Supplementary Information for: Interaction-induced localization of mobile impurities in ultracold systems

Jian Li,[1] Jin An,[1,2] and C. S. Ting[1]

[1]*Texas Center for Superconductivity and Department of Physics,*

University of Houston, Houston, Texas 77204, USA

[2]*National Laboratory of Solid State Microstructures and Department of Physics,*

Nanjing University, Nanjing 210093, China

S-1. THE CRITICAL BEHAVIOR OF THE EXTENDED-LOCALIZED TRANSITION IN l-DIMENSION

In this section we shall derive more precise forms for equation (4) in the text. According to the main text, the optimal localization length λ is determined by $\frac{\partial E}{\partial \lambda} = 0$, where E is given by equation (3) in the text. Then we have equation for λ in l-dimension:

$$-2A_l \frac{1}{\lambda^3} + lB_l \frac{\alpha}{\lambda^{l+1}} - 2lC_l \frac{\beta}{\lambda^{2l+1}} = 0. \tag{S1}$$

where $A_l = l\hbar^2/4m_I$. For $l = 1$ (1D) and $l = 2$ (2D) we can solve λ from the above equation directly and get the energy E:

$$l=1: \quad \frac{1}{\lambda} = \frac{B_1 \alpha}{2(C_1\beta + A_1)}, \qquad E = \frac{-B_1^2 \alpha^2}{4(C_1\beta + A_1)} \tag{S2}$$

$$l=2: \quad \frac{1}{\lambda} = \sqrt{\frac{B_2}{2C_2}} \left(\frac{\alpha - \alpha_c}{\beta}\right)^{\frac{1}{2}}, \quad E = \frac{-B_2^2}{4C_2} \frac{(\alpha - \alpha_c)^2}{\beta} \tag{S3}$$

where $\alpha_c = A_2/B_2$ for $l = 2$.

In 3D, by solving $E = 0$ and $\frac{\partial E}{\partial \lambda} = 0$ simultaneously, we have $\alpha_c = \left(\frac{256\pi^3 \hbar^6 \beta}{3\sqrt{3}m_I^3}\right)^{\frac{1}{4}}$, $\lambda_c^{-1} = \left(\frac{A_3}{3C_3\beta}\right)^{\frac{1}{4}}$. Near the critical point $\alpha = \alpha_c$ we have

$$\frac{1}{\lambda} - \frac{1}{\lambda_c} \approx \frac{\partial \lambda^{-1}}{\partial \alpha}\Big|_{\alpha=\alpha_c} (\alpha - \alpha_c) = \sqrt{\frac{3B_3^2}{A_3 C_3}} \frac{\alpha - \alpha_c}{4\sqrt{\beta}}, \tag{S4}$$

$$E \approx \frac{\partial E}{\partial \alpha}\Big|_{\alpha=\alpha_c} (\alpha - \alpha_c) = \frac{B_3(\alpha_c - \alpha)}{\lambda_c^3}, \tag{S5}$$

where $\frac{\partial \lambda^{-1}}{\partial \alpha}\Big|_{\alpha=\alpha_c}$ and $\frac{\partial E}{\partial \alpha}\Big|_{\alpha=\alpha_c}$ are determined by equation (S1) and (3) in the text.

S-2. THE SOLITON SOLUTIONS

In this section we show that equation (5) in the text has a series of soliton solutions. The localized impurity moving along direction of $\boldsymbol{r}$ has the form of $\Psi(\boldsymbol{r}, t) = \Psi(\boldsymbol{r} - \boldsymbol{v}t)\chi(\boldsymbol{r}, t) = \Psi(\boldsymbol{r} - \boldsymbol{v}t)e^{i[\boldsymbol{k}\cdot\boldsymbol{r} - (\mu + \frac{\hbar^2 k^2}{2m_I})t/\hbar]}$. The right-hand side of equation (5) can be written as

$$
\begin{aligned}
H_{eff}\Psi(\boldsymbol{r}, t) &= -\frac{\hbar^2}{2m_I}\chi(\boldsymbol{r}, t)\frac{\partial^2}{\partial r^2}\Psi(\boldsymbol{r} - \boldsymbol{v}t) - \frac{i\boldsymbol{k}\hbar^2}{m}\chi(\boldsymbol{r}, t)\frac{\partial}{\partial r}\Psi(\boldsymbol{r} - \boldsymbol{v}t) \\
&\quad + [\frac{\hbar^2 k^2}{2m} - 2\alpha|\Psi(\boldsymbol{r}, t)|^2 + 3\beta|\Psi(\boldsymbol{r}, t)|^4]\Psi(\boldsymbol{r}, t) \\
&= -i\hbar\boldsymbol{v}\chi(\boldsymbol{r}, t)\frac{\partial}{\partial r}\Psi(\boldsymbol{r} - \boldsymbol{v}t) \\
&\quad + \{-\frac{\hbar^2}{2m_I}\chi(\boldsymbol{r}, t)\frac{\partial^2}{\partial r^2}\Psi(\boldsymbol{r} - \boldsymbol{v}t) + [\frac{\hbar^2 k^2}{2m} - 2\alpha|\Psi(\boldsymbol{r}, t)|^2 + 3\beta|\Psi(\boldsymbol{r}, t)|^4]\Psi(\boldsymbol{r}, t)\}
\end{aligned}
$$

Notice that in the second step we used relation $\boldsymbol{v} = \frac{\hbar\boldsymbol{k}}{m}$. Since the localized wave function $\Psi(\boldsymbol{r} - \boldsymbol{v}t)$ satisfies equation (2) in the text, i.e.,

$$[-\frac{\hbar^2}{2m_I}\frac{\partial^2}{\partial r^2} - 2\alpha|\Psi(\boldsymbol{r} - \boldsymbol{v}t)|^2 + 3\beta|\Psi(\boldsymbol{r} - \boldsymbol{v}t)|^4]\Psi(\boldsymbol{r} - \boldsymbol{v}t)]\} = \mu\Psi(\boldsymbol{r} - \boldsymbol{v}t),$$

we have

$$H_{eff}\Psi(\boldsymbol{r}, t) = -i\hbar\boldsymbol{v}\chi(\boldsymbol{r}, t)\frac{\partial}{\partial r}\Psi(\boldsymbol{r} - \boldsymbol{v}t) + (\mu + \frac{\hbar^2k^2}{2m_I})\Psi(\boldsymbol{r}, t) \tag{S6}$$

$$= i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r}, t), \tag{S7}$$

as the final form of equation (5).

S-3. CRITICAL PARAMETERS FOR MANY BOSONIC IMPURITIES

For N noninteracting Bosonic impurities, we assume that all the bosons are condensed into a single state, and we have the trial wave function $\Psi_N(\boldsymbol{r}) = \sqrt{N}\Psi(\boldsymbol{r})$. Now the total energy in l-dimension in equation (3) in the text is

$$E_N = N[A_l\frac{1}{\lambda^2} - B_l\frac{N\alpha(N)}{\lambda^l} + C_l\frac{N^2\beta(N)}{\lambda^{2l}}]. \tag{S8}$$

At the critical point for the transition between the extended and localized states, we have $\frac{\partial E_N}{\partial\lambda} = 0$ and $E_N = 0$. Then the critical values of α for different dimensions are obtained as

$$l = 1: \qquad \alpha_c(N) = 0 \tag{S9}$$

$$l = 2: \qquad \alpha_c(N) = \frac{A_2}{B_2N} = \frac{\alpha_c}{N} \tag{S10}$$

$$l = 3: \qquad \alpha_c(N) = (\frac{256\pi^3\hbar^6\beta}{3\sqrt{3}m_I^3N^2})^{\frac{1}{4}} = \frac{\alpha_c}{\sqrt{N}}. \tag{S11}$$

If there exits a weak repulsive interaction $\lambda_{II}\delta(\boldsymbol{r} - \boldsymbol{r}')$ between the background atoms, we thus have an additional energy part $\frac{N^2B_l\lambda_{II}}{2\lambda^l}$. This part can be directly absorbed into α term. Therefore in these cases, the critical value of α gets a shift of $\lambda_{II}/2$, and especially, in 1D it becomes

$$\alpha_c(N) - \frac{1}{2}\lambda_{II} = 0. \tag{S12}$$

S-4. ENERGY OF TWO CORRELATED FERMIONIC IMPURITIES

In this section we shall calculate the total energy of two localized fermionic impurities. The trial wave functions in one, two and three dimension are respectively given by:

$$\psi_{\pm,1d} = \frac{1}{\sqrt{2\lambda\sqrt{\pi}(1 \pm e^{-\frac{a^2}{4\lambda^2}})}}[e^{-\frac{x^2}{2\lambda^2}} \pm e^{-\frac{(x+a)^2}{2\lambda^2}}] \tag{S13}$$

$$\psi_{\pm,2d} = \frac{1}{\sqrt{2\lambda^2\pi(1 \pm e^{-\frac{a^2}{4\lambda^2}})}}[e^{-\frac{x^2+y^2}{2\lambda^2}} \pm e^{-\frac{(x+a)^2+y^2}{2\lambda^2}}] \tag{S14}$$

$$\psi_{\pm,3d} = \frac{1}{\sqrt{2\lambda^3\pi^{\frac{3}{2}}(1 \pm e^{-\frac{a^2}{4\lambda^2}})}}[e^{-\frac{x^2+y^2+z^2}{2\lambda^2}} \pm e^{-\frac{(x+a)^2+y^2+z^2}{2\lambda^2}}] \tag{S15}$$

Here a is the distance between two localized impurities. Notice such trial wave functions become ill-defined when $a/\lambda \ll 1$. When $a/\lambda \to \infty$, which means two localized impurities are far from each other, we have $(E_T - 2E_S) \to 0$. The total energies derived with the trial wave functions are given by

$$E_T^l = \sum_{i=+,-} \int d^l r \psi_i^*(r)[-\frac{\hbar^2}{2m_I}\nabla^2 - \alpha n_I(r) + \beta n_I(r)^2]\psi_i(r) \tag{S16}$$

where $i = +, -$. $l = 1, 2, 3$ represent the dimensions, and $n_I(r) = |\psi_+|^2 + |\psi_-|^2$ is the local density of the impurities. A direct calculation gives the energies for the two impurities in 1D, 2D and 3D.

$$E_T^l = -\frac{\hbar^2}{2m_I}\frac{l\lambda^2(1-\eta)-\frac{a^2}{2}}{(-1+\eta)\lambda^4} - \alpha\frac{2\eta^2+2\eta-8\eta^{\frac{3}{4}}+4}{(2\pi)^{\frac{l}{2}}(-1+\eta)^2\lambda^l} + \beta\frac{2\eta^3-12\eta-6\eta^{\frac{5}{3}}+24\eta^{\frac{2}{3}}-8}{(3\pi^2)^{\frac{l}{2}}(-1+\eta)^3\lambda^{2l}} \tag{S17}$$

where $\eta = e^{\frac{a^2}{2\lambda^2}}$. Notice when $a/\lambda \to \infty$, we have

$$E_T^l = \frac{l\hbar^2}{2m_I\lambda^2} - \frac{\alpha}{(2\pi)^{\frac{l}{2}}}\frac{2}{\lambda^l} + \frac{\beta}{(3\pi^2)^{\frac{l}{2}}}\frac{2}{\lambda^{2l}}, \tag{S18}$$

which is exactly the twice of the energy of single localized impurity given by the Gaussian trial wave function. With the units given by the table in the Methods section, the energies in one, two and three dimension can be rewritten as functions of dimensionless parameters:

$$E_T^1 = -\zeta^2 X_1 - \zeta Y_1 + \beta'\zeta^2 Z_1 \tag{S19}$$

$$E_T^2 = -\zeta^2 X_2 - \alpha'\zeta^2 Y_2 + \zeta^4 Z_2 \tag{S20}$$

$$E_T^3 = -\zeta^2 X_3 - \alpha'\zeta^3 Y_3 + \zeta^6 Z_3 \tag{S21}$$

where $\zeta = a_0/\lambda$, and

$$X_l = -l + \frac{a^2}{2\lambda^2(1-\eta)} \tag{S22}$$

$$Y_l = \frac{2\eta^2 + 2\eta - 8\eta^{\frac{3}{4}} + 4}{(2\pi)^{\frac{l}{2}}(-1+\eta)^2} \tag{S23}$$

$$Z_l = \frac{2\eta^3 - 12\eta - 6\eta^{\frac{5}{3}} + 24\eta^{\frac{2}{3}} - 8}{(3\pi^2)^{\frac{l}{2}}(-1+\eta)^3} \tag{S24}$$

S-5.   MULTI FERMIONIC IMPURITIES IN A 2D LATTICE

In this section we shall solve equation (2) for fermionic impurities with total number N in a two dimensional lattice. Consider a 2D lattice with lattice constant a_0, equation (2) can be rewritten as :

$$\{-\frac{\hbar^2}{2m_I}\nabla^2 - 2\frac{\alpha}{a_0^2}[a_0^2 n_I(x,y)] + 3\frac{\beta}{a_0^4}[a_0^4 n_I(x,y)]\}[a_0\Psi_k(x,y)] = \mu_k[a_0\Psi_k(x,y)], \tag{S25}$$

Notice here k is the index for the k-th impurity. By defining $t_0 = \frac{\hbar^2}{2m_I a_0^2}$, $n_j = a_0^2 n_I(x_j,y_j)$, $\tilde{\alpha} = \frac{\alpha}{a_0^2}$, $\tilde{\beta} = \frac{\beta}{a_0^4}$ and $u_j^k = a_0\Psi_k(x_j,y_j)$, we have the eigenvalue equations

$$\sum_j (-t_{0,\langle ij\rangle} - 2\tilde{\alpha}n_j\delta_{ij} + 3\tilde{\beta}n_j^2\delta_{ij})u_j^k = \mu_k u_i^k, \tag{S26}$$

where t_0 is the hopping integral between nearest neighboring sites and $n_j = \sum_{k=1}^{N}(u_j^k)^* u_j^k$ is the impurity density at the lattice site j. If we choose a_0 as the length unit defined in the Methods section, we have the dimensionless parameters $\alpha' = \frac{2m_I\alpha}{\hbar^2} = \frac{\tilde{\alpha}}{t_0}$ and $\beta' = \frac{2m_I\beta}{\hbar^2 a_0^2} = \frac{\tilde{\beta}}{t_0} = 1$. The total energy of N fermionic impurities can be written as

$$E_N = \sum_{k=1}^{N}\mu_k + \sum_j[\tilde{\alpha}n_j^2 - 2\tilde{\beta}n_j^3] \tag{S27}$$

In our calculation, we use a 50×50 lattice with periodic boundary condition.

S-6.   SINGLE IMPURITY IN A 2D FERMI SUPERFLUID

Given a realistic 2D or 3D system, both of α and β are functions of the IB interaction. According to the Methods section, we have $\alpha \propto \beta^{2/3}$, and this function behavior always has crossing point with the extended-localized transition boundaries in 2D and 3D(see Fig.S1).
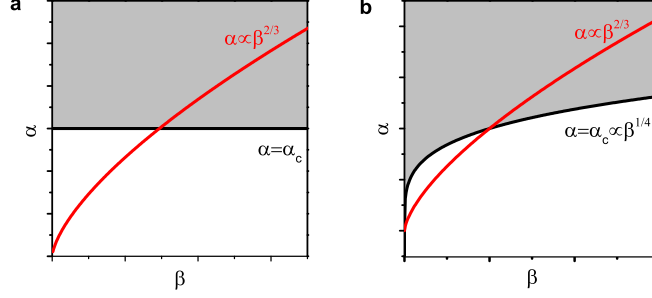
FIG. S1: **Boundary of extended and localized impurity state in 2D and 3D. a**, 2D. **b**, 3D. The black curves indicate the boundary of extended-localized transition, and the red lines represent the relation between α and β in a realistic system. The shadowed regions mark the parameter space for the localized state.

This indicates that the extended-localized transition always occurs in a 2D or 3D system when we increase the IB interaction.

In the following we shall apply our theory to single impurity immersed in a two dimensional Fermi superfluid. For a uniform s-wave superfluid, its ground state energy is given by:

$$E_B = \sum_k (\epsilon_k - \mu - \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}) + \frac{\Omega \Delta^2}{V_0}, \tag{S28}$$

where $\epsilon_k = k^2/2m_B$ is the dispersion of the background atoms, μ is the chemical potential and Ω is the volume of the system. In 2D, the bare attractive interaction of the superfluid V_0 can be regularized by $V_0^{-1} = \sum_k (2\epsilon_k + \epsilon_B)^{-1}$, where ϵ_B is the two-body binding energy. This gives[1]: $\mu = \epsilon_F - \frac{1}{2}\epsilon_B$ and $\Delta = \sqrt{2\epsilon_B \epsilon_F}$, where ϵ_F is the Fermi energy.

According to the Methods section, we have:

$$\alpha = \frac{1}{\Omega} \sum_k \frac{U_{IB}^2 \Delta^2}{2[(\epsilon_k - \mu)^2 + \Delta^2]^{3/2}} \tag{S29}$$

$$\beta = \frac{1}{\Omega} \sum_k \frac{U_{IB}^3 \Delta^2 (\epsilon_k - \mu)}{2[(\epsilon_k - \mu)^2 + \Delta^2]^{5/2}}. \tag{S30}$$

We define $U_{IB} = (1 + \frac{1}{x})\frac{2\pi\hbar^2 a_S}{m_B d}$, where a_S is the 3D scattering length between the impurities and background, length d is due to the strong transverse confinement, and $x = m_I/m_B$.

6

Inserting the results of μ and Δ into equation (S29) and (S30) we have

$$\alpha = \frac{\pi\hbar^2}{m_B}[(1+\frac{1}{x})\frac{a_S}{d}]^2\frac{4\epsilon_F}{2\epsilon_F+\epsilon_B} \tag{S31}$$

$$\beta = \frac{4\pi^2\hbar^2}{3m_Bk_F^2}[(1+\frac{1}{x})\frac{a_S}{d}]^3\frac{16\epsilon_F^2\epsilon_B}{(2\epsilon_F+\epsilon_B)^3}. \tag{S32}$$

Since the boundary of the extended-localized transition is determined by $\alpha' = 2m_I\alpha/\hbar^2 = 2\pi$, we have the parameter region for the localized state: $x[(1+\frac{1}{x})\frac{a_S}{d}]^2 > \frac{1}{2} + \frac{\epsilon_B}{4\epsilon_F}$.

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[1] Randeria, M., Duan, J-M. & Shieh, L-Y. Bound states, Cooper pairing, and Bose condensation in two dimensions. *Phys. Rev. Lett.* **62**, 981 (1989).