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Exact Solution for 1D Spin-Polarized Fermions with Resonant Interactions

Adilet Imambekov,[1] Alexander A. Lukyanov,[2] Leonid I. Glazman,[3] and Vladimir Gritsev[4]

[1]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*
[2]*Abingdon Technology Centre, Schlumberger, Abingdon, OX14 1UJ, United Kingdom*
[3]*Department of Physics, Yale University, New Haven, Connecticut 06520, USA*
[4]*Physics Department, University of Fribourg, Chemin du Musee 3, 1700 Fribourg, Switzerland*

Using the asymptotic Bethe ansatz, we obtain an exact solution of the many-body problem for 1D spin-polarized fermions with resonant p-wave interactions, taking into account the effects of both scattering volume and effective range. Under typical experimental conditions, accounting for the effective range, the properties of the system are significantly modified due to the existence of "shape" resonances. The excitation spectrum of the considered model has unexpected features, such as the inverted position of the particle- and holelike branches at small momenta, and rotonlike minima. We find that the frequency of the "breathing" mode in the harmonic trap provides an unambiguous signature of the effective range.

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Experimental progress in the cooling and trapping of ultracold atomic gases makes it possible to investigate their properties under strong transverse confinement, when the motion of atoms is effectively one dimensional (1D). In such experiments the 1D interaction parameters are precisely known and can be tuned using Feshbach resonances [1] or by varying the harmonic transverse confinement strength. Recent experiments [2,3] have allowed for parameter-free comparison of 1D Bose gas properties with a theoretical description based on the exactly solvable Lieb-Liniger (LL) model [4]. The possibility to compare experimental results with the outcomes of many-body calculations revived an interest in the field of exactly solvable 1D systems: spin-1/2 fermions [5], Bose-Fermi mixtures [6,7], and spinor bosons [8] and fermions [9].

In this Letter, we obtain an exact solution for 1D spin-polarized fermions under resonant scattering conditions [10], which is relevant for ^{40}K and ^{6}Li atoms near p-wave Feshbach resonances [11,12]. Such a 1D experimental system has been realized for ^{40}K [13]. The related 3D problem has also received significant theoretical attention recently [14]. For spin-polarized fermions only scattering in odd partial wave channels is present, and at low energies, p-wave scattering is the strongest. If only the "scattering volume" is taken into account and the "effective range" of p-wave scattering is neglected [see Eq. (1) for definitions], then the projection to 1D [15] results in a fermionic Cheon-Shigehara (CS) model [16], which is dual to the bosonic LL model. For such a model, strongly interacting fermions with resonant interactions are mapped to weakly interacting bosons, the so-called fermionic Tonks-Girardeau (fTG) limit [17]. However, it was shown by L. Pricoupenko [10] that unlike the case of the strongly interacting bosonic TG limit [2,3], the requirements for the observation of the fTG limit are quite stringent, and the effective range of scattering needs to be taken into account. We provide an exact solution that accounts for both scattering volume and effective range, and obtain significant deviations from the CS model [16] due to the "shape" resonance in the p-wave scattering. We find several new effects, such as the inversion of particle- and holelike spectra for low momenta, rotonlike minima in the excitation spectrum, and we calculate density profiles and "breathing" mode frequencies in the harmonic trap.

We use the asymptotic Bethe ansatz (BA) [18] which is justified at sufficiently small densities, when only two-particle collisions are important [19]. The underlying idea goes back to the earlier days of high energy physics and was known as S-matrix theory [20] in the 1950s. The BA method considers the scattering matrix between asymptotic states as an alternative to a Hamiltonian or Lagrangean description. The scattering of ultracold atoms in 1D gases close to resonance can naturally be described by the scattering phase shift, whereas the formulation of a microscopic quantum Hamiltonian is difficult. It can be shown that the scattering matrix close to resonance corresponds to a highly singular, although local, two-body interaction in the spirit of Refs. [16,21]. To avoid difficulties related to the determination of the operators and states in this case, we use an approach based entirely on the scattering phase shift.

Let us start by briefly reviewing the 3D scattering properties in a p-wave channel. At low energies, the phase shift $\delta_p(k)$ can be expanded as [10,22]

$$k^3 \cot\delta_p(k) = -1/w_1 - \alpha_1 k^2 + O(k^4), \tag{1}$$

where w_1 is the scattering volume, α_1 is the effective range, and k is the relative momentum. For $\alpha_1 w_1 < 0$, the scattering length obtained from $\delta_p(k)$ has a very sharp shape resonance at the wave vector [22,23]

$$k_r = 1/\sqrt{-\alpha_1 w_1}. \tag{2}$$

Such resonance is absent for s-wave scattering, but for the p-wave channel it exists due to the presence of the effective range parameter. The higher order terms in Eq. (1) do

not significantly affect the shape resonance, since they are suppressed by powers of the small parameter $kR \ll 1$, where R is the characteristic radius of the 3D potential. For fermions, the typical momenta of scattering particles are of the order of the Fermi momentum $k_F = \pi n$. Therefore, the condition $kR \ll 1$ necessary for neglecting three-particle collisions [19] implies the low-density limit $nR \ll 1$. It is known [10,22,23] that $\alpha_1 \gtrsim 1/R > 0$ does not change significantly at the p-wave Feshbach resonance, while w_1 can be tuned to very large absolute values compared to its characteristic values of the order of $|w_1| \sim R^3$ away from the resonance.

Under transverse harmonic confinement with frequency $\omega_\perp$, only the lowest transverse mode is occupied if the momenta of scattering fermions satisfies

$$ka_\perp \ll 1, \tag{3}$$

where $a_\perp = \sqrt{\hbar/(m\omega_\perp)}$, and m is the atomic mass. Under such conditions, the 1D scattering amplitude in an odd channel is given by [10]

$$f_p^{\text{odd}} = \frac{-ik}{1/l_p + ik + k^2\xi_p}, \tag{4}$$

where [24]

$$l_p = 3a_\perp\left[\frac{a_\perp^3}{w_1} - 3\sqrt{2}\zeta(-1/2)\right]^{-1}, \quad \xi_p = \frac{\alpha_1 a_\perp^2}{3} > 0, \tag{5}$$

and $3\sqrt{2}\zeta(-1/2) \approx -0.88$. The notation adopted is that of Ref. [19]. Using estimates [10,25] of α_1 for ^{6}Li and ^{40}K atoms at resonances with $B_0 \approx 215$ G and 198.6 G, and with transverse frequencies $\omega_\perp = 2\pi \times 200$ kHz and $2\pi \times 30$ kHz [13], we obtain $\xi_p/a_\perp \approx 50$ and ≈ 13, respectively. Thus, under typical experimental conditions needed to achieve the 1D regime $\xi_p \gg a_\perp$ and hence all three terms are significant in the denominator of Eq. (4).

The many-body fermionic wave function $\psi(z_1, \ldots, z_M)$ is antisymmetric, $\psi(\ldots, z_i, \ldots, z_j, \ldots) = -\psi(\ldots, z_j, \ldots, z_i, \ldots)$, and discontinuous when two coordinates coincide [16]. We define its symmetrized version by $\psi_+(z_1, \ldots, z_M) = \prod_{i<j}\text{sgn}(z_i - z_j)\psi(z_1, \ldots, z_M)$, which is continuous. Then Eq. (4) implies the following boundary condition:

$$\lim_{z=z_j-z_i\to 0^+}\left(\frac{1}{l_p} + \partial_z - \xi_p\partial_z^2\right)\psi_+(z_1, \ldots, z_M) = 0. \tag{6}$$

Solving the two-body problem as $\psi_+(z_1, z_2) \propto e^{i\lambda|z_1-z_2|}$, we obtain two roots $\lambda_\pm = (-i \pm \sqrt{-1 - 4\xi_p/l_p})/(2\xi_p)$. For $l_p > 0$, $\text{Im}\lambda_+ > 0$, which corresponds to a bound state. The lowest energy state satisfying the boundary condition (6) can then be constructed as $\psi(z_1, \ldots, z_M) \propto \prod_{i<j}\text{sgn}(z_i - z_j)\prod_{i<j}\exp(i\lambda_+|z_i - z_j|)$. As in the attractive LL model, its energy does not have a proper thermodynamic limit, we will not consider the case where $l_p > 0$. For $l_p < 0$ we construct an exact wave function $\psi_+(z_1, \ldots, z_M)$ as a combination of plane waves, using the BA method in a similar manner to the LL model. In our case, such construction leads to the following periodic boundary conditions on a circle of length L

$$e^{i\lambda_j L} = \prod_{k=1}^{M}\frac{\xi_p(\lambda_j - \lambda_k)^2 - \frac{1}{|l_p|} + i(\lambda_j - \lambda_k)}{\xi_p(\lambda_j - \lambda_k)^2 - \frac{1}{|l_p|} - i(\lambda_j - \lambda_k)}, \tag{7}$$

and the total energy is given in terms of quasimomenta λ_i as $E = \hbar^2/(2m)\sum\lambda_i^2$. We prove that all solutions of Eq. (7) are real by writing the kth term in the product as $\frac{(\lambda_j-\lambda_k-\lambda_+)(\lambda_j-\lambda_k-\lambda_-)}{(\lambda_j-\lambda_k-\lambda_+^*)(\lambda_j-\lambda_k-\lambda_-^*)}$. Since $\text{Im}\lambda_\pm < 0$ for $\xi_p > 0$ and $l_p < 0$, we then have $|\frac{(\lambda-\lambda_+)(\lambda-\lambda_-)}{(\lambda-\lambda_+^*)(\lambda-\lambda_-^*)}| \le 1(\ge 1)$ for $\text{Im}\lambda \le 0(\ge 0)$. After that, the proof simply follows the steps for the LL model described on p. 11 of Ref. [26].

To obtain a thermodynamic limit, we take a logarithm of Eq. (7), which is written as $L\lambda_j + \sum_{k=1}^M\theta(\lambda_j - \lambda_k) = 2\pi n_j$, where n_j are integer quantum numbers for odd M. The phase shift $\theta(\lambda)$ is a monotonic antisymmetric function defined by

$$\theta(\lambda) = 2\text{Arg}(i\lambda - \xi_p\lambda^2 + 1/|l_p|), \tag{8}$$

and belongs to the interval $(-2\pi, 2\pi)$, unlike the LL phase shift, which belongs to the interval $(-\pi, \pi)$. We then directly follow Ref. [27] and show that real solutions of the BA equations exist for any choice of quantum numbers n_j. Their values for the ground state can be fixed by comparison with the LL model [4,26,27], and are given by $n_j = j - (M+1)/2$. Introducing a positive function $K(\lambda, \mu) = \theta'(\lambda, \mu)$,

$$K(\lambda, \mu) = \frac{2|l_p|[1 + |l_p|\xi_p(\lambda - \mu)^2]}{[1 - |l_p|\xi_p(\lambda - \mu)^2]^2 + l_p^2(\lambda - \mu)^2},$$

we pass to the thermodynamic limit, and write an equation for the ground-state quasimomenta distribution in the usual way $2\pi\rho(\nu) - \int_{-q}^{q}K(\nu, \mu)\rho(\mu)d\mu = 1$, where $\pm q$ is the highest (lowest) filled quasimomentum and the normalization is given by $n = M/L = \int_{-q}^{q}\rho(\nu)d\nu$. Apart from new definitions of $\theta(\lambda)$ and $K(\lambda, \mu)$, the structure of the theory remains similar to the LL model, and we can study the ground-state energy, excitation spectra and finite temperature thermodynamics using standard methods [26].

We choose two dimensionless parameters that determine the ground-state properties in the stable region

$$\gamma_1 = -\frac{1}{l_p n} > 0, \qquad \gamma_2 = \frac{1}{\xi_p n} > 0. \tag{9}$$

In Fig. 1 we show the dimensionless ground-state energy functional $e(\gamma_1, \gamma_2)$ obtained by numerically solving the equations for the ground state. The dimensionless form is given by the expression

$$E/L = e(\gamma_1, \gamma_2)(\hbar n)^2/(2m), \tag{10}$$

and reduces to the LL functional $e(\gamma_1)$ for $\gamma_2 \gg 1$, since the CS model [16] obtained in this limit is dual to the LL

model. The function $e(\gamma_1, \gamma_2)$ equals 0 if $\gamma_1 = 0$ or $\gamma_2 = 0$. Expansion by methods of Ref. [28] at $\gamma_1, \gamma_2 \gg 1$ yields $e(\gamma_1, \gamma_2) \approx e(\gamma_1) - 32\pi^4/(15\gamma_1^2\gamma_2)$.

We use the function $e(\gamma_1, \gamma_2)$ obtained numerically to evaluate density profiles in a harmonic trap within the local density approximation [29]. We also use the function $e(\gamma_1, \gamma_2)$ to find the breathing mode frequency ω by solving the hydrodynamic equations [6,30]. The results are shown in Fig. 2 and depend on two dimensionless parameters, $\gamma_1(0)$ and $\gamma_2(0)$, in the center of the cloud. The presence of the effective range significantly affects the shape of the profile compared to the CS model if $\gamma_2(0)$ is small and $\gamma_1(0)$ is not too large. This effect can be understood by using the expansion of $e(\gamma_1, \gamma_2)$ for $\gamma_1, \gamma_2 \ll 1$. The leading term in the Taylor expansion gives $e(\gamma_1, \gamma_2) \propto \gamma_1\gamma_2 \propto 1/n^2$ and hence via Eq. (10) the energy per particle for this term does not depend on density, i.e., the gas has a divergent compressibility. Higher order terms in the expansion of $e(\gamma_1, \gamma_2)$ lead to a finite but large compressibility, which decreases with increasing γ_1 and a constant ratio γ_2/γ_1. Thus, the density profile exhibits a strong peak near the center where γ_1 is smallest.

Since fermions are more strongly correlated for $\gamma_2 \ll 1$ and not too large γ_1 compared to the fTG regime, we suggest calling such a regime a super-fTG gas, analogously to the super-TG gas of bosons [31]. It is realized if

$$\mathrm{Max}\left(\gamma_2, \frac{\gamma_1\gamma_2}{4\pi^2}\right) \lesssim 1. \tag{11}$$

For $|w_1| \ll a_\perp^3$, the second condition corresponds to $k_r \lesssim 2\pi n = 2k_F$. Thus, the super-fTG regime is realized if the largest relative momentum of noninteracting fermions approaches the shape resonance wave vector k_r. In a similar manner to the super-TG gas of bosons, the super-fTG regime can be experimentally identified by measuring the ratio of the squares of the breathing and dipole mode frequencies. In the CS model such a ratio is always larger than 3, similar to the LL model [30], while the inset of Fig. 2 shows the regime where it is smaller than 3. A sharp decrease in this ratio for the super-fTG regime can be easily understood from the "sum rule" approach of Ref. [30], since the cloud density is much more centered in the super-fTG regime than in the fTG regime. We can analytically estimate the value of $-w_1/a_\perp^3$ at which the center of the cloud enters the super-fTG regime, and the drop in $(\omega/\omega_z)^2$ occurs. For that we use Eq. (11) with the free fermion density in the center and obtain $(-w_1/a_\perp^3)|_{\text{super-fTG}} = [(\omega_\perp/\omega_z)/(24N\xi_p/a_\perp)]$, which gives 0.008 for the parameters seen in Fig. 2.

The excitation spectrum $\varepsilon(k)$ in a uniform cloud is also significantly modified in the super-fTG regime compared to predictions of the CS model. In Fig. 3 we illustrate several qualitative features, which appear due to the finite effective range of interactions. First, the system has a regime where the energy of the particlelike excitation is smaller than the energy of the holelike excitation. Since the energy of the particlelike excitation should approach $k^2/(2m)$ at high momenta, there should also be an energy crossing. This crossing will manifest itself as a kink in the k dependence of the lowest energy of the density wave excitations. Second, the spectrum of holelike excitations can have a "roton" minimum (or even an additional maximum, see inset in Fig. 3) at $k \approx k_F$. This minimum can be

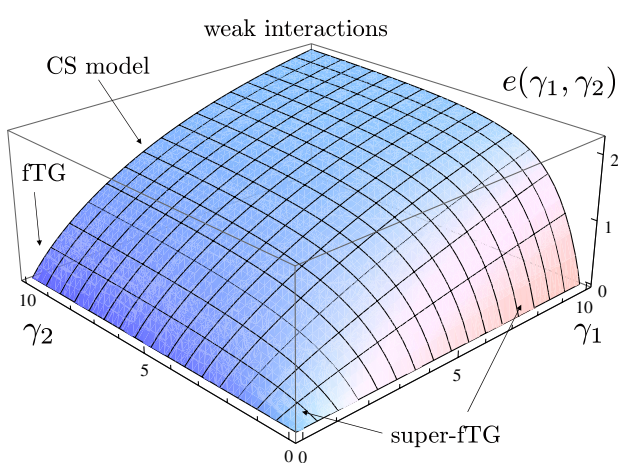

FIG. 1 (color online). Energy functional $e(\gamma_1, \gamma_2)$ as a function of dimensionless parameters γ_1 and γ_2, see Eqs. (9) and (10). Arrows indicate the regimes of weakly interacting fermions, Cheon-Shigehara (CS) model [16], fermionic Tonks-Girardeau (fTG) gas [17], and super-fTG regime [see Eq. (11)] existing due to the finite effective range ξ_p.

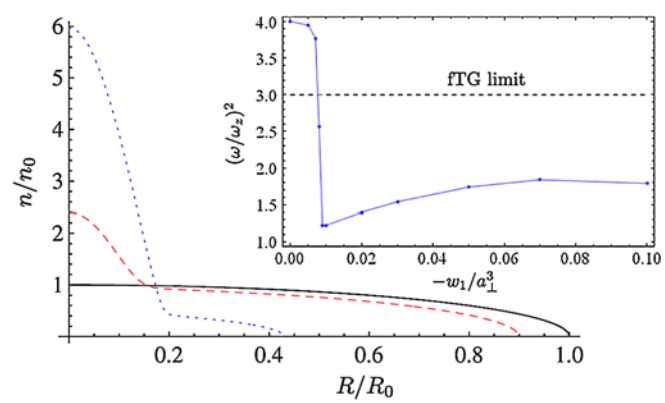

FIG. 2 (color online). Density profiles under harmonic confinement, measured in units of Thomas-Fermi radius R_0 and central density n_0 for the same cloud in the absence of interactions. Different curves correspond to $\{\gamma_1(0), \gamma_2(0)\}$ in the center of the cloud $\{7.5, 0.023\}$ (blue, dotted line), $\{97, 0.058\}$ (red, dashed line), and free fermions (black, solid line). For a cloud of $N = 100$ ^{6}Li atoms with $\omega_\perp = 2\pi \times 200$ kHz and $\omega_z = 2\pi \times 200$ Hz, we get $R_0 = 41$ μm and these curves correspond to $-w_1/a_\perp^3 = 0.05,\ 0.01,\ 0$, respectively. The inset shows the ratio of squares of the breathing and dipole mode frequencies $(\omega/\omega_z)^2$ for the same trap parameters. If a significant part of the cloud is in the super-fTG regime (see text), this ratio drops below the critical value 3 obtained in the fTG limit. A critical value $-w_1/a_\perp^3 \approx 0.008$ corresponds to a detuning from the resonance $\Delta B \approx 50$ mG.

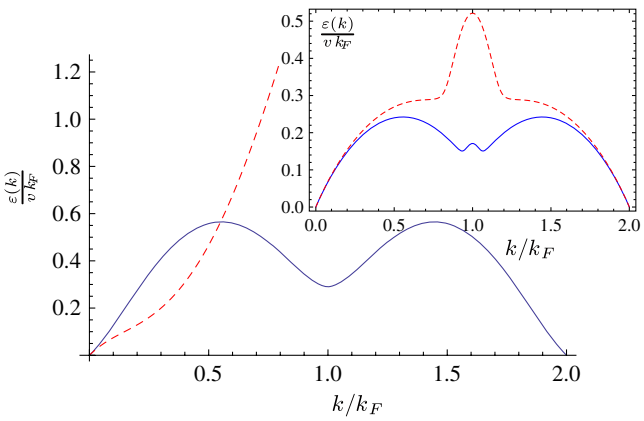

FIG. 3 (color online). Excitation spectrum for $\gamma_1 = 0.5$, $\gamma_2 = 0.005$, where momentum is measured in units of $k_F = \pi n$, and energy is normalized to give a unit velocity $v = \varepsilon'(k)|_{k=0}$. Because of interactions, the particlelike mode (red, dashed line) has energy lower than the holelike mode (blue, solid line) for sufficiently small momenta. Velocities of two modes at $k = 0$ coincide. The inset shows energies of holelike modes for $\gamma_1 = 10.8$, $\gamma_2 = 0.022$ (blue, solid line) and $\gamma_1 = 27.3$, $\gamma_2 = 0.055$ (red, dashed line), normalized to their respective velocities.

understood as a tendency of the system towards pairing when the parameters γ_1, γ_2 approach the boundary of the stable region. Indeed, the energy of the holelike excitation vanishes for $k = 2k_F = 2\pi n$. Since particle density is twice the density of pairs, the vicinity of the paired region manifests itself as a soft mode at $k \approx 2\pi n/2 = k_F$. Dynamic response functions of the system will have power-law divergences at the particle- and holelike modes, which can be calculated using the methods of Ref. [32]. Note however, that the existence of the roton minimum and the inversion of the particle- and holelike spectra lead to modifications of the phenomenology of Ref. [33].

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