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Universal Relations for a Fermi Gas Close to a $p$-wave Interaction Resonance

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We investigate the properties of a spinless Fermi gas close to a $p$-wave interaction resonance. We show that the effects of interaction near a $p$-wave resonance are captured by two contacts, which are related to the variation of energy with the $p$-wave scattering volume $v$ and with the effective range $R$ in two adiabatic theorems. Exact pressure and virial relations are derived. We show how the two contacts determine the leading and sub-leading asymptotic behavior of the momentum distribution ($\sim 1/k^2$ and $\sim 1/k^4$) and how they can be measured experimentally by radio-frequency and photoassociation spectroscopies. Finally, we evaluate the two contacts at high temperature with a virial expansion.

Introduction. In the past decade, degenerate Fermi gases close to scattering resonances have attracted both theoretical and experimental attention [1]. In the unitary Fermi gas close to an $s$-wave resonance, it is understood that thermodynamic properties are universal [2], depending only on a single function, called the “contact” [3–6]. Its manifestations in physical properties have been extensively explored and confirmed in experiments [7–9]. Extension to arbitrary dimensions has been considered [10, 11]. However, so far contact has only been considered for $s$-waves, even though $p$-wave and higher partial waves resonances have been explored experimentally [12–23] and theoretically [24–38].

In this Letter, motivated by the recent radio-frequency (rf) spectroscopic data near a $p$-wave Feshbach resonance in $^{40}$K [39], we generalize the concept of contact to $p$-waves. In the case of an $s$-wave resonance, a single contact, which depends on the $s$-wave scattering length $a_s$, is sufficient for the characterization of universal properties of the system. For example, the two-body binding energy is given by $\hbar^2/Ma^2_s$, where $M$ is the mass of the atoms, and the effective range correction is in general small [40]. In the case of $p$-wave scattering, however, the phase shift is given by $\cot\delta(k) = -1/\epsilon\hbar^2 k - 1/Rk$ for a short-range potential, and the effective range $R$ is of fundamental relevance, in addition to the scattering volume $v$. This can be seen clearly in the binding energy of a shallow $p$-wave bound state $E_b = \hbar^2 R/Mv$ [41], depending crucially on both $v$ and $R$. As a result, to capture the universal properties of a spinless Fermi gas around a $p$-wave resonance, it is necessary to introduce two contacts, related to the variation of $v$ and $R$, separately. We show how two adiabatic theorems [see Eqs. (11) and (12)] can be established and how the two contacts relate to the leading ($\sim 1/k^2$) and the sub-leading ($\sim 1/k^4$) terms of the high-momentum distribution. We also show how the two contacts can be measured spectroscopically. Finally, we use a virial expansion to determine each contact as a function of $T$, $v$, and $R$ at high temperature.

General Formulation. To start, let us consider the two-body problem, where two identical fermions of mass $M$ interact via a short-range potential $U(r)$ of range $r_0$, tuned close to a $p$-wave resonance. The relative wave function in the $p$-wave channel can be written as 

$$\psi_k(r) \equiv \chi_k(r)Y_{1m}(\hat{r})/r,$$

where $m$ labels the projection of angular momentum along $\hat{z}$-direction and $k$ is the relative wave vector. For low-energy $p$-wave scattering, the radial wave function $\chi_k(r)$ can be expanded in powers of $k^2$, $\chi_k(r) \equiv \chi^{(0)}(r) + k^2\chi^{(1)}(r) + \cdots$. In the asymptotic regime where $1/k \gg r \gg r_0$, we fix the normalization such that the explicit form of $\chi_k(r)$ [and hence $\chi^{(0)}$ and $\chi^{(1)}$] is

$$\chi_k(r) = \left(1 - \frac{r^2}{3v}\right) + k^2\left(\frac{r^2}{2} - \frac{r^4}{3R} + \frac{r^4}{30v}\right) + \cdots. \quad (1)$$

It is important to note that the above asymptotic forms for $\chi^{(0,1)}(r)$ also hold for any shallow $p$-wave bound state in the corresponding asymptotic regime. Once the asymptotes are determined through Eq. (1), the short-range form ($r < r_0$) of $\chi^{(0,1)}(r)$ is completely fixed by two-body physics, due to competition between kinetic and potential energy and in particular, independent of the asymptotic wave vector $k$ [5].

To proceed to the many-body case, we first need to derive two important identities, relating the change of $v$ and $R$ to that of the variation of the potential $U(r)$. Consider two slightly different potentials $U_\pm(r) = U(r) \pm \delta U(r)/2$, each with scattering volume $v_\pm$ and effective range $R_\pm$. The radial Schrödinger equation is

$$\left(-\frac{\hbar^2}{M} \frac{d^2}{dr^2} + U_\pm(r) + 2\hbar^2 k_\pm^2 M r^2\right) \chi_\pm(r) = \frac{\hbar^2 k_\pm^2 M}{r^2} \chi_\pm(r). \quad (2)$$

The term $2\hbar^2/(Mr^2)$ gives the $p$-wave centrifugal poten-
The important consequence of such considerations is that, in tension to multiple bound states is straightforward. An energy state with radial wave function 
\[ \phi \]

\[ \text{where} \ \phi \ \text{not rate only on the} \ U \ \text{and} \ \phi \ \text{must be odd. In the region} \ r \ \text{the Fermi wave vector} \ \alpha \ \text{forms an orthonormal set. In a rotationally invariant system, they can be further written as}
\[ \phi_\alpha(r_1, r_2) = \sum_\alpha \frac{1}{\sqrt{\Omega r}} \exp(i\mathbf{P} \cdot \mathbf{r}) \varphi_{j\ell}(r) Y_{\ell m}(\hat{r}), \]

\[ \text{where} \ \mathbf{R} = (r_1 + r_2)/2 \ \text{is the center of mass and} \ r = r_1 - r_2 \ \text{is the relative coordinate and} \ r = |r|, \ P \ \text{can be regarded as the center-of-mass momentum of a pair and} \ j, \ \ell, \ m \ \text{label the quantum numbers of the relative radial direction, the angular momentum, and its projection respectively. Here the index} \ \alpha = \{P, j, \ell, m\} \ \text{is a shorthand for all the quantum numbers that label the pair wave function. In a single-component Fermi gas,} \ \alpha \ \text{must be odd. In the region} \ r \ \rightarrow 0, \ \varphi_{j\ell}(r) \ \sim r^{\ell+1}; \ \text{the} \ p\text{-wave channel has the strongest penetration inside the interaction potential} \ U(r). \ \text{As a result, we shall concentrate only on the} \ p\text{-wave component, since it gives the dominant contribution to the interaction energy of the system.}

The pair wave function \ \phi_\alpha(r_1, r_2), \ \text{and hence} \ \varphi_{j\ell}(r) \ \text{is not an eigenfunction of the two-body Schrödinger equation, but can be expanded in terms of the} \ p\text{-wave functions (setting} \ \ell = 1 \ \text{and neglecting the subscript} \ \ell \ \text{from} \ \varphi_{j\ell} \ \text{thereafter)}
\[ \varphi_{j}(r) = \int_0^\infty dk a_{jk} \chi_\kappa(r) + a_{j\kappa} \chi_\kappa(r), \]

\[ \text{where} \ \{a_{jk}, a_{j\kappa}\} \ \text{are the real expansion coefficients, the integration is taken over all scattering states, and we have also taken into account the possibility of a shallow bound state with radial wave function} \ \chi_\kappa(r) \ \text{and binding energy} \ E_0 = \hbar^2 / 2M = R^2 / (Mv), \ \text{when} \ v > 0 \ \text{and} \ R > 0. \ \text{Extension to multiple bound states is straightforward. An important consequence of such considerations is that, in the asymptotic region where} \ r_0 < r < k_F^{-1}, \ \text{the form of} \ \chi_\kappa(r), \ \text{and hence} \ \varphi_{j}(r), \ \text{when expanded in power of} \ k^2, \ \text{are identical to that of} \ \chi^{(0)} \ \text{and} \ \chi^{(1)}. \ \text{Furthermore, for} \ r < r_0, \ \text{both are uniquely fixed by the two-body physics. Thus, when evaluating the expectation value of any short-range function such as potential} \ U(r), \ \chi^{(0,1)} \ \text{can be taken out of the integration over} \ k. \ \text{The interaction energy of the many-body system can be written in terms of} \ \rho_2 \ \text{as} \ \langle \mathcal{U} \rangle = \int \langle \mathcal{U}(r_1 - r_2) \rangle d^3 r_1 d^3 r_2. \ \text{Using the decomposition Eq. (6) and Eq. (7), we find}
\]

\[ \langle \mathcal{U} \rangle = \sum_m \left[ C_v^{(m)}(1) \int dU(r) |\chi^{(0)}|^2 + C_R^{(m)}(r) \int dU(r) \chi^{(0)}(r) \chi^{(1)}(r) \right]. \]

\[ \text{where we have defined two} \ p\text{-wave contacts} \ \mathcal{C}_v^{(m)} \ \text{for each} \ m,\]

\[ C_v^{(m)} = \sum_{P, j, m} n_{P, j, m} \int \frac{d\mathbf{k}}{2\pi} a_{jk} a_{jk} \left(k^2 + k'^2\right) \]

\[ C_R^{(m)} = \int \frac{d\mathbf{k}}{2\pi} a_{jk} a_{jk} \left(k^2 + k'^2\right). \]

\[ \text{Here the contribution from possible bound states is implicitly included in the integration over} \ k. \ \text{We note that} \ C_v^{(m)} \ \text{has dimension of length, while} \ C_R^{(m)} \ \text{has dimension of inverse length. Just as in the} \ s\text{-wave case,} \ C_v^{(m)} \ \text{encapsulate all the short-range correlations of the many-body system. As a byproduct, the two-body density matrix for} \ r = r_1 - r_2 \ \text{in the asymptotic regime} \ r_0 \ll r < k_F^{-1} \ \text{can be written as}
\]

\[ \rho_2(r_1, r_2) = \frac{1}{\Omega} \sum_m |Y_{\ell m}(\hat{r})|^2 \left[ C_v^{(m)}(r) + C_R^{(m)}(r) \right]. \]

\[ \text{Now suppose that the potential} \ U(r) \ \text{can be controlled via an auxiliary parameter} \ \lambda, \ \text{such that a small change in} \ U(r) \ \text{can be written as} \ (dU/d\lambda) d\lambda. \ \text{We can use the Hellmann-Feynman theorem and write} \ dE/d\lambda = \langle dH/d\lambda \rangle = \langle d\mathcal{U}/d\lambda \rangle, \ \text{where} \ \mathcal{H} = \mathcal{K} + \mathcal{U} \ \text{is the total many-body Hamiltonian with} \ \mathcal{K} \ \text{denoting the kinetic energy, independent of} \ \lambda. \ \text{Using Eqs. (3,4,8), we find}
\]

\[ \frac{dE}{dv} = -\frac{\hbar^2}{2M} \sum_m \frac{C_v^{(m)}}{r^4} \frac{dE}{dv} - \frac{\hbar^2}{M} \sum_m C_R^{(m)}. \]

\[ \| \]

\[ 12 \]

In the simplest case of a shallow} \ p\text{-wave two-body bound state, the wave function in the asymptotic region} \ 1/\kappa \gg r \gg r_0 \ \text{is given by} \ \psi_\kappa(r) = \sqrt{R}(1/r^2 + \kappa/r) \ \text{exp}(-\kappa r) Y_{1m}(\hat{r}) \ \text{with} \ \kappa = \sqrt{R}/v. \ \text{It is then easy to obtain} \ \rho_2(r/2, -r/2) = \Omega r^2 / \rho^2 \ \text{by} \ Y_{1m}(\hat{r})^2 \ |Y_{1m}(\hat{r})|^2 \ \text{for the two-body bound state} \ \psi. \ \text{One can extract directly that} \ C_v^{(m)} = R \ \text{and} \ C_R^{(m)} = -R^2/\kappa \ \text{consistent with the adiabatic theorems Eq. (12). The derivation also applies to thermal equilibrium, in which case, one should replace the energy} \ E \ \text{by the free energy} \ F \ \text{of the system and keep temperature constant} \ [5].
As in the s-wave case, a pressure relation and virial theorem can be found. In a uniform system, the universal hypothesis is that the free energy can be written as \( F(T/T_F, k_B^2 T, k_F R) \) close to a p-wave resonance, where \( T_F \) is the Fermi temperature. Using dimensional analysis \( [5-3, 1] \),

\[
P = \frac{2}{3} \mathcal{E} + \frac{\hbar^2}{3M \Omega \nu} \sum_m C_v^{(m)} + \frac{\hbar^2}{3M \Omega R^2} \sum_m C_R^{(m)},
\]

where \( \mathcal{E} \equiv E/\Omega \) is the energy density and \( E \) is the total energy. In an external harmonic trap \( V(r) = \frac{1}{2}M\omega^2 r^2 \), the free energy can be written as \( F(T/T_F, k_B^2 T, k_F R, \hbar \omega/E_F) \) near resonance, and we find

\[
E = 2\langle V \rangle - \frac{3\hbar^2}{2M} \sum_m C_v^{(m)} - \frac{\hbar^2}{2MR} \sum_m C_R^{(m)},
\]

where \( \langle V \rangle \) denotes the total potential energy due to the harmonic confinement.

**Momentum Distribution.** The correlations encapsulated by the two contacts determine the tail of momentum distribution, which can be measured using time-of-flight imaging \([7]\). Theoretically, the momentum distribution can be obtained by Fourier transforming the single-particle density matrix \( \rho_i(r, r') \equiv N^{-1} \int d^3r' \langle \psi(r') \psi^\dagger(r') \rangle \). Given the structure of the two-body density matrix in the asymptotic regime \([cf. \text{Eq. (11)}]\), we find for \( k_F \ll k \ll 1/r_0 \) \([41]\)

\[
n_k = \sum_m \left[ \frac{16\pi^2 C_v^{(m)}}{\Omega k^2} + \frac{32\pi^2 C_R^{(m)}}{\Omega k^4} \right] |Y_{1m}(\hat{k})|^2,
\]

which shows that \( \sum_m C_v^{(m)} \) and \( \sum_m C_R^{(m)} \) determine the strength of the 1/k2 and 1/k4 tails in the momentum distribution \( n_k \), respectively. We also note that a subleading term in momentum distribution relating to the s-wave effective range is found in Ref. \([40]\).

**Radio-frequency Spectroscopy.** The rf coupling \( H_{rf} = h\Omega_{rf} \int d^3r \psi^\dagger(r) \psi(r) \) transfers fermions into an initially empty spin state \( |e\rangle \), where \( \Omega_{rf} \) is the rf Rabi frequency. For a perturbative \( \Omega_{rf} \), the transfer rate can be written as \( \Gamma_{rf}(\omega) \equiv (2\pi/\hbar) \sum_{i,j} \rho_{ij}(\int [H_{rf}]^2 \delta(h\omega + E_i - E_f), \) where \( i, j \) label the initial and final states, and \( \rho_{ij} \) denotes the initial state distribution. In the region \( E_F \ll \hbar \omega \ll E_R \equiv \hbar^2/4MR^2 \), one finds \([42-44]\)

\[
\Gamma_{rf}(\omega) = \frac{2M\Omega_{rf}^2}{\hbar} \left[ \sum_m C_v^{(m)} \left( \frac{\Omega R}{M\omega} \right)^{1/2} + \frac{3}{2} \sum_m C_R^{(m)} \right].
\]

**Static Structure Factor.** By definition, the static structure factor \( S(q) \) is \( 2\pi \sum_{i,j} \rho_{ij} \int d^3r \rho_i(r) \exp(-i\mathbf{q} \cdot \mathbf{r})/|\mathbf{r}|^2 \) and can be measured by Bragg spectroscopy \([45]\). Here \( \rho_i(r) \) is the density operator and other notations are the same as before. \( S(q) \) can be obtained directly by Fourier transforming \( \rho_2 \), Eq. (11), and diverges linearly in the limit \( q \rightarrow \infty \). It is cut off by the short-range potential \( U(r) \) and will be limited by \( 1/r_0 \).

**Photo-association Spectroscopy.** Photo-association has been used to measure the fraction of closed channel molecules in two-component Fermi gases \([46]\), which is related to the s-wave contact \([5, 6]\). In the case of a p-wave resonance, if the internal wave function \( g_m(r) \) of the relevant excited molecule has a specific projection \( m \) along the \( \hat{z} \) direction, namely \( g_m(r) \sim Y_{1m}(\hat{r}) \), the transition rate is given by \( \Gamma_{pa}^{(m)}(\omega) = 2\pi\hbar^2 \sum_{i,f} \rho_{if} \int d^3r \psi^\dagger(r) \psi^\dagger(r) \psi(r) \psi(r') \langle \hat{g}(\omega + E_i - E_f) \rangle \), with \( \Omega_{pa} \) the Rabi frequency and \( \phi_m(R) \) the molecule creation operator.

Since usually the final molecular state has a finite decay rate \( \gamma \), \( \delta(h\omega + E_i - E_f) \) in the expression of \( \Gamma_{pa}^{(m)}(\omega) \) should be replaced by a Lorentzian \( (h\gamma/2)/(\hbar\omega + E_i - E_f)^2 + (h\gamma/2)^2 \). Typically \( \gamma \sim 10 \text{ MHz} \) \([46]\), much larger than the energy scales associated with the spatial motion of the Fermi gas. As a result, when the \( \omega \) of the photo-association laser is tuned to resonance, \( h\gamma \) dominates over typical values of \( \hbar \omega + E_i - E_f \), and we can approximate the Lorentzian by \( 2/h\gamma \).

\[
\Gamma_{pa}^{(m)}(\omega) = \frac{4\pi}{\gamma} \sum_{i,f} \rho_{if} \int d^3r \psi^\dagger(r) \psi^\dagger(r) \psi(r) \psi(r') \langle \hat{g}(\omega + E_i - E_f) \rangle^2.
\]

The Franck-Condon factor can be computed once \( g_m(r) \) is known. What is important here is that it depends only on two-body physics, so the many-body dependence is encapsulated in \( C_v^{(m)} \). The contribution from \( C_R^{(m)} \) is smaller by a factor \( (k_F r_0)^2 \) if the excited molecular state is of extension \( r_0 \). In the case when the photoassociation process does not distinguish between final molecular states of different \( m \), the total transition rate will be the sum of the individual \( \Gamma_{pa}^{(m)} \).

**Virial Expansion for p-wave Contacts.** At high temperatures, the effects of the interaction can be taken into account by the second virial expansion \([47]\). The change of the free energy of the spinless fermions \( \delta F \equiv F - F_0 \) is given by \( \delta F/k_B T = -2\sqrt{2} \text{N} \lambda^3 b_2 \), where \( F_0 \) is the free energy without interactions and \( \lambda \equiv h/\sqrt{2\pi M k_B T} \). The second virial coefficient is given by

\[
b_2 = 3 \int_0^\infty \frac{dk}{\pi} \frac{d\theta(k)}{dk} e^{-\lambda^2 k^2/2\sigma} + \theta(v)e^{v/k_B T}.
\]

Let \( C_{v,R} = \sum_{m} C_{v,R}^{(m)} \), then by the adiabatic theorems,

\[
\frac{C_v}{N} = 4\sqrt{2}\pi N \lambda \frac{\partial b_2}{\partial v^{-1}}, \quad \frac{C_R}{N} = 4\sqrt{2}\pi N \lambda \frac{\partial b_2}{\partial R^{-1}}.
\]

When \( v^{-1} = 0 \), \( \partial b_2/\partial v^{-1} = (3/\sqrt{2\pi}) \lambda R^2 h_\nu (\lambda/(R\sqrt{2\pi})) \) with

\[
h_\nu(\eta) = \eta + \eta^2 \int_0^\infty dx \left( 1 - e^{-x^2} \right) (\eta^2 + 3x^2) \pi(\eta^2 x + x^3) .
\]
and $\partial b_2/\partial R^{-1} = (3/\sqrt{2\pi})\lambda h_R(\lambda/(R\sqrt{2\pi}))$ with

$$h_R(\eta) = \frac{1}{\sqrt{\pi}} - \eta e^{\eta^2} \text{Erfc}(\eta). \quad (21)$$

Figure 1 shows the dependences of $C_v$ and $C_R$ as a function of $E_b/E_F$ for $T/T_F = 2$ and $k_F R = 1/25$, appropriate for the case of $^{40}$K with a typical density of $2 \times 10^{11}$ m$^{-3}$ at the $p$-wave resonances near $B = 198.5$ G [12]. Here we note that while $C_v$ decreases monotonically as $-E_b/E_F$ increases, $C_R$ shows non-monotonic behavior and reaches a maximum when $-E_b/E_F \sim 2$, where it is comparable to $C_v$, if non-dimensionalized by $k_F$ (see Fig. 1). The temperature dependence of the contacts $C_v$ and $C_R$ at $v^{-1} = 0$ is shown in the inset, for which $C_R$ is much smaller than $C_v$; the magnitude of both grows with increasing $R$. In the temperature regime $T_F \lesssim T \ll h^2/2MR^2$, Eqs. (20) and (21) give $C_v \approx 6\sqrt{2}\pi \eta n R^3 \sim T^{-3/2}$ and $C_R \approx 12\pi warpends 

Away from $p$-wave resonances where the scattering volume $v$ is small, Eq. (18) gives $C_v = 36\pi^2 N n v^2 / \lambda^2$ and $C_R = 180\pi^3 N m v^2 / \lambda^4$ when contribution from the deep bound state is excluded. In this limit, the scaling $C_v \sim v^2$ and $C_R \sim v^2$ is also expected from perturbation calculations for small $v$ [24], which indicates the irrelevance of $C_v$ and $C_R$ in Fermi gases close to an $s$-wave resonance.

**Discussion.** Our derivation of the $p$-wave contacts is based on the single-channel model which does not take into account explicitly the presence of closed-channel molecules, as in the case of a Feshbach resonance. The same results shall be obtained for a two-channel model, provided that the closed-channel molecule is small (comparable to $r_0$), which is typically the case. This is because all the arguments so far depend only on the properties of the two-body wave function or two-body density matrix in the asymptotic regime, which, in our derivation, depend only on the scattering volume $v$ and effective range $R$, irrespective of whether they arise from a shape resonance or a Feshbach resonance. For actual atomic systems, the van der Waals potential modifies the $p$-wave scattering phase shift by introducing a term $\alpha/k^2$ in the effective range expansion [26, 49]. However, close to a Feshbach resonance, it was shown that $\alpha \sim 1/v^2$, whose effects are thus negligible [26, 50]. As a result, we expect that our main results Eqs. (11) to (17) to remain true close to a $p$-wave Feshbach resonance.

Resonances for different $|m|$ can be split due to magnetic dipole-dipole couplings [20]. For $^{40}$K, the $m = 0$ and $m = \pm 1$ resonances around $B = 198.5$ G are split by about 0.5 G [20]. To take this into account, we can introduce phase shifts for different $m$, $\cot(\delta^{(m)}) = -1/v^{(m)}k^3 - 1/R^{(m)}k$. Likewise, we can establish the relation $dE/d(\frac{1}{v^{(m)}}) = -h^2C_v^{(m)}/M$ and $dE/d(\frac{1}{R^{(m)}}) = -h^2C_R^{(m)}/M$ while Eqs. (11) and (15) to (17) stay intact.

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**Note added.** During the final preparation of this manuscript, closely related work by Yoshida and Ueda appeared [51], in which they discuss one of the contacts, $C_v$, using a two-channel model.

[41] See supplementary materials for derivations of the shallow $p$-wave two-body bound states, derivation of equations (3) and (4), and the tail of momentum distribution.