{\rm F}/\pi$, with $k_{\rm F}$ being the Fermi momentum. The interaction between the impurity and other particles is a contact interaction and we only consider the attractive case with negative g.[21] It is a function of the 1D scattering length a with $g = -1/a$.[37]

Introduced by Chevy,[13] a variational wave function for the ground state can be written as

$$|\Psi\rangle = \alpha_0 c^{\dagger}_{p\downarrow}|0\rangle + \sum_{k_1 q_1} \alpha_{k_1 q_1} c^{\dagger}_{p+q_1-k_1\downarrow} c^{\dagger}_{k_1\uparrow} c_{q_1\uparrow}|0\rangle + \ldots, \tag{2}$$

*Supported by the National Natural Science Foundation of China under Grant Nos 11374331, 11304364 and 11534014.

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where $|k_{1(2)}| > k_{\rm F}$ and $|q_1| \leq k_{\rm F}$. The vacuum $|0\rangle$ is defined as a product state of the true vacuum for spin-$\downarrow$ fermion and the Fermi sea for spin-$\uparrow$ fermions. Here p denotes the momentum of the polaron or the whole system. The first two terms describe zero and one particle-hole excitations in the Fermi sea. High order excitations are omitted, and these two terms can give very good results. Minimizing the functional $\langle\Psi|(H-E)|\Psi\rangle$, one can obtain the following two coupled equations[14]

$$\begin{aligned} &-g^{-1}|E|\alpha_0 = \sum_{k_1 q_1} \alpha_{k_1 q_1}, \\ &-g^{-1}E^1_{k_1 q_1}\alpha_{k_1 q_1} = \alpha_0 + \sum_{k_2} \alpha_{k_2 q_1}, \end{aligned} \tag{3}$$

where $E^1 = -E + gn_\uparrow + \epsilon(p+q_1-k_1,\uparrow) + \epsilon(k_1,\uparrow) - \epsilon(q_1,\uparrow)$, and E is the ground-state energy, which is also defined as the energy of the polaron. We have set the ground-state energy for the non-interacting system ($g=0$) to zero. Given a dimensionless parameter $g/n_\uparrow$, one can solve the above coupled equations, obtain α_0, $\alpha_{\rm kq}$ and the ground-state energy E explicitly expressed as

$$E = \sum_{q_1} \frac{1}{\frac{1}{g} + \sum_{k_1} \frac{1}{E^1_{k_1 q_1}}}. \tag{4}$$

When $p \ll k_{\rm F}$, the energy of the polaron under the quasiparticle picture can be written as $E(p) = E_{\rm b} + p^2/2m^*$, which is the ground-state energy for the system with $p=0$, where $E_{\rm b}$ is called the binding energy of the polaron, and m^* is the effective mass of the polaron. These two quantities are the major characteristics of a polaron. However, with the variational wave function one can calculate other quantities, like momentum distributions and correlation functions.

The Hamiltonian Eq. (1) can also be exactly solved by the BA method.[31] In real space, it can be written as

$$\begin{aligned} H = &-\frac{1}{2}\sum_\sigma \int \phi^\dagger_\sigma(x)\frac{d^2}{dx^2}\phi_\sigma(x)dx \\ &+ g\int \phi^\dagger_\downarrow(x)\phi^\dagger_\uparrow(x)\phi_\uparrow(x)\phi_\downarrow(x)dx, \end{aligned} \tag{5}$$

where $\phi^\dagger_\sigma(x)$ is the creation operator of a spin σ fermion at position x. After expanding the many-body wave function with plane waves, the quasi-momenta k_j of fermions under the periodic boundary condition satisfies the BA equations[31]

$$\begin{aligned} &\exp(ik_jL) = \prod_{\alpha=1}^{M}\left(\frac{k_j - \Lambda_\alpha + ig/2}{k_j - \Lambda_\alpha - ig/2}\right), \\ &\prod_{j=1}^{N}\left(\frac{\Lambda_\alpha - k_j + ig/2}{\Lambda_\alpha - k_j - ig/2}\right) = -\prod_{\beta=1}^{M}\left(\frac{\Lambda_\alpha - \Lambda_\beta + ig}{\Lambda_\alpha - \Lambda_\beta - ig}\right), \\ &j = 1,\ldots,N,\ \ \alpha = 1,\ldots,M, \end{aligned} \tag{6}$$

where N is the number of all particles, $M=1$ is the number of spin-$\downarrow$ particles, and Λ_α are additional M quantities which describe down spins. The energy of a state with a set of k_j is given by $E = \sum_j k_j^2/2$. Working in the thermodynamic limit and using the perturbation method, the binding energy $E_{\rm b}$ in the weakly attractive region ($|g|/n_\uparrow \ll 1$) is

$$\frac{E_{\rm b}}{E_{\rm F}} = \frac{2}{\pi}\left[y - \frac{\pi}{2}y^2 + (1+y^2)\arctan(y) + O(y^3)\right], \tag{7}$$

with $y = g/2k_{\rm F}$ and the Fermi energy $E_{\rm F} = k_{\rm F}^2/2$. It agrees with McGuire's calculation.[38] Here y is a dimensionless parameter, which is a scaled $g/n_\uparrow$. On the other hand, in the strongly attractive region ($|g|/n_\uparrow \gg 1$), the binding energy and the effective mass are

$$\frac{E_{\rm b}}{E_{\rm F}} = -2y^2 - 1 - \frac{4}{3\pi y} + O(y^{-2}), \tag{8}$$

$$m^* = 2 + \frac{2}{\pi y} + O(y^{-2}). \tag{9}$$

In the strongly attractive limit $y = -\infty$, the impurity forms a very tight pair with a particle in the Fermi sea, and the effective mass equals 2. In general, for a finite system one can solve the above coupled BA equations directly and obtain quasi-momenta k_j. Then with the many-body wave function one can calculate the binding energy, the effective mass and so on. In our numerical calculations, $L=1$ for the sake of simplicity and the number of spin-$\uparrow$ fermions equals 21.

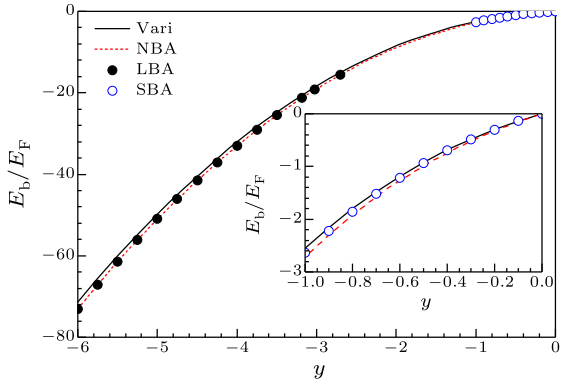

Fig. 1. The binding energy of polaron versus dimensionless parameter $y = g/2k_{\rm F}$, calculated by the variational method (Labeled by Vari), the numerical BA method (NBA), the small interaction (SBA) and the large interaction (LBA) perturbations (Eqs. (7) and (8)). Inset: Enlargement of the weakly attractive region.

In Fig. 1 we show the binding energy as a function of the dimensionless parameter y (the scaled interaction strength). The results obtained from different methods agree with each other very well. The relative error $(E_{\rm b}^{\rm Vari}(y) - E_{\rm b}^{\rm NBA}(y))/E_{\rm b}^{\rm NBA}(y)$ for Fig. 1 is less than 3.3%. Compared with the BA method, the variational method gives a very good binding energy, which can also be seen in Ref. [25]. In the weakly attractive region ($|y| \ll 1$), the impurity slightly interacts with

particles in the Fermi sea, and under the mean field approximation the binding energy $E = gn_\uparrow = (2y/\pi)E_\mathrm{F}$, which is the leading order of Eq. (7). As the attraction $|y|$ increases, the binding between the impurity and particles in the Fermi sea becomes stronger and the binding energy $|E_\mathrm{b}|$ increases. In the strongly attractive region, one can think that the impurity forms a tightly bound pair with a particle in the Fermi sea. From the two-particle physics the binding energy $E = -g^2/2 = -2y^2E_\mathrm{F}$, which is the leading order of Eq. (8).

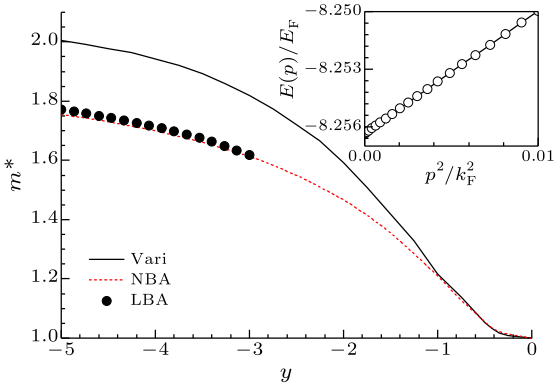

Fig. 2. The effective mass of polaron. Inset: The ground-state energy versus p^2 for a system with dimensionless parameter $y = -2$.

Not only the binding energy, we also calculate the ground-state energy for systems with finite p. After linearly fitting the energy versus p^2, one can obtain the effective mass of polaron. In the inset of Fig. 2 we show the ground-state energy versus p^2 for a typical system, and a linear relation indeed shows up. In Fig. 2 we show the effective mass versus the dimensionless parameter y. The maximal relative error is around 10%. Compared with the BA method, the variational method gives quite good results, especially if the relative error is less than 2.8% when $|y| < 1$. The effective mass $m^* > 1$ because the impurity is dressed by particles in the Fermi sea. As the attraction $|y|$ increases, the impurity is more entangled with the Fermi sea and harder to move with a larger effective mass. In the strongly attractive region, the impurity is tightly paired with a particle in the Fermi sea, and the effective mass $m^* \to 2$.

With the ground-state energy, one can obtain the variational wave function by solving Eq. (3). Then other quantities can also be calculated. In Fig. 3 we show momentum distributions of the major component for systems with $p = 0$ and different attractions. It is defined as $n_\uparrow(k) = \langle \Psi | c_{k\uparrow}^\dagger c_{k\uparrow} | \Psi \rangle$. Distributions are symmetric about $k = 0$, and we only show the right half. For systems with $p \neq 0$, momentum distributions are asymmetric, but as the attraction increases they have the same behavior as for systems with $p = 0$. When the attraction is weak ($|y| \ll 1$), the momentum distribution is basically a step function, and particle-hole excitations concentrate on the Fermi surface. As the attraction increases, particles in the Fermi sea are more entangled with the impurity, and more inner particles are excited to higher momentum states. However, there is only one impurity, and no matter how large the attraction is the overall number of excitations in the Fermi sea is still small. We think this is the intrinsic reason why the variational method can work so well. In the inset of Fig. 3 we show the corresponding momentum distributions for the impurity, which are defined as $n_\downarrow(k) = \langle \Psi | c_{k\downarrow}^\dagger c_{k\downarrow} | \Psi \rangle$. There is a discontinuity at $k = 0$, and $n_\downarrow(k = 0) = |\alpha_0|^2$, which is the residue of impurity that remains un-excited. The residual has a significant weight, which also indicates that the fraction of excited particles is relatively small. In the strongly attractive region ($|y| > 1$), every particle in the Fermi sea has almost the same chance to be excited out, and there is a peak at finite momentum in the distribution for impurity.

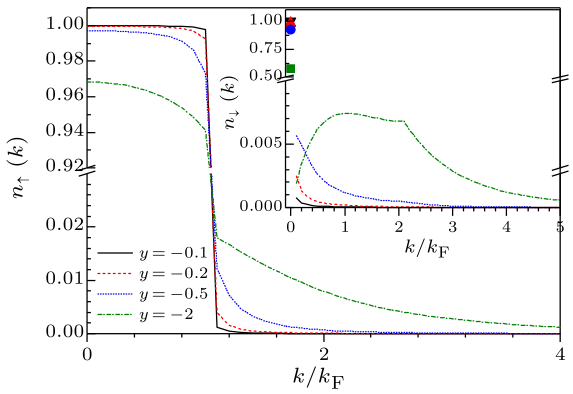

Fig. 3. Momentum distributions $n_\uparrow(k)$ for systems with different y. Inset: the corresponding momentum distributions for the impurity.

Now we come to study the Tan contact. For the 1D Fermi polaron, it is defined as

$$C = g^2 \int dx \langle \Psi | \phi_\uparrow^\dagger(x) \phi_\downarrow^\dagger(x) \phi_\downarrow(x) \phi_\uparrow(x) | \Psi \rangle, \qquad (10)$$

which measures the probability of finding two particles with different spins at the same place.[37] Compared with Eq. (5), the Tan contact is highly related to the interaction energy and the local density-density correlation function. Using the variational wave function Eq. (2), the Tan contact can be calculated directly by being transformed into momentum space. In addition to the direct calculation, the Tan contact can also be extracted from the momentum distribution. One of Tan's universal relations is

$$n_\downarrow(k \gg k_\mathrm{F}) = n_\uparrow(k \gg k_\mathrm{F}) = \frac{C}{k^4}, \qquad (11)$$

where C is the Tan contact. There is a linear relation between $\ln n_\sigma(k)$ and $\ln k$ when $k \gg k_\mathrm{F}$ (an example is shown in the inset of Fig. 4). After linearly fitting, one can extract the Tan contact.

Furthermore, from Tan's relation between adiabatic energy and the scattering length, the Tan con-

tact can be calculated by $C = dE/da$.[34] This equation also suggests that given a Tan contact one can determine the free energy and any thermodynamic quantity at zero temperature, which makes the Tan contact a very important quantity in the thermodynamics. With the above BA resulted Eqs. (7) and (8), the Tan contact is

$$\frac{C}{k_{\rm F}E_{\rm F}} = \frac{4}{\pi}[2y^2 - \pi y^3 + 2y^3 \arctan(y) + O(y^4)], \quad |y| \ll 1, \tag{12}$$

$$\frac{C}{k_{\rm F}E_{\rm F}} = 2\Big[-4y^3 + \frac{4}{3\pi} + O(y^{-1})\Big], \ |y| \gg 1. \tag{13}$$

In Fig. 4 we show the Tan contact versus dimensionless parameter y, calculated by different methods. All results agree with each other very well. The relative errors are less than 3.7%. Then compared with the BA method, the variational method can also give very good thermodynamic properties.

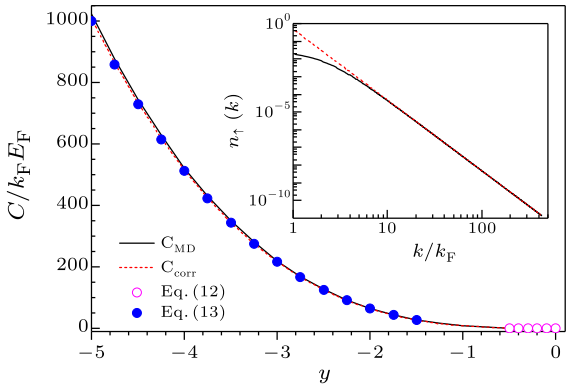

Fig. 4. The Tan contact versus dimensionless parameter y. Here $C_{\rm MD}$ is obtained from fitting the momentum distribution tail, $C_{\rm corr}$ is obtained from Eq. (10) with the variational wave function. Inset: log-log plot of $n_\uparrow(k)$ for a system with $y = -2$. The dotted straight line is a fitting function in form $\propto 1/k^4$.

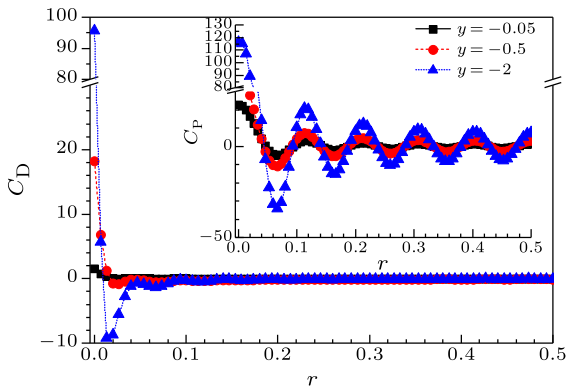

Fig. 5. Density-density correlation functions for systems with different y. Inset: the corresponding pair correlation functions.

Finally, we use the variational method to calculate the correlation functions which are currently out of reach for the BA method. The density-density correlation function between different spins is defined as $C_{\rm D}(r) = \langle\Psi|n_\uparrow(r)n_\downarrow(0)|\Psi\rangle - \langle\Psi|n_\uparrow(r)|\Psi\rangle\langle\Psi|n_\downarrow(0)|\Psi\rangle$ with $n_\sigma(r) = \phi^\dagger_\sigma(r)\phi_\sigma(r)$ the density operator. Translation invariance has been used and only the relative coordinate matters. In Fig. 5 we show density-density correlation functions for systems with different attractions. Correlation functions are symmetric about $r = 0$ and we only show the right half. In the absence of interaction ($y = 0$), there is no correlation between two components. As the attraction increases, a peak immediately emerges at the center ($r = 0$) and becomes more sharp. This signature indicates the formation of a polaron. The impurity only has significant correlations with nearby spin-↑ particles. The decay rate of the correlation function indicates the size of a polaron. As the attraction increases, the central peak becomes higher and narrower, which indicates that the polaron becomes more tightly bound with a smaller size. In the inset of Fig. 5 we show the corresponding pair correlation functions, which are defined as $C_{\rm P}(r) = \langle\Psi|\phi^\dagger_\uparrow(r)\phi^\dagger_\downarrow(r)\phi_\downarrow(0)\phi_\uparrow(0)|\Psi\rangle$. The pair correlation shows oscillatory decay, the same as the Friedel oscillation,[39] and the same as the density-density correlation function, the pair correlation function becomes stronger as the attraction increases.

In summary, an impurity, immersed in a Fermi sea with attractive interactions between them, will be dressed up by surrounding particles to form a polaron. It becomes more tightly bound as the attraction increases. We used both the variational method and the exact Bethe ansatz method to study properties of the 1D Fermi polaron. Explicitly, we have studied the binding energy, effective mass, momentum distributions, Tan contact and correlation functions for systems with different attractions. Compared with the Bethe ansatz method the variational method gives very good results. Especially, they give almost the same Tan contact, which means the same thermodynamic properties. The variational method is totally qualified to study properties of 1D Fermi polaron. The reason why the variational method can work so well is that there is only one impurity and the number of caused particle-hole excitations in the Fermi sea is rather small. It is reasonable to think that the variational method is also good for other 1D impurity systems and even for the two- or three-dimensional polaron. For example, for the two-impurity system one just needs to replace the one impurity creation operator $c^\dagger_{p\downarrow}$ by $c^\dagger_{p_1\downarrow}c^\dagger_{p_2\downarrow}$ in the variational wave function.

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