Long-range interacting Fermi polaron

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We construct the simplest density functional for the problem of a single impurity interacting with a Fermi gas via a long-ranged potential using the Thomas-Fermi approach. We find that the Fermi polaron is fully bosonized in two dimensions, as the model results in the Landau-Pekar functional known from the Bose polaron problem, and in its many-image extension in other dimensions. We discuss applications of our theory for the two-dimensional exciton-polaron and the ionic polaron problem and compute the effective mass for these cases, finding a self-trapping transition with order dependent on the dimensionality.

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I. INTRODUCTION

Polarons are quasiparticles that emerge from dressing of impurities with the excitations of the quantum many-body medium that they are embedded in. Their introduction was motivated mainly by modeling the motion of electrons in solids [1–4]. However, the idea of dressed states with modified energy and effective mass is general regardless of the medium nature [5]. Polarons are nowadays among the central concepts in understanding quantum transport [6]. Experiments with ultracold atomic gases have enabled the study of polarons in both bosonic and fermionic media and provided the possibility of tuning the interaction strength via Feshbach resonances, as well as new detection schemes which have greatly advanced the field [7].

One of the most intriguing aspects of the impurity problem is the calculation of the effective mass, an important quantity characterizing the polaron along with its energy and quasiparticle residue. For strong interactions, as well as for strongly correlated media, the mass renormalization can be exponentially large and diverge with the coupling constant [8]. Furthermore, a self-localization effect occurs in some approaches where the effective mass becomes infinite at finite interaction strength [9–12]. It is still under debate whether such transition can occur in realistic polaron models.

The simplest variational ansatz for the polaron wave function would consist of the free particle dressed with a single medium excitation [13]. However, the interactions need not be perturbative [14]. A full description of the system has to take into account the possibility of forming few- and many-body bound states and losing the quasiparticle picture, making fully numerical treatment such as Monte Carlo methods, necessary [15]. Field theoretical and variational approaches still do give valuable insights into the nature of the system [16–18]. While the polaron problem is actively investigated, most studies to date have been devoted to the case of contact interactions between the impurity and the bath. A particularly interesting case occurs when the impurity-medium interaction is instead long-ranged. This can be realized using, e.g., ions embedded in cold gases [19,20] and in the bosonic case results in the formation of many-body bound states [20,21]. Similar phenomena could be expected for excitons in a Fermi sea of electrons, as the electron-exciton interaction has the same nature as the ion-atom one and exciton polarons have already been observed [22–26]. Other possible examples include dipolar interactions [27] and Rydberg impurities [28–30]. Ions are important in this context since their position can be controlled effectively using external fields. It is thus important to study how their motion is affected by the surroundings. In this work, we construct a simple model that takes the fermionic nature of the bath and the nonzero range of the potential into account in a natural way. It results in a series of interesting effects, such as bosonization in two dimensions and the localization transition of dimension-dependent order, which we connect to bound-state formation in the system. Importantly, the model allows for a relatively simple extraction of the effective mass, which follows the lines of the localization transition.

II. THE MODEL

We consider a system of N free fermions of mass m_F and spin s and one impurity particle of mass m_I in d dimensions enclosed in a large box of volume L^d at zero temperature. The impurity interacts with the fermions via a two-body potential V which we assume to be bounded, to be symmetric, and to vanish sufficiently fast at infinity, but at the same time to be slowly varying, such that the system can be described using the Thomas-Fermi approximation with the functional

$$\mathcal{H}(\psi,\rho)=\frac{\hbar^2}{2m_I}\int|\nabla\psi(x)|^2dx+\frac{d\epsilon_{\mathrm{F}}\rho^{-\frac{2}{d}}}{d+2}\int\rho(x)^{1+\frac{2}{d}}dx+\iint\rho(x)V(x-y)|\psi(y)|^2dxdy \tag{1}$$

to be minimized with the normalization constraints $\int\rho(x)dx=N$ and $\int|\psi(x)|^2dx=1$, with $\int dx$ always denoting the multidimensional integral over the box. In the above, $\rho=NL^{-d}$ is the density of the uniform gas, and $\epsilon_{\mathrm{F}}=(\frac{\Gamma(\frac{d+2}{2})}{2s+1})^{\frac{2}{d}}\frac{2\pi\hbar^2}{m_F}\rho^{2/d}$ is the corresponding Fermi level, while ψ is the wave function of the impurity, and $\rho(x)$ is the local density of fermions at point x. This approach

appears natural in the context of long-range forces: in fact, the system described by Eq. (1) is essentially a collection of infinitesimally small boxes, each filled with the free Fermi gas with local density $\rho(x)$ having internal energy $\sim\rho(x)^{1+\frac{2}{d}}dx$ due to the Fermi pressure and subject to an external potential with a source whose position is smeared out due to the quantum nature of the impurity, $\int|\psi(y)|^2V(x-y)dy$. Since Thomas-Fermi theory is asymptotically correct in the limit of large atoms in quantum chemistry [31] where the electrons are "tightly spaced," it might be expected that Eq. (1) correctly describes our problem in a suitable scaling limit.

We first optimize the functional in Eq. (1) over ρ at fixed ψ. This immediately results in

$$\rho_\psi(x)=\rho\left(\frac{\mu-V_\psi(x)}{\epsilon_{\mathrm{F}}}\right)^{\frac{d}{2}}\Theta[\mu-V_\psi(x)], \tag{2}$$

where

$$V_\psi(x)=(|\psi|^2*V)(x)=\int V(x-y)|\psi(y)|^2dy, \tag{3}$$

Θ denotes the Heaviside Θ function, and μ is the chemical potential, satisfying

$$\rho\int\left(\frac{\mu-V_\psi(x)}{\epsilon_{\mathrm{F}}}\right)^{\frac{d}{2}}\Theta[\mu-V_\psi(x)]dx=N. \tag{4}$$

The Θ functions can be removed, provided that the number of fermions, and hence the chemical potential, are large enough. The optimized ρ_ψ can now be plugged back into Eq. (1), which yields a nonlinear functional of ψ alone. In what follows, we shall perform this procedure in different dimensions separately.

A. Bosonization in two dimensions

The resulting equations are particularly simple for $d=2$. In fact, for fixed N, we can easily determine μ from Eq. (2):

$$\mu=\epsilon_{\mathrm{F}}+\frac{1}{L^2}\int V_\psi(x)dx=\epsilon_{\mathrm{F}}+\langle V\rangle\,, \tag{5}$$

where $\langle V\rangle$ denotes the mean value of the potential, which is independent of ψ if the box is suitably large compared to the range of the potential, such that the integration might be extended to infinity.

Using the resulting density profile as well as the expression for the Fermi level ϵ_{F} in two dimensions, the total energy can be written as

$$\mathcal{H}(\psi,\rho_\psi)=E_{\mathrm{F}}\left(1+\frac{\langle V\rangle}{\epsilon_{\mathrm{F}}}\right)^2+\mathcal{E}^{\mathrm{Pek}}(\psi), \tag{6}$$

where $E_{\mathrm{F}}=\frac{1}{2}N\epsilon_{\mathrm{F}}$ is the ground-state energy of the uniform Fermi gas, and the *Pekar functional* $\mathcal{E}^{\mathrm{Pek}}(\psi)$ reads

$$\mathcal{E}^{\mathrm{Pek}}(\psi)=\frac{\hbar^2}{2m}\int|\nabla\psi(x)|^2dx - \frac{g_s m_F}{4\pi\hbar^2}\iint|\psi(x)|^2V^{(2)}(x-y)|\psi(y)|^2dxdy, \tag{7}$$

where we introduced the spin degeneracy factor $g_s=2s+1$ as well as the notation

$$V^{(2)}(x)=V*V(x)=\int V(x-y)V(y)dy\,. \tag{8}$$

Equation (7) is precisely the well-known Pekar functional describing the semiclassical theory of impurities interacting with *bosonic* fields [1], arising on top of the Fröhlich model which provides an asymptotically correct theory for long-range interactions [32]. Thus, at the semiclassical level, which provides a description of the long-range case, the Fermi polaron in two dimensions is essentially equivalent to the Bose polaron in the same dimension (see Appendix D). This is not surprising, given the similarities displayed by the corresponding ideal gases in two dimensions, e.g., their virial expansions differ only in one term [33].

B. Other dimensions—The polaronic Droste effect

In dimensions different than two, Eq. (2) for the chemical potential cannot be solved as easily. However, a perturbative expansion of the nonlinear functional may be applied in this case in the regime when the local potential or its spatial variations are small, i.e., for $|V_\psi-\langle V\rangle|\ll\epsilon_{\mathrm{F}}$. Then $\mu\approx\epsilon_{\mathrm{F}}+\langle V\rangle$ and one can solve for μ and find the energy by expanding the density in $|V_\psi-\langle V\rangle|/\epsilon_{\mathrm{F}}$. We provide the details of this calculation in Appendix C. The result is

$$\mathcal{H}(\psi,\rho_\psi)=\frac{d}{d+2}N\epsilon_{\mathrm{F}} + N\langle V\rangle\left(1+\frac{d\langle V\rangle}{4\epsilon_{\mathrm{F}}}+\frac{(d-2)(d-4)\langle V\rangle^2}{12\epsilon_{\mathrm{F}}^2}\right) + \mathcal{E}^{\mathrm{Pek}}_{(3)}(\psi), \tag{9}$$

with the following generalized version of the Pekar functional:

$$\mathcal{E}^{\mathrm{Pek}}_{(3)}(\psi)=\frac{\hbar^2}{2m}\int|\nabla\psi(x)|^2dx - \frac{d}{4}\frac{\rho}{\epsilon_{\mathrm{F}}}\left(1+\frac{(d-2)(d-4)\langle V\rangle}{2d\epsilon_{\mathrm{F}}}\right)W_2(\psi) + \frac{(d-2)(d-4)}{24}\frac{\rho}{\epsilon_{\mathrm{F}}^2}W_3(\psi), \tag{10}$$

with the already encountered two-body interaction

$$W_2(\psi)=\int_{(\mathbb{R}^d)^{\times2}}|\psi(x_1)|^2V^{(2)}(x_1-x_2)|\psi(x_2)|^2 \tag{11}$$

and a newly emerging *three-body interaction*,

$$W_3(\psi)=\int_{(\mathbb{R}^d)^{\times3}}|\psi(x_1)|^2|\psi(x_2)|^2|\psi(x_3)|^2V^{(3)}(x_1,x_2,x_3), \tag{12}$$

with the three-body potential

$$V^{(3)}(x_1,x_2,x_3)=\int V(x_1-y)V(x_2-y)V(x_3-y)dy. \tag{13}$$

The main observation is that the three-body term appears which is not present in the two-dimensional (2D) Pekar functional for fermions, or for bosons in any dimensionality. The

inclusion of further terms in the series in inverse powers of ϵ_F yields a functional with the general structure

$$\mathcal{E}^{\mathrm{Pek}}_{(\infty)}(\psi) = \frac{\hbar^2}{2m}\int |\nabla\psi(x)|^2 dx + \sum_{k=1}^{\infty}\frac{\rho}{\epsilon_F^k}\int_{\mathbb{R}^{d(k+1)}} G^{(k)}(x_1,\ldots,x_{k+1})\prod_{i=1}^{k+1}|\psi(x_i)|^2, \tag{14}$$

with appropriate $k+1$-body kernels $G^{(k)}(x_1,\ldots,x_{k+1})$ depending on V. In the pictorial language of Pekar's theory, the fermionic correlations lead to an emergence of infinite mirror images of the impurity imprinted in the Fermi medium. Borrowing from the fine arts language, we describe this phenomenon as the *polaronic Droste effect* [34].

III. EFFECTIVE MASS AND LOCALIZATION

A. Definition of effective mass via frequency shifts

Apart from the computation of the ground-state energy of the polaron, an important quantity to estimate is its effective mass. We adopt an approach to the effective mass problem inspired by Ref. [35]. The idea is to place the impurity particle into a very shallow harmonic trap of low-frequency ω, such that the Thomas-Fermi functional reads now

$$\mathcal{H}(\psi,\rho;\omega) = \frac{\hbar^2}{2m_I}\int|\nabla\psi(x)|^2dx + \frac{d\epsilon_F\rho^{-\frac{2}{d}}}{d+2}\int\rho(x)^{1+\frac{2}{d}}dx + \iint\rho(x)V(x-y)|\psi(y)|^2dxdy + \frac{m_I\omega^2}{2}\int x^2|\psi(x)|^2dx. \tag{15}$$

If the polaron is indeed formed and the impurity and the gas behave as one entity with effective mass M_{eff}, then the difference between the ground-state energies of the functional (15) at small ω and $\omega=0$ should be well described by the ground-state energy of the Hamiltonian $\frac{\hbar^2}{2M_{\mathrm{eff}}}(-i\nabla_x)^2 + \frac{m_I\omega^2}{2}x^2$, namely, $\frac{d}{2}\hbar\omega\sqrt{\frac{m_I}{M_{\mathrm{eff}}}}$. Accordingly, we define the effective mass as

$$M_{\mathrm{eff}} = \lim_{\omega\to0}\frac{d^2m_I\hbar^2\omega^2}{4[E^{\mathrm{TF}}(\omega)-E^{\mathrm{TF}}(0)]^2}, \tag{16}$$

with $E^{\mathrm{TF}}(\omega)$ being the minimum energy of the functional (15), assuming the limit exists. In other words, we expect a shift in the frequency of oscillations of the impurity immersed in a Fermi gas as compared to the motion in vacuum, and we attribute this shift to the mass renormalization. This directly corresponds to possible experimental effective mass measurements in ultracold atomic setups. In practice, we are going to estimate $E^{\mathrm{TF}}(\omega)-E^{\mathrm{TF}}(0)$, e.g., by variational methods and fit the results to a parabolic curve for sufficiently small ω. The limit (16) can then be obtained from the value of the fitted parameter in front of the linear term.

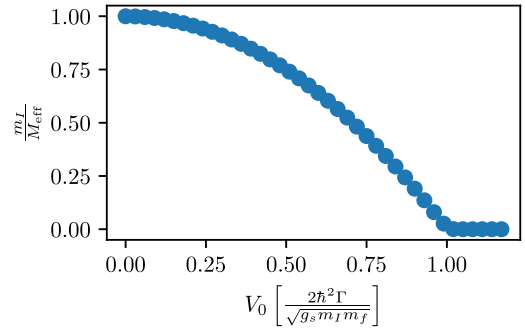

FIG. 1. Inverse effective mass of the two-dimensional Fermi polaron in units of the impurity mass as a function of the coupling strength in units of $2\hbar\Gamma/\sqrt{g_s m_I m_F}$. The mass diverges continuously at critical coupling, and thus the self-trapping transition is of *second order*.

B. Localization

To gain some insight into the problem, let us test the above procedure on a simple example of a Gaussian-type potential and trial wave function. It is instructive to follow the simple calculations that emerge in this case: they are presented in Appendix B. The results are summarized in Figs. 1 and 2. The main conclusion here is the presence of a sharp *localization transition*: the effective mass is *finite* for small couplings and infinite for larger ones, with the divergence occurring at the respective critical value of V_0. Moreover, in $d=2$ the divergence is continuous while in $d=3$ it is abrupt. Accordingly, the transition is second order in two dimensions and first order in three dimensions.

The behavior of the effective mass reflects the existence or nonexistence of a minimizer for the respective Pekar functional. In particular, we observe that in $d=2$ the transition takes place and a minimal value of the coupling is necessary to induce binding, even though all two-body attractive potentials have bound states in two dimensions. This is not an artifact of the variational calculation and the particular choice but a genuine property of the functional, anchored in its

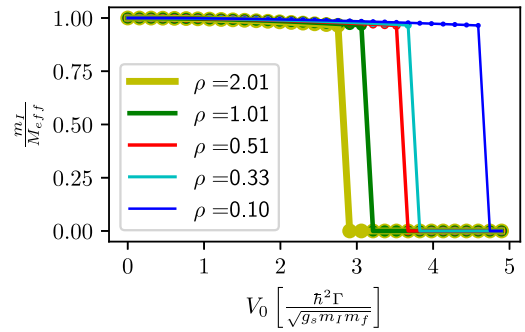

FIG. 2. Inverse effective mass of the three-dimensional Fermi polaron in units of the impurity mass, plotted against the coupling. The solid lines present the results obtained from the Pekar functional with three-body terms included, the dots indicate truncation to two-body terms (no Droste effect). The densities are given in units of the volume set by the potential range $\Gamma^{3/2}$. As the effective mass jumps to infinity discontinuously at critical coupling, the trapping transition is of *first order*.

nonlinearity. We provide a rigorous proof of this fact in Appendix A, where we show that the Pekar functional

$$\mathcal{E}(\psi) = \frac{\hbar^2}{2m}\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 dx - g\iint_{\mathbb{R}^d\times\mathbb{R}^d} |\psi(x)|^2\eta(x-y)|\psi(y)|^2 dxdy \quad (17)$$

does not admit a bound state for g small enough and for sufficiently fast decaying potentials η, in both two and three dimensions. This is in contrast to the linear case where a bound state always exists for negative potentials. The value of the critical coupling g necessary for binding can be estimated from the proof: trapping does not occur for $g < g_*$, which can be written

$$g_* = \frac{\hbar^2 S_{2D}^{(d)}}{2m\|\eta\|_{d/2}}, \quad (18)$$

with $\|\eta\|_{d/2} = (\int |\eta(x)|^{d/2}dx)^{2/d}$, for some explicit constants $S_{2D}^{(d)}$ dependent on the dimensionality. In our problem, $\eta = V^{(2)} = V * V$, where V is the original impurity-fermion potential, while $g = \frac{d}{4}\frac{\rho}{\epsilon_F}$. The proof gives the estimate $g^* \sim \frac{\hbar^2}{m\|V^{(2)}\|_{d/2}}$. Assuming V comes with a characteristic strength V_0 and range R, we have $\|V^{(2)}\|_{d/2} \sim V_0^2 R^{d+2}$ and thus the critical value of V_0 can be estimated as

$$V_{0,c} \sim \sqrt{\frac{\hbar^2}{2mR^{d+2}g^*}} = \sqrt{\frac{\epsilon_F}{\rho R^d}\frac{\hbar^2}{2mR^2}} = \sqrt{\frac{\epsilon_F T_R}{N_R}}, \quad (19)$$

where $N_R = \rho R^d$ is the mean number of fermions in the range of the potential and $T_R = \frac{\hbar^2}{2mR^2}$ is the characteristic kinetic energy of the impurity self-trapped in volume R^d. Note that both ϵ_F and N_R increase with the density, with $\epsilon_F \sim \rho^{2/d}$ and $N_R \sim \rho$; in three dimensions, the ratio results in a critical coupling that decreases with the density while in $d = 2$ the density cancels out.

Let us finally discuss how the transition found could be linked to the well-known polaron-to-molecule transition in Fermi polarons with contact interactions [13,36], with the system behaving like a quasi-free-particle with a definite effective mass for small couplings (polaronic phase) and forming many-body bound states with the fermions for large couplings, leading to the infinite value of the effective mass under our definition. In fact, by Weyl's law, the number of bound states of an attractive potential is approximately given by the classical phase-space volume corresponding to negative energies [37]. In our case and with $d = 3$, this volume is proportional to the integral $\int |V_\psi(x)|^{3/2}dx$. This integral scales with the box volume as $L^{-3/2}$ in the polaronic regime and is thus very small; for the bound states to appear in the potential V_ψ forming a well for the fermions, ψ must be localized. This supports the interpretation of the transition in terms of cluster formation. In particular, in this model polarons and bound clusters can coexist in three dimensions where the transition is of first order but not in two dimensions where it is continuous.

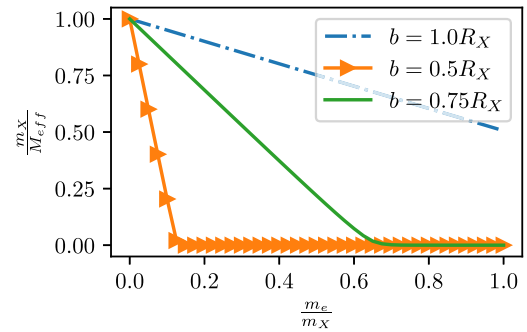

FIG. 3. The inverse effective mass of the 2D exciton polaron as a function of the electron to exciton mass ratio in the material, for different values of the length scale b. Here, $R_X = \sqrt{C_4 m_X}/\hbar^2$, with m_X being the exciton mass.

IV. APPLICATIONS

We now apply the model to two simple and experimentally relevant cases in which the impurity-fermion pair consists of a charge and a neutral polarizable entity, such that the underlying two-body potential at long range comes from electrostatic induction and decays as r^{-4}. We use a regularized interaction with a finite depth,

$$V(r) = -\frac{C_4}{(r^2+b^2)^2}, \quad (20)$$

where $b > 0$ is the regularizing length scale, while $C_4 = \frac{1}{2}q^2\alpha$, with q being the charge and α the polarizability of the neutral object in question. This potential comes along with the length and energy scales $R^* = \sqrt{2m_r C_4/\hbar^2}$ and $E^* = \hbar^2/(2m_r R^{*2})$, respectively, with m_r denoting the reduced mass of the impurity-fermion pair. Using a Feshbach resonance it is possible to tune experimentally the scattering length of the potential, which we model by tuning the value of b.

First we study the exciton-polaron problem in two dimensions, i.e., a mobile exciton interacting with free electrons in a 2D layer, taking the functional (7) with the potential (20) and using Gaussian trial functions. Assuming that the exciton polarizability is independent of its mass and neglecting any external potentials, the relevant parameter quantifying the coupling is given by the ratio of the effective masses of the electron and the exciton in the material. In Fig. 3 we present the effective mass of the exciton-polaron as a function of the electron to exciton mass ratio at different values of the regularizing scale b. As in the simple Gaussian model, we encounter a self-trapping transition of second order.

Second, we use the 3D Pekar functional with the potential (20) for the ionic Fermi polaron problem, again with a Gaussian trial function and without the inclusion of many-body terms. As we are interested principally in the computation of the effective mass, the latter approximation should be enough for our purpose, even at moderate densities (see Fig. 2). We apply the theory for the case of equal masses as well as to the experimentally more interesting mass-imbalanced case of a Ba ion immersed in a cold gas of ^{6}Li atoms [38]. The energy of the equal mass case is depicted in Fig. 4(b) and is compared to the result of Christensen *et al.* [20], who calculated the polaron energy within the ladder approximation. We note that the

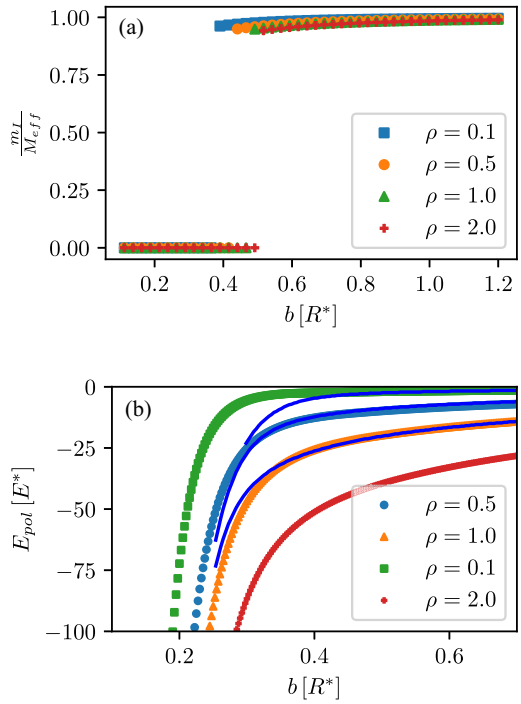

FIG. 4. (a) The inverse of the effective mass of the 3D ionic polaron in the case where the impurity and the (polarized) fermions are of equal mass. (b) The ground-state energy of the polaron. The thin solid lines are the results of the ladder approximation at the same densities [20]. Dimer formation in the two-body problem occurs at $b \sim 0.6R^*$ [20]. The densities are given in units of $(R^*)^{-3}$.

two curves agree perfectly in the large-b limit where the potential is very shallow and mean field theory should be strict. For deeper potentials both approaches provide qualitatively similar results. The effective mass again diverges for values of b close to the ones corresponding to dimer formation in the two-body problem, cf. Fig. 4(a), which marks the presence of the self-trapping transition of first order. We remark that recent Monte Carlo calculations of the effective mass of the ionic polaron [39] display an abrupt increase for values of b in the same range, validating the use of the semiclassical theory. For the mass-imbalanced case we obtain similar results, with a moderate mass increase of up to 3% in the polaron regime for experimentally realistic parameter values.

V. SUMMARY

We have developed a basic theory of an impurity interacting with a free Fermi gas via a long-range potential, applying the Thomas-Fermi approximation for the gas density. We found that in two dimensions this leads to the nonlinear Pekar functional known from the bosonic counterpart of the problem, describing a self-interacting impurity. In dimensions other than two, a perturbative expansion gives rise to a new functional with multiple self-interactions of the impurity with its own images. Interestingly, we found that a localization transition takes place in the system, as a particle forms either a polaron with renormalized mass or an immobile many-body bound state. The presence of such a transition marks a boosted version of the smooth crossover between polarons and many-body clusters which is likely to be found in the full quantum treatment and in the laboratory. We expect our results to act as useful benchmarks for future experiments and theories to follow, in particular, the measurements of the effective mass in various dimensions and its dependence on the gas density and the impurity-fermion mass ratio. All these parameters can easily be varied within our approach, while the model itself remains open to further analysis and extensions such as including thermal effects and nonequilibrium dynamics of the impurity.

ACKNOWLEDGMENTS

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APPENDIX A: PROOF OF THE LOCALIZATION TRANSITION FOR THE PEKAR FUNCTIONAL WITH REGULAR POTENTIALS

In the main text, we have shown results of simple variational calculations that revealed the self-trapping transition in the Pekar functionals under study. Here we prove rigorously that the transition is not an artifact of the variational method but is inherent to the Pekar functional with two-body terms, provided that the potential is sufficiently regular—we assume that it is bounded and integrable in the proof, but it may be expected that these assumptions can be relaxed. In fact, we show that whenever the interaction potential is weak enough the energy cannot be strictly minimized using normalized wave functions. This is different than in the case of the standard quantum mechanical particle in a well: in $d = 2$, there is always a bound state with negative energy for arbitrarily weak potentials.

Theorem. Let $g > 0$ be a coupling constant and consider the Pekar functional, defined for L^2-normalized wave functions that are in the $H^1(\mathbb{R}^d)$ class (which means that both the function and its distributional gradient are square integrable) as

$$\mathcal{E}(\psi) = \frac{\hbar^2}{2m}\int_{\mathbb{R}^d} |\nabla\psi(x)|^2 dx - g\iint_{\mathbb{R}^d\times\mathbb{R}^d} |\psi(x)|^2\eta(x-y)|\psi(y)|^2 dxdy \qquad \text{(A1)}$$

in $d = 2$ and $d = 3$, and assume that the interaction potential is bounded and integrable, i.e., $\eta \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. Then there exists $g_* > 0$ such that for $g < g_*$ the functional (A1) has no minimizer in $H^1(\mathbb{R}^d)$, and its minimal possible energy equals 0.

Proof. Let us first note that there exists a sequence of normalized L^2 functions ψ_j such that $\lim_{j\to} \mathcal{E}(\psi_j) = 0$. Indeed, it is enough to consider $\psi_j(x) = j^{-d/4}e^{-\pi x^2/(2j)}$; then it can be computed explicitly that $\lim_{j\to\infty}\int_{\mathbb{R}^d} |\nabla\psi_j(x)|^2 dx = 0$,

while, with the hat denoting the Fourier transform,

$$-\iint_{\mathbb{R}^d\times\mathbb{R}^d}|\psi_j(x)|^2\eta(x-y)|\psi_j(y)|^2dxdy = \int e^{-j\pi k^2}\hat{\eta}(k)dk \to 0 \tag{A2}$$

as $j \to 0$, where the equality follows the Parseval's identity, and the limit is taken by dominated convergence. Thus, the infimum of (A1) is at least 0. Next, we show that for sufficiently small couplings, for all localized wave functions one has $\mathcal{E}(\psi) > 0$, so that no minimizing bound state exists.

Let us first consider the case $d = 2$: then, using the Cauchy-Schwarz inequality and Young's inequality for convolutions $\|f * g\|_r \leqslant \|f\|_p\|g\|_q$ if $p^{-1} + q^{-1} = 1 + r^{-1}$, $1 \leqslant p, q, r \leqslant \infty$ [40] for $r = 2$, $p = 1$, and $q = 2$, we can bound

$$\iint_{\mathbb{R}^d\times\mathbb{R}^d}|\psi(x)|^2v(x-y)|\psi(y)|^2dxdy \leqslant \|\psi\|_4^2\|\eta * |\psi|^2\|_2 \leqslant \|\psi\|_4^4\|\eta\|_1. \tag{A3}$$

[here, $\|f\|_p = (\int |f|^p dx)^{1/p}$ denotes the p-norm of a function f]. Moreover, the Sobolev inequality for gradients in $d = 2$ states that for all $q \geqslant 2$ there exists a constant $S_q^{(2)}$ such that for all L^2-normalized functions

$$\|\nabla\psi\|_2^2 + 1 \geqslant S_q^{(2)}\|\psi\|_q^2. \tag{A4}$$

From this, it follows that

$$\|\nabla\psi\|_2^2 \geqslant \frac{\left(S_4^{(2)}\right)^2}{4}\|\psi\|_4^4. \tag{A5}$$

In fact, for any ψ, let $\psi_\lambda(\cdot) = \lambda\psi(\lambda\cdot)$ for some $\lambda > 0$. Then $\|\nabla\psi_\lambda\|_2^2 = \lambda^2\|\nabla\psi\|_2^2$ and $\|\psi_\lambda\|_4^2 = \lambda\|\psi\|_4^2$, and thus for all $\lambda > 0$ and all ψ, the quadratic form $\lambda \mapsto \lambda^2\|\nabla\psi\|_2^2 - S_4\lambda\|\psi\|_4^2 + 1$ is positive definite, from which Eq. (A5) follows. Combining this with the bound (A3), we have that

$$\mathcal{E}(\psi) \geqslant \frac{\hbar^2}{2m}\|\nabla\psi\|_2^2 - g\|\eta\|_1\|\psi\|_4^4 \geqslant \left(\frac{\hbar^2\left(S_4^{(2)}\right)^2}{8m} - g\|\eta\|_1\right)\|\psi\|_4^4, \tag{A6}$$

which is strictly positive for all ψ if $g < g_* = \frac{\hbar^2 S_4^{(2)2}}{8m\|\eta\|_1}$. This proves the statement for $d = 2$: no localized wave function yields energy precisely 0 for $g < g_*$ while 0 must be the infimum in this case by the previous argument.

The case of $d = 3$ is similar: instead of the bound (A5), we use the standard Sobolev inequality for gradients in $d = 3$ to bound the kinetic energy from below as

$$\|\nabla\psi\|_2^2 \geqslant S_6^{(3)}\|\psi\|_6^2 \tag{A7}$$

for some universal constant $S_6^{(3)} > 0$. For the interaction energy, we use the Young's inequality in the different form [40]

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3}|f(x)|^2\eta(x-y)|g(y)|^2dxdy \leqslant \|f\|_p\|\eta\|_q\|g\|_r \tag{A8}$$

for $(1/p) + (1/q + (1/r) = 2$, $p, q, r \geqslant 2$. We choose $p = 3$, $q = 3/2$, and $r = 1$ to find for $f = g = |\psi|^2$

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\psi(x)|^2\eta(x-y)|\psi(y)|^2dxdy \leqslant \||\psi^2|\|_3\|\eta\|_{3/2} \tag{A9}$$

as $\||\psi|^2\|_1 = 1$ since ψ is normalized. Since $\||\psi^2|\|_3 = \|\psi\|_6^2$, the last two inequalities combined yield

$$\mathcal{E}(\psi) \geqslant \left(\frac{\hbar^2 S_6^{(3)}}{2m} - g\|\eta\|_{3/2}\right)\|\psi\|_6^2, \tag{A10}$$

which is again strictly positive for all ψ if $g < g_* = \frac{\hbar^2 S_6^{(3)}}{2m\|\eta\|_{3/2}}$. This completes the proof. ■

APPENDIX B: SELF-TRAPPING WITHIN THE GAUSSIAN ANSATZ

The previous Appendix is devoted to showing that the self-trapping is a genuine feature of our model. With this knowledge, we proceed to gain some insight into the details of the transition on a simple example, using the Gaussian-type potential which is commonly chosen as a model of finite-ranged interaction,

$$V(x) = -V_0\exp(-\Gamma x^2), \tag{B1}$$

with the coupling amplitude $V_0 > 0$ and the inverse range squared Γ.

Then a simple calculation shows that

$$V^{(2)}(x) = \frac{\pi V_0^2}{2\Gamma}\exp\left(-\frac{\Gamma}{2}x^2\right). \tag{B2}$$

As indicated in the main text, we estimate the ground-state energy of $\mathcal{E}^{\text{Pek}}$ using a one-parameter trial wave function,

$$\psi_u(x) = \left(\frac{2u}{\pi}\right)^{d/4}\exp(-ux^2), \quad u > 0. \tag{B3}$$

We start with $d = 2$. The resulting energy is very easy to calculate and reads

$$E(u) \equiv \mathcal{E}^{\text{Pek}}(\psi_u) = \frac{\hbar^2}{m_I}u - \frac{g_s m_F V_0^2}{8\Gamma\hbar^2}\frac{u}{u+\frac{\Gamma}{2}}. \tag{B4}$$

Already this simple approach leads to the occurrence of a localization transition, i.e., the phenomenon that a bound state appears only for sufficiently strong couplings. In fact, the positive root of the derivative of $E(u)$ is given by

$$u_+ = \frac{1}{2}\left(\frac{V_0}{2\hbar}\sqrt{g_s m_I m_F} - \Gamma\right) \tag{B5}$$

and appears if and only if [comp. (19)]

$$V_0 \geqslant V_c = \frac{2\Gamma\hbar^2}{\sqrt{g_s m_F m_I}}. \tag{B6}$$

Otherwise, the lowest energy attainable by means of ψ_u equals 0 and corresponds to the ground state of the free particle in the box. Thus, for $V_0 < V_c$, the surrounding gas does not localize the particle. At $V_0 > V_c$ binding does occur, and the particle

gets trapped by the surrounding medium. If we now again take (B1) as the particle-impurity potential and define also

$$E(u;\omega) = \mathcal{E}^{\mathrm{Pek}}(\psi_u) + \frac{m_I\omega^2}{2}\int x^2|\psi_u(x)|^2dx,$$
$$E_0(\omega) = \inf_{u>0} E(u,\omega), \tag{B7}$$

with ψ_u denoting the class of functions (B3), then the effective mass in the *Gaussian* approach will be

$$M^{\mathrm{G}}_{\mathrm{eff}} = \lim_{\omega\to 0}\frac{d^2 m_I\hbar^2\omega^2}{4[E_0(\omega)-E_0(0)]^2}. \tag{B8}$$

In two dimensions, it is then straightforward to find

$$E(u;\omega) = \frac{\hbar^2}{m_I}u - \frac{g_s m_F V_0^2}{8\Gamma\hbar^2}\frac{u}{u+\frac{\Gamma}{2}} + \frac{m_I\omega^2}{4u}. \tag{B9}$$

The condition for the zero of the derivative

$$\frac{\hbar^2}{m} - \frac{g_s m_F V_0^2}{16\hbar^2}\frac{1}{\left(u+\frac{\Gamma}{2}\right)^2} - \frac{m_I\omega^2}{4u^2} = 0 \tag{B10}$$

leads to the quartic equation

$$\frac{\hbar^2}{m}u^2\left(u+\frac{\Gamma}{2}\right)^2 - \frac{g_s m_F V_0^2}{16\hbar^2}u^2 - \frac{m_I\omega^2}{4}\left(u+\frac{\Gamma}{2}\right)^2 = 0, \tag{B11}$$

whose unperturbed ($\omega = 0$) nonnegative solutions are $u_p = 0$ in the unbound regime ($V_0 < V_c$) and $u_b = u_+$ in the bound ($V_0 > V_c$) regime. In the unbound regime, we solve (B11) by treating ω as small and by setting $u = u_p + \delta = \delta$, where δ is the first-order correction to the unperturbed solution, and retaining only leading order terms in δ and ω. This leads to

$$u = \frac{\frac{m_I\omega}{2\hbar}}{\sqrt{1-\left(\frac{V_0}{V_c}\right)^2}} + o(\omega) \tag{B12}$$

and the minimizing energy at small ω reads

$$E_0(\omega) = \sqrt{1-\left(\frac{V_0}{V_c}\right)^2}\hbar\omega, \tag{B13}$$

so that the effective mass equals

$$M^{\mathrm{G}}_{\mathrm{eff}} = \frac{m_I}{1-\left(\frac{V_0}{V_c}\right)^2} \tag{B14}$$

and diverges as the amplitude V_0 approaches the localization point. In contrast, beyond the localization point and at ω small, it is easy to see the lowest-order approximate solution of Eq. (B11) is $b = b_+ + \delta$, with $\delta \sim \omega^2$, and consequently $E_0(\omega) - E_0(0) \sim \omega^2$. The limit (B8) is then infinite, and one can say that the localized particle has infinite effective mass under the definition adopted here.

Now we pass to the case $d = 3$ and study the (pure) Pekar functional in three dimensions,

$$\mathcal{E}^{\mathrm{Pek}}_{(2)}(\psi) = \frac{\hbar^2}{2m}\int|\nabla\psi(x)|^2dx$$
$$-\frac{3}{4}\frac{\rho_0}{\epsilon_{\mathrm{F}}}\iint|\psi(x_1)|^2V^{(2)}(x_1-x_2)|\psi(x_2)|^2dx_1dx_2, \tag{B15}$$

which, with our choice of the potential and wave function, evaluates to the function

$$E_2(b) = \frac{3}{2}\frac{\hbar^2}{m_I}u - \frac{3\rho V_0^2}{4\epsilon_{\mathrm{F}}}\left(\frac{\pi}{2\Gamma}\right)^{\frac{3}{2}}\left(\frac{2u}{2u+\Gamma}\right)^{\frac{3}{2}}. \tag{B16}$$

Now, the two-body Gaussian functional (B16) admits a simple calculation of the critical coupling strength for the localized state to appear as a global minimum of the untrapped system. The condition for the zero of the derivative of Eq. (B16) leads to the equation

$$\frac{(2u)^{1/2}}{(2u+\Gamma)^{5/2}} = \frac{2\hbar^2\epsilon_{\mathrm{F}}}{3m_I V_0^2\rho\Gamma}\left(\frac{2\Gamma}{\pi}\right)^{\frac{3}{2}} \tag{B17}$$

that can be solved only if $|V_0| \geqslant \sqrt{\frac{25\sqrt{5}}{24}\left(\frac{2}{\pi}\right)^{\frac{3}{2}}\frac{\hbar^2\Gamma^{\frac{5}{2}}\epsilon_{\mathrm{F}}}{m_I\rho}}$ which is the minimal value of $|V_0|$ for which *metastable* localized states appear. The minimal value of $|V_0|$ required for *stable* localization can be found by using Eq. (B17) together with the condition $E_2(u) = 0$, as the localized and delocalized state coexist as stable minima at this value of V_0. This gives (compare the estimate $V_c \sim \sqrt{\frac{\epsilon_{\mathrm{F}}T_R}{N_R}}$ in the main text, wherein the symbols are also explained)

$$|V_c| = \sqrt{\left(\frac{6}{\pi}\right)^{\frac{3}{2}}\frac{\hbar^2\Gamma^{\frac{5}{2}}\epsilon_{\mathrm{F}}}{2m_I\rho}}. \tag{B18}$$

Unfortunately, the effective mass cannot be found explicitly, as the relevant equation for small ω is a quintic one, rather than quartic as in two dimensions, and thus it does not admit a closed solution. It can be, however, computed numerically from the slope of the energy difference $E_0(\omega) - E_0(0)$ at small frequencies.

APPENDIX C: PERTURBATION EXPANSION FOR THE DROSTE EFFECT

We shall give a few more details about the perturbation expansion which leads to the polaronic Droste effect described by the Pekar functional with many-body terms.

As pointed out in the main text, the regime we are interested in corresponds to situations where the chemical potential is close to ϵ_{F}, which is its value for the free Fermi gas at zero temperature. For simplicity, we shift the interaction potential $V \to V - \langle V\rangle$ and work with a V that has a mean value of 0. When considering the final result, one simply has to add a constant term $N\langle V\rangle$ to the energy functional. Further, in order to control the expansion, we substitute $V_\psi \to \lambda V_\psi$ where $\lambda > 0$ is meant to be a small dimensionless parameter measuring the smallness of V_ψ resulting either from the weakness of the potential V itself or the large spread of the wave function ψ, in which case V_ψ is indeed small as we assume that V has a mean value of 0. At the end of the expansion, λ is set equal to unity.

Accordingly, we write

$$\mu = \epsilon_{\mathrm{F}}\left(1 + \frac{\lambda}{\epsilon_{\mathrm{F}}}\mu_0 + \left(\frac{\lambda}{\epsilon_{\mathrm{F}}}\right)^2\mu_1 + \left(\frac{\lambda}{\epsilon_{\mathrm{F}}}\right)^3\mu_2 + o[(\lambda/\epsilon_{\mathrm{F}})^4]\right) \tag{C1}$$

and plug this into the formula for the optimal density profile given ψ, i.e.,

$$\rho_\psi(x) = \rho\left(\frac{\mu - \lambda V_\psi}{\epsilon_{\mathrm{F}}}\right)^{\frac{d}{2}} \tag{C2}$$

[the Heaviside function can be dropped since in the assumed regime of validity of the expansion it clearly holds that $\mu > \lambda V_\psi(x)$ for all x]. The application of the generalized binomial expansion

$$(1+x)^\alpha = \sum_{k=0}^{\infty}\frac{\Gamma(\alpha+1)}{\Gamma(\alpha+1-k)k!}x^k \equiv \sum_{k=0}^{\infty}\binom{\alpha}{k}x^k \tag{C3}$$

with $\Gamma(\cdot)$ denoting the Euler Γ function yields

$$\begin{aligned}\rho_\psi(x) = \rho\Bigg(&1 + \frac{\lambda}{\epsilon_{\mathrm{F}}}D[\mu_0 - V_\psi(x)] \\ &+ \frac{\lambda}{\epsilon_{\mathrm{F}}}^2\left[D\mu_1 + \binom{D}{2}[\mu_0 - V_\psi(x)]^2\right] + \\ &- \left(\frac{\lambda}{\epsilon_{\mathrm{F}}}\right)^3\Bigg\{2\binom{D}{2}\mu_1[\mu_0 - V_\psi(x)] + D\mu_2 \\ &+ \binom{D}{3}[\mu_0 - V_\psi(x)]^3\Bigg] + o[(\lambda/\epsilon_{\mathrm{F}})^4]\Bigg\},\end{aligned}$$

where we introduced $D = \frac{d}{2}$ for the sake of transparency. Then $\int \rho_\psi(x)dx - N$ is a polynomial in λ. Since $\int \rho_\psi(x)dx = N$, all coefficients of this polynomial have to vanish, which leads to

$$\begin{aligned}\mu_0 &= 0, \\ \mu_1 &= -\frac{1}{D}\binom{D}{2}\frac{\int V_\psi(x)^2dx}{L^d}, \\ \mu_2 &= \frac{1}{D}\binom{D}{3}\frac{\int V_\psi(x)^3dx}{L^d}.\end{aligned}$$

We plug these back into the density profile and compute the resulting energy from the functional $\mathcal{H}(\rho, \psi)$. With the use of Eq. (C3), the internal energy of the fermions is then evaluated as

$$\begin{aligned}&\frac{d}{d+2}\epsilon_{\mathrm{F}}\rho^{-\frac{2}{d}}\int \rho(x)^{1+\frac{2}{d}}dx \\ &= \frac{d}{d+2}N\epsilon_{\mathrm{F}} + \frac{\lambda^2}{\epsilon_{\mathrm{F}}}\frac{d}{d+2}\binom{D'}{2}D^2\int V_\psi(x)^2dx \\ &\quad - \frac{\lambda^3}{\epsilon_{\mathrm{F}}^2}\left[\binom{D'}{3}D^3 + 2\binom{D}{2}\binom{D'}{2}D\right]\int V_\psi(x)^3dx \\ &\quad + o\big(\lambda^4\epsilon_{\mathrm{F}}^{-3}\big),\end{aligned}$$

where $D' = 1 + \frac{2}{d}$. The interaction energy at the same order reads

$$\begin{aligned}\lambda\int \rho(x)V_\psi(x)dx = &-\frac{\lambda^2}{\epsilon_{\mathrm{F}}}\rho D\int V_\psi(x)^2dx \\ &+ \frac{\lambda^3}{\epsilon_{\mathrm{F}}^2}\rho\binom{D}{2}\int V_\psi(x)^3dx + o\big(\lambda^4\epsilon_{\mathrm{F}}^{-3}\big).\end{aligned}$$

After simple manipulations, we arrive at the final expression

$$\begin{aligned}\mathcal{H}(\psi, \rho_\psi) = &\frac{\hbar^2}{2m_I}\int |\nabla\psi(x)|^2dx \\ &- \frac{d}{4}\frac{\rho}{\epsilon_{\mathrm{F}}}\int \tilde{V}_\psi(x)^2dx \\ &+ \frac{(d-2)(d-4)}{24}\frac{\rho}{\epsilon_{\mathrm{F}}^2}\int \tilde{V}_\psi(x)^3dx + N\langle V\rangle,\end{aligned} \tag{C4}$$

where we have put $\lambda = 1$ and denoted explicitly the shifted potential $\tilde{V}_\psi = V_\psi - \langle V\rangle$. By noting that $\int V_\psi^2dx = W_2(\psi)$ and $\int V_\psi^3dx = W_3(\psi)$, it is straightforward to arrive at the form given in the main text. It is evident from the procedure sketched that at higher orders in λ, many-body terms will emerge from expressions like $\int V_\psi(x)^k dx$ which appear at higher orders in the binomial expansion of the energy.

APPENDIX D: SEMICLASSICAL THEORY OF THE BOSE POLARON

In order to illustrate the point of our result in $d = 2$, which we describe as the bosonization of the semiclassical Fermi polaron, we recall the corresponding results for the Bose polaron. We start with the Fröhlich Hamiltonian describing an impurity of mass m immersed in a superfluid Bose gas,

$$\begin{aligned}\mathbb{H} = &\int \hbar c|k|b_k^\dagger b_k dk + \frac{\hbar^2}{2m}\big(-\nabla_x^2\big) \\ &+ \int\left(\frac{|k|w_k}{\sqrt{2m_B\hbar c|k|}}b_k e^{ikx} + \mathrm{H.c.}\right)dk,\end{aligned} \tag{D1}$$

where c is the critical velocity of the gas, w_k is the Fourier transform of the impurity-boson potential W, and m_B is the mass of the bosons. Such a Hamiltonian arises if one applies the Bogoliubov approximation to the full quantum mechanical many-body problem, and it is known to be asymptotically correct in appropriate scaling regimes [32,41,42]. Its semiclassical theory is provided by taking the expectation value of $\mathbb{H}$ on product states of the type $|\psi\rangle \otimes |z\rangle$, where ψ is some impurity wave function and $|z\rangle$ is a coherent state. Minimization over all possible coherent states yields the functional

$$\begin{aligned}\mathcal{E}_B^{\mathrm{Pek}}(\psi) = &\frac{\hbar^2}{2m}\int |\nabla\psi(x)|^2dx \\ &- \frac{1}{2m_Bc^2}\iint |\psi(x)|^2W^{(2)}(x-y)|\psi(y)|^2dxdy,\end{aligned} \tag{D2}$$

with $W^{(2)} = W * W$. As we see, the resulting semiclassical theory has the precise same structure as we found for our model of the semiclassical Fermi polaron, provided that

$d = 2$. It is, in fact, known that in this particular dimension the difference between free fermions and free bosons is least prominent; for example, their virial expansions are identical up to one term [33]. It is known that the two systems map exactly to each other provided that suitable interactions are present [43]. Thus, our findings suggest that the Bose and Fermi polarons in two dimensions should display certain similarities not present in other dimensions.

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