Theory of spinor Fermi and Bose gases in tight atom waveguides

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Divergence-free pseudopotentials for spatially even and odd-wave interactions in spinor Fermi gases in tight atom waveguides are derived. The Fermi-Bose mapping method is used to relate the effectively one-dimensional fermionic many-body problem to that of a spinor Bose gas. Depending on the relative magnitudes of the even and odd-wave interactions, the N-atom ground state may have total spin $S = 0$, $S = N/2$, and possibly also intermediate values, the case $S = N/2$ applying near a p-wave Feshbach resonance, where the N-fermion ground state is space-antisymmetric and spin-symmetric. In this case the fermionic ground state maps to the spinless bosonic Lieb-Liniger gas. An external magnetic field with a longitudinal gradient causes a Stern-Gerlach spatial separation of the corresponding trapped Fermi gas with respect to various values of $S$.

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I. INTRODUCTION

When an ultracold atomic vapor is placed into an atom waveguide with sufficiently tight transverse confinement, its two-body scattering properties are strongly modified. This occurs in a regime of low temperatures and densities where transverse oscillator modes are frozen and the dynamics is described by a one-dimensional (1D) Hamiltonian with zero-range interactions [1, 2], a regime which has already been reached experimentally [3–5]. In addition, a regime with chemical potential $\mu$ less than transverse level spacing $\hbar \omega_\perp$ but $k_B T > \hbar \omega_\perp$ has been achieved [6, 7]. We assume herein that both $\mu < \hbar \omega_\perp$ and $k_B T < \hbar \omega_\perp$ as in [3–5]. Nevertheless, virtually excited transverse modes renormalize the effective 1D coupling constant via a confinement-induced resonance, as first shown for bosons [1, 8] and recently for spin-polarized fermionic vapors by Granger and Blume [9].

The dynamics of an optically trapped Fermi gas is richer than that of a magnetically trapped one, since the spin is not polarized. A Fermi-Bose mapping first used to solve the 1D hard-sphere Bose gas [10, 11] was recently shown [12] to provide an exact duality between effective zero-range 1D fermionic and bosonic interactions and applied to spin-polarized Fermi gases [9, 13]. It will be shown here that this mapping and Fermi-Bose duality also hold for spinor Fermi gases. This mapping will be exploited to reduce the degenerate spatially antisymmetric fermionic ground states to that of a spinless Bose gas, which, in the 1D, zero-range interaction regime, is the Lieb-Liniger model which is exactly solvable in the absence of longitudinal trapping [14, 15] and well approximated by a local equilibrium approach in the trapped case [16]. It will be shown that in the presence of longitudinal trapping, this fermionic ground state can be Stern-Gerlach spatially decomposed by a longitudinal magnetic field gradient into components with various values of total longitudinal spin.

II. TWO-BODY PROBLEM FOR FERMIONS IN A TIGHT WAVEGUIDE

Consider first the three-dimensional two-body scattering problem for spin-$\frac{1}{2}$ fermionic atoms. There are both s-wave scattering states, which are space symmetric and spin antisymmetric with spin eigenfunctions of singlet form $\frac{1}{\sqrt{2}}(\downarrow \downarrow - \downarrow \uparrow)$, as well as p-wave scattering states which are space antisymmetric and spin symmetric with spin eigenfunctions of triplet form $\uparrow \uparrow$ or $\downarrow \downarrow$ or $\frac{1}{\sqrt{2}}(\downarrow \uparrow + \uparrow \downarrow)$. s-wave scattering cannot occur in a spin-polarized Fermi gas, but it is usually dominant in a spinor Fermi gas since p-wave spatial antisymmetry suppresses short-range interactions. However, both s-wave and p-wave interactions can be greatly enhanced by Feshbach resonances [17, 18]. Assume until further notice that the Hamiltonian does not depend on spin. Then the spin dependence of wave functions need not be indicated explicitly and they can be written as the sum of spatially even and odd parts $\psi_e$ and $\psi_o$. When such an atomic vapor is confined in an atom waveguide with tight transverse trapping, the dynamics becomes effectively 1D [1]. The effective 1D interactions are determined by 1D scattering lengths $a_{1D}^s$ for spatially even waves $\psi_e(z) = \psi_e(-z)$ related to 3D s-wave scattering and spatially odd waves $\psi_o(z) = -\psi_o(-z)$ related to 3D p-wave scattering; here $z$ is the relative coordinate $z_1 - z_2$ for 1D scattering. These determine the $k \to 0$ behavior just outside the range $z_0$ of the interaction:

\begin{align*}
\psi_e'(z_0) &= -\psi_e(-z_0) = -(a_{1D}^s - z_0)^{-1}\psi_e(\pm z_0) \\
\psi_o(z_0) &= -\psi_o(-z_0) = -(a_{1D}^p - z_0)\psi_o'(\pm z_0). \quad (1)
\end{align*}

$a_{1D}^s$ is a known [1] function of the 3D s-wave scattering length $a_s$, and $a_{1D}^p$ is a known [9, 19] function of the 3D p-
wave scattering volume $V_p = a_p^3 = -\lim_{k \to 0} \tan \delta_p(k)/k^3$ [20]:

$$a_{1D}^\rho = \frac{-2a_\|}{a_\|^2} [1 - (a_\|/a_\|)|\zeta(1/2)|]^{-1}$$
$$a_{1D}^o = \frac{6V_e}{a_\|^2} [1 + 12(V_e/a_\|^2)\zeta(-1/2, 1)]^{-1}$$  \hspace{1cm} (2)$$

where $a_\| = \sqrt{\hbar/\mu \omega_\perp}$ is the transverse oscillator length for the relative motion, $\mu$ is the effective mass, $\zeta(1/2) = -1.460 \cdots$ is a Riemann zeta function, and $\zeta(-1/2, 1) = -0.2079 \cdots$ is a Hurwitz zeta function [21].

In the zero-range limit $z_0$ approaches $0^+$ and $-z_0$ approaches $0^-$, and Eqs. (1) reduce to “contact conditions” which relate a discontinuity in $\psi_e$ at contact $z = 0$ to $\psi_e(0)$, and a discontinuity of $\psi_o$ to $\psi_o(0)$. Although a discontinuity in the derivative is a well-known consequence of the zero-range delta function pseudopotential and plays a crucial role in the solution of the Lieb-Liniger model [14], discontinuities of $\psi$ itself have received little attention, although they have been discussed previously by Cheon and Shigehara [12] and are implicit in the recent work of Granger and Blume [9]. For an odd wave $\psi_o$ the discontinuity $2\psi_o(0^+)$ is a trivial consequence of antisymmetry together with the fact that a nonzero odd-wave scattering length cannot be obtained in the limit $z_0 \to 0$ unless $\psi_o(0^+ \pm) \neq 0$. These discontinuities are rounded off when $z_0 > 0$, since the interior wave function interpolates smoothly between the values at $z = -z_0$ and $z = 0$. A general 1D two-body wave function $\psi(z)$ is the sum of even and odd parts: $\psi(z) = \psi_e(z) + \psi_o(z)$, and the zero-range limit of Eqs. (1) can be combined into

$$\psi'(0^+) - \psi'(0^-) = (a_{1D}^o)^{-1} [\psi(0^+) + \psi(0^-)]$$
$$\psi(0^+) - \psi(0^-) = (a_{1D}^e)^{-1} [\psi'(0^+) + \psi'(0^-)]$$ \hspace{1cm} (3)$$

III. EVEN AND ODD-WAVE PSEUDOPOTENTIALS

Take the Hamiltonian to be

$$\hat{H}_{1D} = -\left(h^2/2\mu\right)\partial_z^2 + v_{1D}^e + v_{1D}^o$$ \hspace{1cm} (4)$$

where $v_{1D}^e$ and $v_{1D}^o$ are even- and odd-wave pseudopotentials to be determined. $\partial_z^2$ is nonsingular for $z \neq 0$, but at the origin there are singular contributions. The first derivative is $\partial_z \psi(z) = \psi'(z \neq 0) + [\psi(0^+) - \psi(0^-)] \delta(z)$. The second derivative then has two contributions in addition to $\psi'(z \neq 0)$, one because in general $\psi'(0^+) \neq \psi'(0^-)$ and the other from the derivative of the delta function:

$$\partial_z^2 \psi(z) = \psi''(z \neq 0) + [\psi'(0^+) - \psi'(0^-)] \delta(z) + [\psi(0^+) - \psi(0^-)] \partial_z \delta(z)$$ \hspace{1cm} (5)$$

$\delta(z)$ term is standard in the theory of zero-range even-wave interactions, the derivative discontinuity in $\psi(z)$ being chosen to cancel a zero-range even-wave interaction proportional to $\delta(z)$, but the $\delta'(z)$ term is new. To cancel it an odd-wave pseudopotential proportional to $\delta'(z)$ suggests itself. However, the discontinuity in $\psi$ leads to unwanted products of delta functions unless regularizing operators are included. Define two linear operators $\hat{\partial}_\pm$ by

$$\hat{\partial}_\pm \psi(z) = (1/2)[\psi(0^+) + \psi(0^-)] \delta(z)$$
$$\hat{\partial}_\pm \psi(z) = (1/2)[\psi'(0^+) + \psi'(0^-)]$$ \hspace{1cm} (6)$$

where $\delta(z)$ is the usual Dirac delta function. The divergence-free even and odd-wave pseudopotential operators are then

$$v_{1D}^e = \hat{g}_{1D}^e \hat{\partial}_\pm \ , \ \ v_{1D}^o = \hat{g}_{1D}^o \delta'(z) \hat{\partial}_\pm \ .$$ \hspace{1cm} (7)$$

They satisfy convenient projection properties $v_{1D}^e \psi_o = v_{1D}^o \psi_e = 0$ on the even and odd parts of $\psi$, and their matrix elements are $\langle \chi | v_{1D}^e \psi | \chi \rangle = 1/\lambda \langle \chi | \psi(0^+) + \psi(0^-) \rangle$ and $\langle \chi | v_{1D}^o \psi | \chi \rangle = -1/\lambda \langle \chi | \psi(0^+) - \psi(0^-) \rangle$. They are unambiguous and connect only even to even and odd to odd wave functions if we stipulate that $\chi(0) = 0$ [the average of $\chi(0^+)$ and $\chi(0^-)$] if $\chi$ is odd and $\chi(0) = 0$ [the average of $\chi(0^+)$ and $\chi(0^-)$] if $\chi$ is even. In fact, the wave function and its derivative at $z = 0$ refer to the internal wave function as modified by the potential, whereas $z = 0^+$ and $z = 0^-$ refer to the wave function just outside the range of the potential, and the above values at $z = 0$ follow from the way the internal wave function interpolates between the contact conditions on the exterior wave function (see below). Terms in $\delta(z)$ and $\delta'(z)$ cancel from $\hat{H}_{1D}$ if

$$\hat{g}_{1D}^e \psi(0^+) + \psi(0^-) = (h^2/\mu) [\psi(0^+) - \psi(0^-)]$$
$$\hat{g}_{1D}^o [\psi'(0^+) + \psi'(0^-)] = (h^2/\mu) [\psi'(0^+) - \psi'(0^-)]$$ \hspace{1cm} (8)$$

and these are equivalent to the contact conditions (3) if $\hat{g}_{1D}^e = -h^2/\mu a_{1D}^e$ and $\hat{g}_{1D}^o = -h^2/\mu a_{1D}^o$.

The physical significance is clarified by starting from a nonsingular square well. Take the potential $v(z)$ to be $-V_0$ when $-z_0 < z < 0$ and zero when $|z| > z_0$. (The odd-wave interaction $v_{1D}^o$ in $\hat{H}_{1D}$ is negative definite in the regime of interest, where $\hat{g}_{1D}^o > 0$.) The antisymmetric solution $\psi_o$ of the zero-energy scattering equation $[(-h^2/2\mu)\partial_z^2 + v(z)]\psi_o(z) = 0$ inside the well is $\sin(kz)$ with $k = \sqrt{\mu V_0/\hbar^2}$. The odd-wave scattering length $a_{1D}^o$ is defined by the second Eq. (1), which is satisfied in the limit $z_0 \to 0^+$ if $V_0$ scales with $z_0$ as $\kappa = (\pi/2z_0)[1 + (2/\pi)^2 (z_0/a_{1D}^o)]$. In that limit the boundary conditions reduce to the second Eq. (3). Inside the well the kinetic and potential energy terms are $(-h^2/2\mu)\partial_z^2 \psi_o(z) = -(\hbar^2 k^2/2\mu) \sin(kz)$ and $v(z)\psi_o(z) = -V_0 \sin(kz)$. For $|z| < z_0$, $\cos(kz)$ is proportional to a representation of $\delta(z)$ as $z_0 \to 0$, since $\int_{-z_0}^{z_0} \cos(kz) f(z) dz \to f(0) \int_{-z_0}^{z_0} \cos(kz) dz = f(0) 2k^{-1} \sin(kz_0) \to 2zf(0)$. Then its derivative
−(κ/2z₀)sin(κz) is a representation of δ′(z). Noting that κz₀ → π/2 as z₀ → 0 we have −(ℏ²/2µ)∂²/∂z²ψ₀(z) = −(ℏ²κ²/2µ)sin(κz) → (πℏ²/2µ)δ(z) which agrees with the kinetic energy term −ℏ²⟨ψ₀|ψ₀⟩ − ℏδ′(z) from Eq. (5) when ψ₀(z) and ψ₀(−z) are interpreted as ψ₀(z₀) and ψ₀(−z₀) as z₀ → 0+. Next consider the potential energy term inside the well as z₀ → 0+: −V₀sin(κz) → −V₀(−2z₀/κ)δ(z) → (πℏ²/2µ)δ(z). Comparing this with ℏκzψ₀(z) from Eq. (7), using the expression for g_D^n, noting that ψ(0±) in Eq. (6) are to be interpreted as ψ′(±z₀), one finds that the two expressions for the potential energy term agree in the limit z₀ → 0+.

IV. FERMION-BOSE MAPPING

The two-body states ψ(z) considered so far are fermionic, i.e., the spatially even part ψ_e(z) contains an implicit spin-odd singlet spin factor, and the spatially odd part ψ_o(z) contains implicit spin-even triplet spin factors. To emphasize the combined space-spin fermionic antisymmetry, these will now be denoted by ψ_F(z) = ψ_e(z) + ψ_o(z). States of combined space-spin bosonic symmetry can be defined by the mapping ψ_B(z) = sgn(z)ψ_F(z) where sgn(z) is +1 if z > 0 and −1 if z < 0. This maps the spatially even fermionic function ψ_e to a spatially odd bosonic function ψ_B and the spatially odd fermionic function ψ_o to a spatially even bosonic function ψ_B while leaving the spin dependence unchanged, and the corresponding scattering lengths are also unchanged: a^e_D,B = a^e_D,F and a^o_D,B = a^o_D,F. Then the even-wave contact conditions for a^e_D,B follow from the odd-wave contact conditions for a^o_D,F and the odd-wave contact conditions for a^e_D,B follow from the even-wave contact conditions for a^o_D,F.

The bosonic Hamiltonian is of the same form as the fermionic one (4) but with mapped coupling constants g_D^n_B = ℏ²/µ²g_D^n,F and g_D^o_B = ℏ²/µ²g_D^o,F, the first of which agrees with the low-energy limit of Eq. (25) of [9, 19]. In the limit g_D^n_B = +∞ arising when V_p → 0−, this is the N = 2 case of the original mapping [10, 11] from hard sphere bosons to an ideal Fermi gas, now generalized to arbitrary coupling constants and spin dependence. This generalizes to arbitrary N: Fermionic solutions ψ_F(z₁, σ₁; · · · ; z_N, σ_N) are mapped to bosonic solutions ψ_B(z₁, σ₁; · · · ; z_N, σ_N) via ψ_B = A(z₁, · · · , z_N)ψ_F(z₁, σ₁; · · · ; z_N, σ_N) where A = Π₁≤j≤N sgn(z_j) is the same mapping function used originally [10, 11] and the spin z-component arguments σ_j take on the values ↑ and ↓. The N-fermion and N-boson Hamiltonians are both of the form ˆH_D = −(ℏ²/2m)J_j + ˆJ_J_j + ˆJ_J_j generalizing (4) and (7), where the linear operators ˆJ_j and ˆJ_J_j are defined on the Hilbert space of N-particle wave functions ψ by ˆJ_jψ = (1/2)|ψ⟩z_j = z{+} + |ψ⟩z_j = z{−} and ˆJ_J_jψ = (1/2)[∂/∂z_j]|ψ⟩z_j = z{±} − ∂/∂z_j|ψ⟩z_j = z{±}. On fermionic states ψ_F, ˆg_D^n and ˆg_D^o are ˆg_D^n_B and ˆg_D^o_B, whereas on the mapped bosonic states ˆψ_F = Ψ_F they are ˆg_D^n_B = ℏ²/µ²g_D^n_B and ˆg_D^o_B = ℏ²/µ²g_D^o_B.

V. N-PARTICLE GROUND STATE

Assume that both g_D^n_B ≥ 0 and g_D^o_B ≥ 0. If g_D^n_B is zero or negligible, then it follows from a theorem of Lieb and Mattis [22] that the fermionic ground state has total spin S = 0 (assuming N even), as shown in the spatially uniform case by Yang [23] and with longitudinal trapping by Ashcroft et al. [24]. If g_D^n_B is not negligible then the ground state may not have S = 0. In fact, if g_D^n_B is zero or negligible then one can apply a theorem of Eisenberg and Lieb [25] to the mapped spinor boson Hamiltonian, with the conclusion that the degenerate Bose ground state is totally spin-polarized, has S = N/2, and is the product of a symmetric spatial wave function ψ_B and a symmetric spin wave function. ψ_B is the ground state of the Lieb-Liniger gas [14, 15] which is known for all positive g_D^n_B (hence all positive mapped g_D^n_B) in the absence of longitudinal trapping. The inverse mapping then yields the N-fermion ground state, which has a totally space-antisymmetric and spin-symmetric wave function, which is (N + 1)-fold degenerate since S_z ranges from −N/2 to N/2. Define dimensionless bosonic and fermionic coupling constants by γ_B = mg_D^n_B/ℏ² and γ_F = mg_D^o_Bn/ℏ² where n is the longitudinal particle number density. They satisfy γ_Bγ_F = 4. The energy per particle ϵ is related to a dimensionless function ϵ(γ) available online [26] via ϵ = (ℏ²/2m)n²ϵ(γ) where γ is related to γ_F herein by γ = γ_F = 4/γ_F. This is plotted as a function of γ_F in Fig. 1. For g_D^n_B → ∞ as occurs at a p-wave Feshbach resonance, one has a “fermionic TG gas” [13] mapping to a zero-energy ideal Bose gas, a fermionic analog of the “TG gas” of impenetrable point bosons mapping to an ideal Fermi gas [1, 3, 7, 10, 11, 27]. Any S = 0 state has a higher energy in this case; in fact, for N > 2 the mapped Bose gas is partially space-antisymmetric, raising its energy by the exclusion principle.

In the presence of a uniform external magnetic field the directional degeneracy is lifted and the above N-particle state is the (now nondegenerate) ground state with field quantization direction parallel to the field, and the ground state energy is lowered by an amount Nµ_Bℏ/2 where µ_Bℏ/2 is the magnetic moment of each spin-1/2 atom.

So far we have considered only the extremes of an S = 0 ground state (large g_D^n_B) or one with S = N/2 (large g_D^n_B). The determination of the state of lowest energy for arbitrary values of these coupling constants is as yet
only partially solved, although we have recently obtained exact results for the phase diagram of ground-state total spin [28].

VI. RESPONSE TO A MAGNETIC FIELD GRADIENT

Suppose that the spinor Fermi gas is longitudinally trapped by an optical potential \( V_{\text{trap}} = \sum_j \frac{1}{2} \hbar^2 \omega_{\text{long}}^2 z_j^2 \), and that there is also a longitudinal magnetic field \( h(z) = cz \) with constant gradient \( c \), adding an interaction term \( V_{\text{space-spin}} = -\mu_B c \sum_j \hat{s}_j z_j \) to the \( N \)-particle Hamiltonian \( H^L_{D,e} \), where \( \hat{s}_j \) is the spin \( z \)-component operator for the \( j \)th particle. The space-spin interaction terms can be eliminated by a canonical transformation \( \hat{U}^{-1} \hat{s}_j \hat{U} = \hat{s}_j - \alpha \hat{s}_j z_j \), \( \hat{U}^{-1} \hat{p}_j \hat{U} = \hat{p}_j \), \( \hat{U}^{-1} \hat{s}_j \hat{U} = \hat{s}_j \) which leave the canonical commutation relations invariant. Noting that \( \hat{U}^{-1} V_{\text{space-spin}} \hat{U} = V_{\text{space-spin}} + \frac{1}{2} N \mu_B c \alpha \) and \( \hat{U}^{-1} V_{\text{trap}} \hat{U} = \sum_j \frac{1}{2} m \omega_{\text{long}}^2 (z_j - \alpha \hat{s}_j z_j)^2 \), one finds that the space-spin coupling terms cancel from \( \hat{U}^{-1} H^L_{D,e} \hat{U} \) with the choice \( \alpha = -\mu_B c / (m \omega_{\text{long}}^2) \), leading to a transformed Hamiltonian \( \hat{U}^{-1} H^B_{ID} \hat{U} = H^B_{ID}(c = 0) - N(\mu_B c)^2 / (8m \omega_{\text{long}}^2) \) where \( \hat{H}^B_{ID}(c = 0) \) does not include \( \hat{V}_{\text{space-spin}} \). The ground state \( \phi_{B0}(z_1, s_1; \cdots, z_N, s_N) \) of \( \hat{U}^{-1} H^B_{ID} \hat{U} \) is the same as that of \( H^B_{ID}(c = 0) \). The corresponding single-particle density \( n_0(z) \) is centered on \( z = 0 \). It is not known analytically in the presence of longitudinal trapping, but accurate numerical results have been calculated by a local density method [16]. In the presence of \( V_{\text{space-spin}} \) the single-particle density \( n(z) \) is \( \langle \phi_{B0}(\hat{U}^{-1} \hat{n}(z) \hat{U}) | \phi_{B0} \rangle \) where \( \hat{n}(z) = \sum_j \delta(z - z_j) \). The state \( | \phi_{B0} \rangle \) is a simultaneous eigenstate of the longitudinal spin operator \( \hat{S}_z = \sum_j \hat{s}_j z_j \), which has eigenvalues \( S_z = -N/2, -N + 1/2, \cdots, N - 1/2, N \). The ground state of \( H^B_{ID} \), which now includes \( V_{\text{space-spin}} \), is \( \hat{U} | \phi_{B0} \rangle \), and the \((N + 1)\)-fold degeneracy is not lifted by the magnetic field gradient so long as the magnetic field vanishes at \( z = 0 \). One has \( \hat{U}^{-1} \hat{U} = \hat{U}^{-1} \hat{n}(z) \hat{U} = \delta(z - z_j - \frac{\mu_B c}{m \omega_{\text{long}}^2} \hat{s}_j z_j) \), whose expectation value is \( N^{-1} n_0(z = 0) \) when the eigenvalue of \( \hat{s}_j \) is \( \pm \frac{1}{2} \), where \( z_0 = \frac{\mu_B c}{2m \omega_{\text{long}}^2} \). If the eigenvalue of \( \hat{S}_z \) is \( \pm \frac{1}{2} \), then \( wN \) of the \( \hat{s}_j \) have eigenvalue \( \frac{1}{2} \) and \((1 - w)N \) have eigenvalue \( -\frac{1}{2} \), where the fraction \( w \), which satisfies \( 0 \leq w \leq 1 \), is \( u = N - N \hat{S}_z + \frac{1}{2} \). It follows that the single-particle density \( n(z) \) in a ground state \( \hat{U} | \phi_{B0} \rangle \) with longitudinal spin \( \hat{S}_z \) is a weighted average of the extremal densities: \( n(z) = w n_0(z - z_0) + (1 - w) n_0(z + z_0) \). The ground state wave function of the corresponding spinor Fermi gas differs by a factor \( A \), the previously-given mapping function. It has the same longitudinal spin eigenvalues and same degeneracy, and since \( A^2 = 1 \) these fermionic ground states have the same density profiles as the bosonic ones.

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