Supplemental Material: "Polaron-to-polaron transitions in the radio-frequency spectrum of a quasi-two-dimensional Fermi gas"

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In this supplemental material, we discuss the calculation of the radio-frequency spectra arising from confinement-induced dimers and polarons in a quasi-two-dimensional Fermi gas. We determine the dimer binding energies, including both the tight axial confinement and the nonzero transverse confinement. We provide the probabilities for dimer-to-dimer transitions and the shape of the dimer-to-scattering state spectrum. We also find the energy and quasi-particle weights for polarons in the two-dimensional gas and the corresponding resonance frequencies for polaron-to-polaron transitions.

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We begin by reviewing briefly in § I the radio-frequency spectrum arising from confinement-induced pairs, including final state interactions, but ignoring many-body effects, using the method employed for the three-dimensional case by Chin and Julienne [1]. We consider mixtures of the three lowest hyperfine states of ^{6}Li, denoted $|1\rangle$, $|2\rangle$, $|3\rangle$. For the conditions of our experiments in a 12 mixture at 720 G, the observed $2 \rightarrow 3$ threshold spectrum is well described by a 12-dimer-to-13-scattering-state transition. In contrast, at 834 G, the predicted dimer spectrum is in marked disagreement with the data. In particular, we find that the difference between the ground and excited state dimer energies is too small. In § II we determine the energies for noninteracting confinement-induced polarons. We find that the locations of the observed resonances for a 12 mixture near 834 G are well modeled by the predicted energy difference between isolated state 2 polarons and state 3 polarons, in a bath of atoms in state 1.

I. CONFINEMENT-INDUCED DIMERS

A simple golden rule calculation gives the radio-frequency-induced transition rate out of the initial state to all possible final states $R_i(\omega_{rf}) = \sum_F R_{f \leftarrow i}$, where $R_{f \leftarrow i} = (2\pi/\hbar)|\tilde{H}'_{fi}|^2 \delta(E_f - E_i - \hbar\omega_{rf})$, with $\tilde{H}'_{fi} = \hbar\Omega_{fi}\langle F|I\rangle/2$. Here, Ω_{fi} is the Rabi frequency for changing the hyperfine state of a single atom from the chosen populated state (i) to the initially unpopulated state (f) and $\langle F|I\rangle$ is the overlap between the initial and final wave-functions for the relative motion of the atom-pair. Since the center of mass energy does not change in the rf transition, $E_f - E_i$ is the total change in the atomic hyperfine energy ($\equiv \hbar\omega_{fi}$) plus the change in the energy of the relative motion of the pair $E_F - E_I$. Since $\sum_F |\langle F|I\rangle|^2 = 1$, $\int d\omega_{rf} R_i(\omega_{rf}) = (\pi/2)\Omega_{fi}^2$. We define a normalized spectrum $I(\omega)$ where $R_i(\omega_{rf}) = (\pi/2)\Omega_{fi}^2 I(\omega)$ and $\omega_{rf} = \omega_{fi} + \omega$, with ω the frequency relative to the (unshifted) free-atom hyperfine transition frequency. Then, $I(\omega) = \sum_F |\langle F|I\rangle|^2 \hbar\delta(E_F - E_I - \hbar\omega)$

and $\int d\omega I(\omega) = 1$.

For transitions between bound dimer states, we determine the resonance frequencies from the difference between the binding energies for the initial and final dimer states. In a 1-2 mixture, for transitions from an occupied state 2 to an initially empty state 3, the expected bound-to-bound transition frequency is then determined by the difference between the 1-2 dimer and 1-3 dimer binding energies. We note that interactions arising from $2 - 3$ scattering do not shift the $2 \rightarrow 3$ transition frequency [2, 3].

To determine the spatial wavefunctions and the pair binding energies, we note that the range of the two-body interaction is small compared to the interparticle spacing as well as to the harmonic oscillator confinement scale $l_z \equiv \sqrt{\hbar/(m\omega_z)}$. In this case, interactions between atoms in two different spin states are well described by the s-wave pseudopotential in three dimensions [4], $V(r) = (4\pi\hbar^2 a/m)\,\delta(r)\partial_r(r...)$, where r is the distance between the atoms, m is the mass of a single atom and a is the magnetically tunable s-wave scattering length. The spatial wavefunctions are readily written in terms of the Green's function $G_E(\mathbf{r})$ for the relative motion of the two atoms in the confining potential, which we take to be harmonic, with ground state energy E_0. The two-atom scattering states with energy $E = E_0 + E_s$, where $E_s \geq 0$, take the form $\psi_s(\mathbf{r}) = \psi_{E_s}^{(0)}(\mathbf{r}) - a\,G_{E_s}(\mathbf{r})\,u'_s(0)$, where $\psi_{E_s}^{(0)}$ is the input state and $\psi = u/r$ with u regular at $r = 0$. For the bound states, where there is no input, we have $\psi_b(\mathbf{r}) = -a\,G_{E_b}(\mathbf{r})\,u'_b(0)$, where $E = E_0 - E_b$ with $E_b > 0$. Using $\partial_r[r\psi_b(r)]_{r\to 0} = u'_b(0)$ yields the equation for the binding energy [4], $1 = -a\,\partial_r[rG_{E_b}(\mathbf{r})]_{r\to 0}$, where the right side projects out the regular part of G at $r = 0$. For a three dimensional harmonic trap, the Green's function is

$$G_\epsilon(\mathbf{r}) = \frac{i}{l_z\sqrt{4\pi}} \int_0^\infty d\eta\, e^{i\epsilon\eta} \prod_j e^{i\cot(\beta_j\eta)\left(\frac{x_j}{2l_j}\right)^2} f_j(\eta), \quad (1)$$

where $E = E_0 + \epsilon\,\hbar\omega_z$, with $\epsilon = -\epsilon_b$ for bound states and $\epsilon > 0$ for scattering states. Here, $f_j(\eta) = \sqrt{2\beta_j/(1 - e^{-2i\beta_j\eta})}$, with $\beta_z \equiv 1$, $\beta_{x,y} = \omega_{x,y}/\omega_z$ and

$l_j = l_z/\sqrt{\beta_j}$. After subtracting the irregular part of G and changing to real variables, we determine the dimer binding energies $E_b = \epsilon_b \hbar\omega_z > 0$ from

$$\frac{l_z}{a} = \int_0^\infty \frac{du}{\sqrt{4\pi u^3}} \left\{ 1 - \prod_j \left(\frac{2\beta_j u}{1 - e^{-2\beta_j u}} \right)^{1/2} e^{-\epsilon_b u} \right\}. \quad (2)$$

The dimer binding energy is significantly increased for nonzero transverse confinement. At resonance, where $l_z/a \to 0$, for $\nu_\perp/\nu_z = 0$ we obtain $E_b = 0.245\, h\nu_z$, while for $\nu_\perp/\nu_z = 1/25$ we obtain $E_b = 0.290\, h\nu_z$. At 842 G in the shallowest trap, the binding energy of the 13 dimer is increased from 0.15 kHz without transverse confinement to 0.78 kHz with transverse confinement. We compute the pair binding energy $E_b \equiv \epsilon_b\, \hbar\omega_z$ as a function of magnetic field using the s-wave scattering lengths a measured in Ref. [5].

The scattering state is determined using $u_s'(0) = u_s'^{(0)}(0)/\{1 + a\, \partial_r[rG_{E_s}(\mathbf{r})]_{r\to 0}\}$. Using the relation (one-to-one correspondence) between the scattering length and the bound state energy, we have $u_s'(0) = u_s'^{(0)}(0)/\{a\,[G_{E_s}(\mathbf{r}) - G_{E_b}(\mathbf{r})]_{r\to 0}\}$, where E_b is the binding energy corresponding to the scattering length a and we have used $\partial_r\{r[G_{E_s}(\mathbf{r}) - G_{E_b}(\mathbf{r})]_{r\to 0}\} = [G_{E_s}(\mathbf{r}) - G_{E_b}(\mathbf{r})]_{r\to 0}$, which is regular at $r = 0$. Then, the scattering state takes the form

$$\psi_s(\mathbf{r}) = \psi_{E_s}^{(0)}(\mathbf{r}) - \frac{G_{E_s}(\mathbf{r})\, u_s'^{(0)}(0)}{[G_{E_s}(\mathbf{r}) - G_{E_b}(\mathbf{r})]_{r\to 0}}, \quad (3)$$

where $u_s'^{(0)}(0) = \psi_{E_s}^{(0)}(0)$, since the input state is regular at $r = 0$.

For $2 \to 3$ transitions in a 12 mixture at 834 G, the binding energies are small compared to the energy difference between symmetric axial states $2\hbar\omega_z$, which are coupled by the s-wave scattering interaction. In this case, the Green's functions, and hence the 1-2 and 1-3 bound states and the 1-3 scattering states, are well approximated by axial ground state component. For the scattering state Green's function, ignoring the transverse confinement in Eq. 1 and taking $E_s = \epsilon_\perp \hbar\omega_z = \hbar^2 k_\perp^2/m$, the axial ground state component is $G_{\epsilon_\perp}^{(0)}(z,\rho) = \phi_0(z) \int dz' \phi_0(z')\, G_{\epsilon_\perp}(z',\rho)$, where $\phi_0(z)$ is the axial ground vibrational state for the relative motion (reduced mass $\mu = m/2$), which is real. It is easy to show by direct integration that

$$G_{\epsilon_\perp}^{(0)}(z,\rho) = \phi_0(z)\, \phi_0(0) \left\{ \pi\, i\, H_0^{(1)} \left(\frac{\rho\sqrt{\epsilon_\perp}}{l_z} \right) \right\}, \quad (4)$$

where $\sqrt{\epsilon_\perp}/l_z = k_\perp$ is the transverse wavevector. For a bound state, the axial ground state Green's function is $G_{\epsilon_b}^{(0)}(z,\rho) = \phi_0(z) \int dz' \phi_0(z')\, G_{\epsilon_b}(z',\rho)$, which is readily obtained from Eq. 1 and corresponds to taking $\sqrt{\epsilon_\perp} \to i\sqrt{\epsilon_b}$ in Eq. 4. We obtain

$$G_{\epsilon_b}^{(0)}(z,\rho) = \phi_0(z)\, \phi_0(0) \left\{ 2\, K_0 \left(\frac{\rho\sqrt{\epsilon_b}}{l_z} \right) \right\}. \quad (5)$$

Eq. 5 yields the normalized bound state,

$$\psi_{\epsilon_b}(z,\rho) = \phi_0(z)\, \frac{\kappa}{\sqrt{\pi}}\, K_0(\kappa\rho), \quad (6)$$

where $E_b = \epsilon_b\, \hbar\omega_z$ is the pair binding energy for the given scattering length, and $\hbar^2\kappa^2/m = E_b$, i.e., $\kappa = \sqrt{\epsilon_b}/l_z$. The 1-2 bound state to 1-3 bound state transition strength is then determined by the overlap between of the modified Bessel functions, $K_0(\kappa_{12}\rho)$ and $K_0(\kappa_{13}\rho)$, where $\kappa_{12(13)}$ is determined by $\epsilon_b^{12(13)}$. The 1-2 bound to 1-3 bound contribution to the lineshape is then given by

$$I_{bb}(\nu) = \epsilon_{bb}(q)\, \delta[\nu - (\epsilon_b^{12} - \epsilon_b^{13})\nu_z], \quad (7)$$

where ν_z is the axial harmonic oscillator frequency in Hz and ν is the rf frequency in Hz, relative to the bare 2-3 hyperfine transition frequency of $\simeq 83$ MHz. For the axial ground state, the frequency integrated bound to bound transition strength can be written compactly in terms of $q \equiv \ln(\epsilon_b^{13}/\epsilon_b^{12})$,

$$\int d\nu\, I_{bb}(\nu) \equiv \epsilon_{bb}(q) = \frac{q^2}{4\sinh^2(q/2)}. \quad (8)$$

We plot ϵ_{bb} as a function of magnetic field in Fig. 1 for the general case, valid for both weak and tight binding of the $1-2$ or $1-3$ dimers, including the contribution of the first 50 even axial states. For comparison, we show the
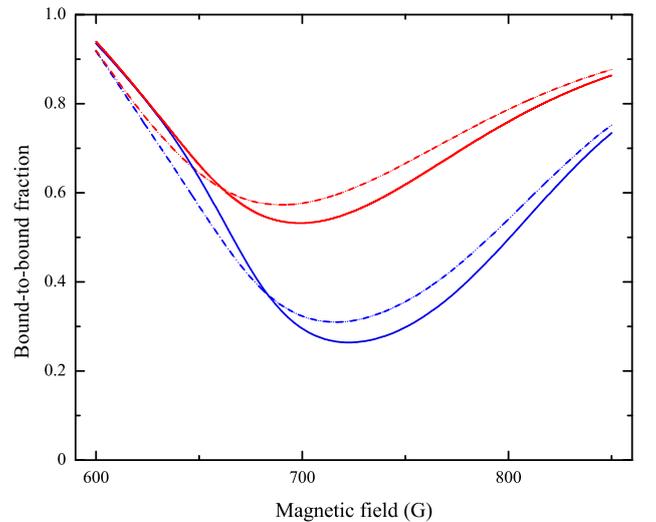
FIG. 1: Bound 12 dimer to bound 13 dimer transition fraction versus magnetic field for $\nu_\perp/\nu_z = 1/25$. Upper curves (red online): Trap depth $U_0 = 280\,\mu$K, $\nu_z = 82.5$ kHz; Lower curves (blue online) $U_0 = 21\,\mu$K and $\nu_z = 24.5$ kHz. Solid lines denote the square of Frank-Condon overlap integral, including the first 50 even axial states. Dashed lines denote the corresponding results using only the ground axial state, Eq. 8.

weak binding approximation given by Eq. 8, which includes only the ground axial vibrational state. For small binding energies, increasing the trap depth significantly

increases the pairing energy, increasing the overlap integral for bound-to-bound transitions.

From Fig. 1, we see that for a trap depth $U_0 = 21\,\mu\text{K}$ at 720 G, the $2 \rightarrow 3$ transition in a 12 mixture is dominated by bound-to-free transitions. In contrast, at 834 G, the corresponding bound-to-bound transition is dominant and increases with increasing trap depth.

In the same weak binding approximation as used for the bound states, again neglecting the transverse confinement, the two dimensional box-normalized (to area A) 1-3 scattering state takes the form $\psi_{\epsilon_\perp}(z,\rho) = \phi_0(z)\,\psi_{\epsilon_\perp}(\rho)$, with $E_s = \epsilon_\perp \hbar\omega_z = \hbar^2 k_\perp^2/m$. Assuming that the incident transverse state is the azimuthally-symmetric part ($l = 0$) of a box normalized plane-wave state $\exp(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp)/\sqrt{A}$, i.e., $J_0(k_\perp\rho)/\sqrt{A}$, Eq. 3 with $u'^{(0)}_s(0) = \phi_0(0)/\sqrt{A}$ gives

$$\psi_{\epsilon_\perp}(\rho) = \frac{1}{\sqrt{A}}\left\{ J_0(k_\perp\rho) - \frac{\pi i}{\ln(\epsilon_b/\epsilon_\perp) + \pi i}\,H_0(k_\perp\rho) \right\}, \tag{9}$$

where we have used

$$[\pi i\,H_0^{(1)}(\rho\sqrt{\epsilon_\perp}/l_z) - 2\,K_0(\rho\sqrt{\epsilon_b}/l_z)]_{\lim \rho \to 0}$$
$$= \pi i + \ln(\epsilon_b/\epsilon_\perp).$$

We determine the overlap integral of the 1-2 bound state Eq. 6 with the 1-3 scattering state Eq. 9 and integrate the transition rate using the density of transverse states, $A/(2\pi)^2\,2\pi k_\perp\,dk_\perp$, to obtain the 1-2 bound to 1-3 scattering state contribution to the lineshape, which takes the form of a threshold function,

$$I_{bf}(\nu) = \frac{\epsilon_b^{12}\nu_z}{\nu^2}\,\frac{q^2\,\theta(\nu - \epsilon_b^{12}\nu_z)}{\left[q - \ln\left(\frac{\nu}{\epsilon_b^{12}\nu_z} - 1\right)\right]^2 + \pi^2}. \tag{10}$$

Note that $\int d\nu\,I_{bf}(\nu) = 1 - \epsilon_{bb}(q)$, as it should. We find that Eq. 10 well fits the radio frequency spectra obtained at 720 G, where the dimer binding energy is larger than the transverse Fermi energy.

II. POLARONS IN A TWO-DIMENSIONAL FERMI GAS

For radiofrequency $2 \rightarrow 3$ spectra obtained near 834 G in a 12 mixture, we find that the difference between the calculated dimer binding energies significantly underestimates the observed frequency shifts, as shown in Figs. 2, 3, and 4 of the main paper. We consider the possibility that the spectra may arise from transitions between polaronic states, as the atom produced in state 3 is naturally an impurity. Further, the polaron energy is significantly more negative than the corresponding dimer energy when the transverse Fermi energy is larger than the dimer binding energy and is therefore energetically preferred [6].

To estimate the polaron energies, we consider either an isolated impurity atom in state 2 or in state 3, immersed in a bath of atoms in state 1. We note that for the $2 \rightarrow 3$ transition, the interaction between states 2 and 3 does not affect the transition frequency of the coherently rotated hyperfine state. We employ the method described for polarons in three dimensions in the supplementary material of Schirotzek at al. [7], which is based on the zero momentum polaron wavefunction proposed by Chevy [8], which for a polaron in state $i = 2, 3$ takes the form

$$|E_i\rangle = \varphi_{0i}|0\rangle_i\,|FS\rangle_1 + \sum_{q < k_F < k} \varphi_{\mathbf{kq}}|\mathbf{q} - \mathbf{k}\rangle_i\,c_{\mathbf{k}1}^\dagger c_{\mathbf{q}1}\,|FS\rangle_1. \tag{11}$$

Here, the first term describes an impurity i of zero momentum in a Fermi sea of atoms in state 1 for which the net momentum is zero. Collisions between the impurity and the background atoms couple the zero momentum impurity state to that with momentum $\mathbf{q} - \mathbf{k}$, producing a particle-hole pair from the Fermi sea of atoms in state 1 with net momentum $\mathbf{k} - \mathbf{q}$, conserving the total zero momentum.

For the 2D calculations, we replace the box normalization volume in the supplementary material of Schirotzek at al. [7] by the corresponding area A, so that the polaron energy in 2D takes the form

$$E_{pi} = \frac{1}{A}\sum_{q < k_F} f(E_{pi}, q), \tag{12}$$

where

$$f^{-1}(E_{pi}, q) = \frac{1}{g_0} + \frac{1}{A}\sum_{k > k_F}\frac{1}{\epsilon_\mathbf{k} - \epsilon_\mathbf{q} + \epsilon_{\mathbf{q}-\mathbf{k}} - E_{pi}}. \tag{13}$$

Here, $\epsilon_k = \hbar^2 k^2/(2m)$ and k_F is the local Fermi wavevector with $E_F = \hbar^2 k_F^2/(2m)$ the corresponding local transverse Fermi energy.

Following Zöllner et al., Ref. [6], we assume that the effective bare interaction U arises from a short range 2D potential, so that the matrix elements $U_{\mathbf{kk'}} = g_0/A$ are momentum independent. g_0 can be rewritten using the physical two-body T-matrix element in 2D, $1/g_0 = 1/T_{2B}(\mathbf{k}_0) - (1/A)\sum_\mathbf{k} 1/(2\epsilon_k - 2\epsilon_{k_0})$. This method is similar to that employed previously [6, 9, 10]. Here, we choose the T-matrix element $T_{\mathbf{k'k_0}} = T_{2B}(\mathbf{k}_0)/A$ so that the scattering rate calculated using the generalized Golden rule reproduces the scattering rate obtained from the 2D flux corresponding to Eq. 9. Then $T_{2B}(\mathbf{k}_0) = \hbar^2 f(k_0)/m$, with $f(k_0) = 4\pi/[\pi i + \ln(E_b/\epsilon_\perp)]$. Here, $\epsilon_\perp = 2\epsilon_{k_0}$ and $E_b = \epsilon_b\hbar\omega_z$ is the dimer binding energy calculated from Eq. 2. Both the πi term and the k_0 dependence in $T_{2B}(\mathbf{k}_0)$ are canceled by corresponding terms in the sum $(1/A)\sum_\mathbf{k} 1/(2\epsilon_k - 2\epsilon_{k_0})$, so that $f^{-1}(E_{pi}, q)$ is independent of k_0 as it should be. For attractive polarons with energy $E_{pi} < 0$, we then obtain the simple integral equation $\epsilon(L_i) = \Sigma(L_i, \epsilon_i)$, where

$$\Sigma \equiv \int_0^1 \frac{-2\,du}{-L + \ln[\sqrt{(1 - \frac{\epsilon}{2})^2 - u} + (1 - \frac{\epsilon}{2} - \frac{u}{2})]}. \tag{14}$$

Here, $\epsilon(L_i) \equiv \epsilon_i = E_{pi}/E_F$ and $L_i = ln(E_b^{1i}/E_F)$ for an impurity in state i. Eq. 14 yields the polaron energies $E_{pi} = \epsilon_i E_F$ for the initial and final states $i = 2, 3$, using the binding energies $E_b^{1i} = \epsilon_b^{1i}\hbar\omega_z$ determined from Eq. 2.

Fig. 2 shows the attractive polaron energies obtained from Eq. 14, which agree with the numerical results of Ref. [6] and the approximate analytic result of Ref. [11]. We see that the polaron energy E_p is a large fraction of the local Fermi energy, which can be much larger than the corresponding dimer binding energy E_b.
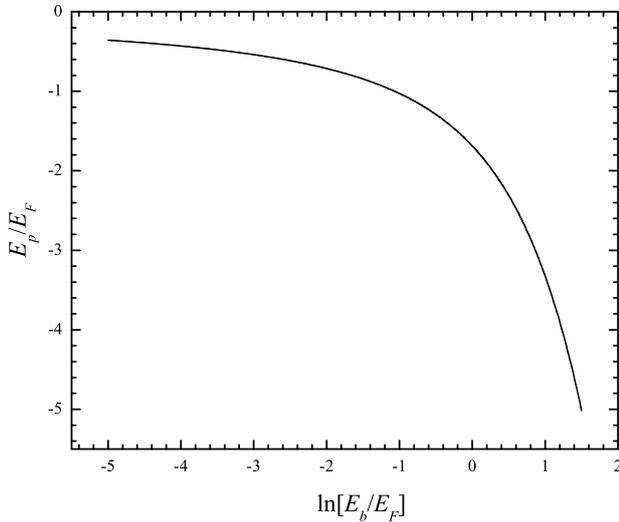
FIG. 2: Polaron energy E_p/E_F versus $\ln[E_b/E_F]$, where E_b is the dimer binding energy and E_F is the local Fermi energy.

For radiofrequency transitions between impurity states $2 \rightarrow 3$ in a bath of atoms in state 1, the momentum of the impurity does not change. We therefore assume the coherent part of the spectrum is given by

$$I(\hbar\omega) = Z_2 Z_3 \, \delta[\hbar\omega - E_{p3} + E_{p2}], \qquad (15)$$

where $|\varphi_{03}^* \varphi_{02}|^2 = Z_2 Z_3$ is the square of the overlap integral between the part of the initial and final polaron states that yields the coherent part of the spectrum. We determine $Z_2 = |\varphi_{02}|^2$ using $Z_2^{-1} = 1 - \partial\Sigma(L_2, \epsilon)/\partial\epsilon$, with $\epsilon \rightarrow E_{p2}/E_F$, as described in Ref. [7] for the 3D problem, and similarly for $Z_3 = |\varphi_{03}|^2$. Fig. 3 shows the quasiparticle weight Z obtained from Eq. 14. For the dimer binding energies in a 12 mixture near 834 G, Table 1 of the main paper, we find that $Z_2 \simeq 0.85$ and $Z_3 \simeq$

0.94 for the shallowest trap depth, both close to unity. Hence, we expect that the overlap between the initial and final polaron states is strong and that transitions between polaron states should make an important contribution to the spectrum.

In the limit that the dimer binding energy is small compared to the local Fermi energy, i.e., $E_b \ll E_F$, one verifies from Eq. 14 that the corresponding polaron energy yields the limiting form [6, 11]

$$E_p \simeq \frac{-2\,E_F}{\ln(2\,E_F/E_b)}, \qquad (16)$$
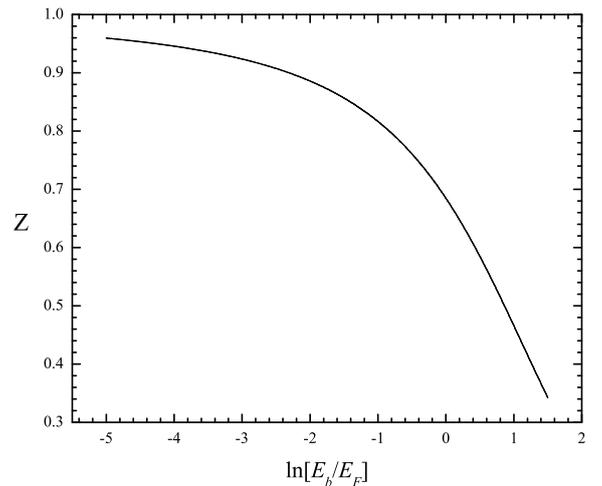
FIG. 3: Polaron quasiparticle weight Z versus $\ln[E_b/E_F]$, where E_b is the dimer binding energy and E_F is the local Fermi energy.

which can be interpreted as an effective mean field shift, since E_F is proportional to the 2D density $n_\perp(\rho)$. At 842 G, where the dimer binding energy is reasonably small compared to the transverse Fermi energy in our experiments, this formula overestimates the magnitude of the polaron energy difference $E_{p3} - E_{p2}$ by about 10% for the most shallow trap. At 811 G, it overestimates the energy difference by about 40%. As E_b is not small compared to E_F for most of the data, it is not surprising that E_F cannot be adjusted in Eq. 16 to give the measured frequency differences.

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