Finite-range effects in the two-dimensional repulsive Fermi polaron

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(Dated: August 25, 2020)

We study the repulsive Fermi polaron in a two-component, two-dimensional system of fermionic atoms inspired by the results of a recent experiment with 173 Yb atoms [N. Darkwah Oppong et al., Phys. Rev. Lett. 122, 193604 (2019)]. We use the diffusion Monte Carlo method to report properties such as the polaron energy and the quasi-particle residue that have been measured in that experiment. To provide insight on the quasi-particle character of the problem, we also report results for the effective mass. We show that the effective range, together with the scattering length, is needed in order to reproduce the experimental results. Using different model potentials for the interaction between the Fermi sea and the impurity, we show that it is possible to establish a regime of universality, in terms of these two parameters, that includes the whole experimental regime. This illustrates the relevance of quantum fluctuations and beyond mean-field effects to correctly describe the Fermi polaron problem.

The problem of a single particle surrounded by a medium plays a crucial role in many different quantum many-body systems. Some examples are the Kondo effect and Anderson’s orthogonality catastrophe. Because of this, it has been studied in different fields of physics, such as condensed matter and neutron matter. In particular, an impurity coupled to a Fermi sea leads to the formation of a quasi-particle, known as Fermi polaron. The properties of such quasi-particle can differ drastically from the properties of the bare particle.

Ultracold atoms constitute an excellent platform for the investigation of the properties of the Fermi polaron, mainly due to their high tunability. Specifically, the interaction between the impurity and the bath can be controlled by means of a Feshbach Resonance. Experimentally, two-component mixtures of ultracold gases with a very small concentration of one of the components are used to study the physics of the Fermi polaron. This includes mixtures of two different hyperfine levels of the same atom and of different atoms. While initially only alkali atoms were employed, the recent discovery of Orbital Feshbach resonance (OFR) in 173 Yb has made it possible to study the quantum degenerate regime also with these systems. The interactions between these atoms open the possibility of studying new phenomena, such as spin exchange and SU(N)-symmetric collisions. Under these conditions, it has been possible to spectroscopically probe the energies of the repulsive and attractive branches of the two-dimensional (2D) polaron, and to measure the quasi-particle residue by driving Rabi oscillations.

Previous diffusion Monte Carlo (DMC) calculations reveal the existence of a universal regime in terms of the gas parameter $n a_s^2$ for the 2D repulsive Fermi polaron, that stands for values $n a_s^2 \leq 10^{-3}$, with $n$ the particle density and $a_s$ the 2D s-wave scattering length. These results contrast with the ones reported for unpolarized two-dimensional, two-component Fermi system where the universal regime stands for $n a_s^2 \lesssim 10^{-2}$, which reflects the enhanced relevance of quantum fluctuations in the Fermi polaron problem.

Remarkably, the energy of the 2D polaron and the quasi-particle residue have been measured recently outside of the universal regime exploiting the OFR in 173 Yb. As a consequence, mean-field theory and its first perturbative correction (the Lee-Huang-Yang -LHY- term), which are functions of only the scattering length, are unable to accurately describe this problem. As is commonly done in literature, here we study the Fermi polaron in terms of the Fermi momentum times the scattering length $k_F a_s$, that has a direct relationship with the gas parameter $k_F a_s = \sqrt{4\pi n a_s^2}$.

With the aim of extending the regime of universality, in this Letter we study the 2D Fermi polaron problem with a model in which the two-body potential is constructed taking into account both the s-wave scattering length and the effective range. We fix both quantities to values compatible with the experiment of Ref. We perform our calculations with two different model potentials, detailed below, in order to check if the scattering length and the effective range are sufficient to quantitatively describe the system in the regime of $k_F a_s$ considered. A similar approach has been carried out in other systems, where good agreement with experimental results has been found, see

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for example Refs. [25,27] for results regarding quantum droplets in Bose-Bose mixtures. Our results show that the explicit consideration of the finite range of the interaction allows for an excellent agreement with experimental data. Interestingly, we observe a regime of universality in terms of the two scattering parameters that covers the experimental regime of Ref. [22] for the 2D Fermi polaron.

Our microscopic approach is based on the diffusion Monte Carlo (DMC) method. DMC allows to accurately describe the ground state of quantum systems both in the dilute and in the strongly correlated regimes. Starting from a variational ansatz, the initial wave function $\Psi_T(R)$ is propagated in imaginary time keeping its nodal surface constant. In this way, one keeps the Fermi sign problem under control, leading to a statistical representation of the best possible wave function within a nodal surface constraint (fixed-node approximation (FN) [28]).

As a consequence, FN-DMC produces variational results whose quality is related to the accuracy of the model nodal surface. For the trial wave function, we use a Jastrow-Slater ansatz, which consists of a product of an antisymmetric part $\Psi_A(R)$ times a Jastrow factor $\Psi_J(R)$, that is symmetric to the exchange of particles. It reads

$$\Psi_T(R) = \Psi_A(R_\uparrow)\Psi_J(R), \quad (1)$$

where $R = \{r_1, \ldots, r_N, r_i\}$ is the set of all $N_\uparrow + 1$ particle coordinates, and $R_\uparrow$ accounts only for the coordinates of the $N_\uparrow$ particles of the bath. The antisymmetric term corresponds to a Slater determinant of plane waves, which is accurate enough for the low densities considered in this work [29]. The Jastrow term in Eq. (1) is chosen as a product of two-body correlation functions, which are taken as the ground-state wave function of the two-body problem at short distances matched with a phonon-like long-range term [29]. The propagator that we employ is a Jastrow-Slater ansatz, which consists of a product of two-body correlation functions, which are taken as the ground-state wave function of the two-body problem at short distances matched with a phonon-like long-range term [29]. The propagator that we employ is the Jastrow-Slater ansatz, which consists of a product of two-body correlation functions, which are taken as the ground-state wave function of the two-body problem at short distances matched with a phonon-like long-range term [29].

To describe the 2D Fermi polaron, we study a system of $N = N_\uparrow + 1$ particles composed by a Fermi sea of $N_\uparrow$ non-interacting fermions and a spin $\downarrow$ impurity, all with the same mass $m$. The Hamiltonian of the $N$-particle system reads

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_\uparrow^2 - \frac{\hbar^2}{2m} \sum_{i=1}^{N_\uparrow} \nabla_i^2 + \sum_{j=1}^{N_\uparrow} V^{\text{int}}(r_{ij}), \quad (2)$$

where $r_{ij} \equiv |r_i - r_j|$ is the distance between a bath particle at $r_i$ and the impurity position $r_j$. The two-body potential $V^{\text{int}}(r)$ models the interaction of the polaron with the bath. We use two different models: The first one is a Square-Well-Soft-Core (SWSC) potential, which reads

$$V(r) = \begin{cases} -U_0, & 0 < r < R_0, \\ U_1, & R_0 < r < R_1, \\ 0, & R_1 < r < \infty, \end{cases} \quad (3)$$

with all the parameters $(R_0, R_1, U_0, U_1)$ being positive. The second model is a Soft-Core (SC) potential, that can be considered a limiting case of the previous one by setting $R_0$ and $U_0$ to zero, and thus it is uniquely described by $U_1$ and $R_1$. The values of the parameters of Eq. (3) are reported in Table II. These values are chosen so that the potential reproduces the experimental results from Ref. [30], which corresponds to setting $a_{3D} = 187a_0$ and $r_{\text{eff}}^{3D} = 216a_0$, with $a_0$ the Bohr radius [31,32]. In Ref. [34], it is reported a second value for the effective range, which is smaller ($r_{\text{eff}}^{3D} = 126a_0$), but we checked with DMC that experimental data are only reproduced by choosing the larger value, $r_{\text{eff}}^{3D} = 216a_0$.

One of the most relevant quantities in the study of the polaron is the polaron energy, which is in fact the chemical potential of the impurity. Within the DMC framework, it can be evaluated by means of the energy difference

$$\varepsilon_p = [E(N_\uparrow, 1) - E(N_\uparrow, 0)]_V, \quad (4)$$

where $E(N_\uparrow, 0)$ is the energy of the $N_\uparrow$-particle pure system and $E(N_\uparrow, 1)$ is the one obtained when the impurity is added, keeping the volume constant. Within the mean-field approximation, the polaron energy is given by

$$\varepsilon_{\text{MF}} = \frac{4\pi\hbar^2 n}{m \ln(c_0/n a_0^2)}, \quad (5)$$

with $c_0$ a free parameter [33] that is related to the energy scale of the system. Following previous works [29,30,31], we fix it so that the choice for the energy scale corresponds to that of the free Fermi system $(E_F = \frac{\hbar^2 k_F^2}{2m} = 2\hbar^2 \pi n/m)$, which results into $c_0 = e^{2\gamma} \pi /2 \simeq 4.98$, where $\gamma \simeq 0.577$ is the Euler’s gamma constant.

In order to benchmark the present results, we compare our DMC energies for the SWSC and SC models to those obtained with a hard-disk (HD) potential (from Ref. [23]) and to the mean-field prediction [3]. While the hard-disk potential shares the same scattering length

| Potential | $R_0 [a_{3D}]$ | $R_1 [a_{3D}]$ | $U_0 [\hbar^2 / (ma_{3D}^2)]$ | $U_1 [\hbar^2 / (ma_{3D}^2)]$ |
|-----------|----------------|----------------|----------------|----------------|
| SC        | 0.91627        | 2.29069        | 0.62099        | 0.576351       |
| SWSC      | 0.91627        | 2.29069        | 0.62099        | 0.576351       |
Experiment

with the SWSC and SC potentials, its effective range is different and cannot be imposed in the construction of the model potential because the HD potential has only one free parameter, that is the diameter of the disk.

We report in Fig. 1 our DMC results for the polaron energy corresponding to the SWSC and SC potentials. In the same figure, we include the mean field prediction, the HD model results, and the experimental results of Ref. [22]. As it can be seen in the plot, both mean-field theory and the HD model fail to reproduce the experimental data. On the other hand, our two present models, in which both scattering length and effective range are fixed at the same time, show good agreement between them and with the experimental measurements [22]. Therefore, the dimensionless parameter \( k_F a_s \) is not the only relevant quantity to quantitatively describe the system and, to this end, finite range effects need to be included. Moreover, the independence on the specific shape of the potential, when both scattering length and effective range are reproduced, shows a universal behavior in these two quantities for the range of \( k_F a_s \) values shown in the figure.

To better characterize the Fermi polaron, we evaluate properties that are related its quasi-particle character. First, we study the quasi-particle residue \( Z \), which is defined as the overlap between the wave function of the system, featuring an interacting impurity, and the wave function of a pure system with a non-interacting impurity with zero momentum. Following previous works [23, 26, 37], we evaluate the quasi-particle residue from the long-range asymptotic behavior of the one-body density matrix when the interacting polaron moves in the Fermi bath. In our DMC implementation, this is obtained from the following estimator

\[
Z = \lim_{|r'_i - r_j| \to L/2} \frac{\langle \Psi_T(R, r'_i) \rangle}{\langle \Psi_T(R, r_j) \rangle}.
\]

In Fig. 2, we show DMC results for \( Z \) using the SWSC, SC, and HD potentials. In the same figure, we include the experimental results of Ref. [22] for this quantity. For values of \( k_F a_s < 0.2 \), we find that the results of the three models coincide, in agreement to the universal regime for this observables, as reported in Ref. [23]. However, as \( k_F a_s \) is increased, the results of the SWSC and SC models, for which the effective range and scattering length are fixed simultaneously, show good agreement with the experimental data of Ref [22] and a clear discrepancy with the HD short-range model. These results reinforce the ones for the polaron energy and remark the importance of going beyond the usual mean-field prescription in order to provide an accurate description of the two-dimensional Fermi polaron.

For the calculations presented here, \( \Phi^{N_1} = |\text{FS} + 1\rangle \), which stands for a Fermi sea (FS) with an added non-interacting impurity with zero momentum. Following previous works [23, 26, 37], we evaluate the quasi-particle residue from the long-range asymptotic behavior of the one-body density matrix when the interacting polaron moves in the Fermi bath. In our DMC implementation, this is obtained from the following estimator

\[
Z = \lim_{|r'_i - r_j| \to L/2} \frac{\langle \Psi_T(R, r'_i) \rangle}{\langle \Psi_T(R, r_j) \rangle}.
\]
As can be seen from the figure, both models agree within mass of the polaron. Similarly to previous reported quasi-particle energy, as defined in Eq. (4).

Experimentally accessed through its low-momenta excitation spectrum, the quasi-particle, formed by the impurity “dressed” by the medium, which propagates freely. In the DMC algorithm, the effective mass can be obtained by evaluating the low imaginary-time asymptotic behavior of the diffusion coefficient of the impurity throughout the bath [3, 39].

$$m = \lim_{\tau \to \infty} \frac{1}{4\tau} D^2(\tau),$$

with $D_0 = \frac{\hbar^2}{2m}$ corresponding to the free-particle diffusion constant and $D^2(\tau) = \langle (r_r(\tau) - r_r(0))^2 \rangle$ the mean squared imaginary-time displacement of the impurity in the medium. The effective mass of the polaron can be experimentally accessed through its low-momenta excitation spectrum,

$$\varepsilon_p(k) = \varepsilon_p(k = 0) + \frac{\hbar^2}{2m^*} k^2 + \mathcal{O}(k^4)$$

with $\varepsilon_p(k)$ being the polaron energy corresponding to a state with momentum $k$ and $\varepsilon_p(k = 0)$ the ground state polaron energy, as defined in Eq. (6).

We present in Fig. 3 our DMC results for the effective mass of the polaron. Similarly to previous reported quantities, we show results for the SWSC and the SC models. As can be seen from the figure, both models agree within the statistical error, coming from the MC sampling, for $k_F a_s \in [10^{-2}, 1]$. As expected, the effective mass increases as $k_F a_s$ approaches to one and the contribution of polaron-medium correlations are enhanced. However, the observed increase of the effective mass with $k_F a_s$ is less pronounced that the one predicted by T-matrix theory [35], relying only in the s-wave scattering length. Unfortunately, we are not aware of any measurement of $m^*$ in this range of densities to compare with.

In conclusion, inspired by a recent experiment with $^{173}$Yb [22], we have addressed the two-dimensional repulsive Fermi polaron problem by means of the DMC technique. With the aim of reproducing the experimental results of Ref. [22], which are outside of the universal regime for this problem in terms of the gas parameter [29], we include, through the two-body interaction potential, information of the effective range of the impurity-bath interaction. Our results for the polaron energy and the quasi-particle residue show agreement between two different model potentials with the same scattering length and effective range, and are in good agreement with the experimental ones. Thus, it hints at the existence of a universal regime in terms of two parameters: the Fermi momentum and the effective range. This assertion seems to be confirmed when the effective mass of the polaron is evaluated.

It is worth to remark that a similar attempt has been made recently with the aim of extending the current state of the art theory. In Ref. [40] the authors present a model that, by effectively including finite-range effects, is able to reproduce the Rabi oscillations of the Fermi polaron both from the three [18] two-dimensional [22] Fermi polaron experiments. On the other hand, although the quasi-particle residue that they report improves previous theoretical results, it is still unable to correctly reproduce them.

Therefore, we have shown that the employment of ab initio quantum Monte Carlo techniques offer insight into the polaron problem once the universality limit is surpassed. Similar results have been shown recently in the formation of droplets in Bose-Bose mixtures [22] and in the description of dipolar droplets of Dysprosium atoms [41]. We strongly believe that the observation of many-body effects, going beyond the simple mean-field approach, will stimulate further theoretical and experimental work in the field of ultracold atoms, with the advantage of the high tunability of interactions and the versatility that they offer to work in reduced dimensionalities practically at will.

ACKNOWLEDGMENTS

This work has been partly supported by the MINECO (Spain) Grant No. FIS2017-84114-C2-1-P. We acknowledge financial support from Secretaría d’Universitats i Recerca del Departament d’Empresa i Coneixement de la Generalitat de Catalunya, co-funded by the European Union Regional Development Fund within the ERDF Operational Program of Catalunya (project QuantumCat, ref. 001-P-001644). V. C. acknowledges financial support from the Project HPC-EUROPA3 (INFRAIA-2016-1-730897), with the support of the EC Research Innovation Action under the H2020 Programme. J. S-B. acknowledges the FPU fellowship with reference FPU15/01805.
