Supplemental Material for "Itinerant ferromagnetism in 1D two-component Fermi gases"

Yuzhu Jiang,[1] D.V. Kurlov,[2] Xi-Wen Guan,[1,3] F. Schreck,[2] and G.V. Shlyapnikov[1,2,4,5]

[1] *State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China*
[2] *Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*
[3] *Department of Theoretical Physics, Research School of Physics and Engineering, Australian National University, Canberra ACT 0200, Australia*
[4] *LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France*
[5] *Russian Quantum Center, Novaya Street 100, Skolkovo, Moscow Region 143025, Russia*

In the Supplemental Material we first discuss the scattering of identical fermions in 1D, obtain the expression for the odd-wave off-shell scattering amplitude, and derive two-body and many-body contributions to the odd-wave interaction energy of a 1D Fermi gas. We then describe our calculation of the momentum distribution in the antiferro- and paramagnetic states.

Scattering amplitude in 1D. The off-shell scattering amplitude, defined by Eq.(2) of the main text, is the sum of the even-wave and odd-wave partial amplitudes:

$$f(k',k) = f_{even}(k',k) + f_{odd}(k',k), \tag{S.1}$$

where

$$f_{even}(k',k) = \int_{-\infty}^{\infty} dx' \cos k'x'\, V(x')\, \psi_{even}(k,x'), \quad f_{odd}(k',k) = -i\int_{-\infty}^{\infty} dx' \sin k'x'\, V(x')\, \psi_{odd}(k,x'), \tag{S.2}$$

and ψ_{even}, ψ_{odd} are the partial wavefunctions of the relative motion in the even-wave and the odd-wave channels, respectively. For $|k'| = |k|$ one has the on-shell amplitudes, which follow from Eq. (S.2) putting $k' = k$. These amplitudes enter the asymptotic expression for the wavefunction of the relative motion at interparticle separations $|x| \to \infty$ (see, e.g., [S1]):

$$\psi_k(x) = e^{ikx} - \frac{im}{2\hbar^2 k} e^{ik|x|}\big(f_{even}(k) + \mathrm{sign}(x) f_{odd}(k)\big). \tag{S.3}$$

In the quasi1D regime obtained by tightly confining the motion of particles in two directions to zero point oscillations, the on-shell scattering amplitude in the odd-wave channel was calculated in Ref. [S1], and it reads:

$$f_{odd}(k) = \frac{2\hbar^2}{m}\frac{k^2}{1/l_p + ik + \xi_p k^2}, \tag{S.4}$$

where parameters l_p and ξ_p are defined in the main text.

We now proceed with the derivation of the odd-wave off-shell scattering amplitude. The asymptotic form of the wavefunction $\psi_{odd}(k,x)$ at $|x| \to \infty$ can be written as

$$\psi_{odd}(k,x) \propto \mathrm{sign}(x) \sin\big(k|x| - \delta_{odd}(k)\big), \tag{S.5}$$

where $\delta_{odd}(k)$ is the scattering phase shift. The relation between the odd-wave phase shift and the corresponding scattering amplitude follows from Eq. (S.5) and the odd-wave part of Eq. (S.3):

$$f_{odd}(k) = \frac{2\hbar^2 k}{m}\frac{\tan\delta_{odd}(k)}{1 + i\tan\delta_{odd}(k)}, \tag{S.6}$$

with

$$\delta_{odd}(k) = \arctan\{l_p k / \big(1 + l_p \xi_p k^2\big)\}. \tag{S.7}$$

Let us rewrite the wavefunction of the odd-wave channel $\psi_{odd}(k,x)$ in the following form:

$$\psi_{odd}(k,x) = \frac{i\,\tilde{\psi}_{odd}(k,x)}{1 + i\tan\delta_{odd}(k)}, \tag{S.8}$$

where $\tilde{\psi}_{odd}(k,x) = \sin kx - \mathrm{sign}(x)\tan\delta_{odd}(k)\cos kx$ is real. Then, the odd-wave off-shell scattering amplitude can be represented as

$$f_{odd}(k',k) = \frac{\tilde{f}_{odd}(k',k)}{1 + i\tan\delta_{odd}(k)}, \tag{S.9}$$

where $\tilde{f}_{odd}(k',k)$ is also real:

$$\tilde{f}_{odd}(k',k) = \int_{-\infty}^{\infty} dx' \sin k'x' V(x')\tilde{\psi}_{odd}(k,x'). \tag{S.10}$$

Assuming that the phase shift is small, one obtains the following relation:

$$f_{odd}(k',k) = \tilde{f}_{odd}(k',k) - \frac{im}{2\hbar^2 k}\tilde{f}_{odd}(k',k)\tilde{f}_{odd}(k). \tag{S.11}$$

Substituting $k' = k$ into Eqs. (S.9)-(S.11) we obtain similar relations for the on-shell amplitudes $f_{odd}(k)$ and $\tilde{f}_{odd}(k)$. In the case of low-energy scattering we may put $\sin k'x' \approx k'x'$ and $\sin kx' \approx kx'$ in the expressions for $\tilde{f}_{odd}(k',k)$ and $\tilde{f}_{odd}(k)$, which shows that in the odd-wave channel one obtains the off-shell amplitude from the on-shell amplitude by simply replacing k in the first multiple of Eq. (S.6) with k'. Then, using Eqs. (S.6) and (S.9) we arrive at Eq. (**??**) of the main text for the odd-wave off-shell scattering amplitude $\tilde{f}_{odd}(k',k)$.

Two-body and many-body contributions to the interaction energy. An infinitely strong even-wave contact repulsion can be transferred to the boundary condition for the wavefunction. The interaction part of the Hamiltonian then contains only the odd-wave interaction, which in our case is present solely between ↑-state particles:

$$\hat{\mathcal{H}}_{int} = \frac{1}{2L}\sum_{k_1,k_2,q} V(q)\,\hat{a}^\dagger_{k_1+q}\hat{a}^\dagger_{k_2-q}\hat{a}_{k_2}\hat{a}_{k_1}, \tag{S.12}$$

where $\hat{a}^\dagger_k, \hat{a}_k$ are the creation and annihilation operators of ↑-fermions, and $V(q)$ is the Fourier transform of the interaction potential:

$$V(q) = \int_{-\infty}^{\infty} dx\, V(x)e^{-iqx}. \tag{S.13}$$

Then, the first-order correction is given by the diagonal matrix element of $\hat{\mathcal{H}}_{int}$:

$$E^{(1)} = \frac{1}{2L}\sum_{k_1,k_2}\left[V(0) - V(k_2 - k_1)\right] N(k_1)\, N(k_2)\,. \tag{S.14}$$

The second-order correction to the energy of a state $|j\rangle$ is given by

$$E^{(2)}_j = \sum_{m\neq j}\frac{V_{jm}V_{mj}}{E_j - E_m}, \tag{S.15}$$

where the summation is over the eigenstates of the non-interacting system, and the non-diagonal matrix element $V_{jm} = \langle m|\,\hat{\mathcal{H}}_{int}\,|j\rangle$ is related to the scattering of two particles from the initial state k_1, k_2 to an intermediate state k_1', k_2'. In our case, the symbol j corresponds to the ground state, and the symbol m to excited states. Then, taking into account the momentum conservation law $k_1 + k_2 = k_1' + k_2'$, we obtain the following expression for the quantity $V_{jm}V_{mj}$:

$$V_{jm}V_{mj} = \frac{1}{(2L)^2}\sum_{k_1,k_2}\left[V(k_1' - k_1) - V(k_2' - k_1)\right]\left[V(k_1 - k_1') - V(k_1 - k_2')\right] N(k_1)\, N(k_2)\left(1 - N(k_1')\right)\left(1 - N(k_2')\right),$$

and the second-order correction becomes:

$$E^{(2)} = \frac{1}{(2L)^2}\sum_{k_1,k_2,k_1'}\frac{\left[V(k_1' - k_1) - V(k_2' - k_1)\right]\left[V(k_1 - k_1') - V(k_1 - k_2')\right]}{\hbar^2(k_1^2 + k_2^2 - k_1'^2 - k_2'^2)/2m} N(k_1)\, N(k_2)\left(1 - N(k_1')\right)\left(1 - N(k_2')\right). \tag{S.16}$$

It is evident that the second-order correction diverges at large k_1' because of the term proportional to $N(k_1)\,N(k_2)$. This artificial divergence can be eliminated if one expresses $E^{(1)}$ and $E^{(2)}$ in terms of a real physical quantity — the scattering amplitude. The relation between the Fourier component of the interaction potential and the off-shell scattering amplitude is given by [S2]

$$f(k',k) = V(k'-k) + \frac{1}{L}\sum_{k''}\frac{V(k'-k'')f(k'',k)}{E_k - E_{k''} + i0}, \tag{S.17}$$

where $k=(k_1-k_2)/2$, $k'=(k_1'-k_2')/2$, and $k''=(k_1''-k_2'')/2$ are relative momenta, E_k and $E_{k''}$ are relative collision energies, and we have $E_k - E_{k''} = \hbar^2(k^2-k''^2)/m = \hbar^2(k_1^2+k_2^2-k_1''^2-k_2''^2)/2m$, with k_1, k_2 (k_1'', k_2'') being the momenta of colliding particles in the initial (intermediate) state. Equation (S.17) allows us to rewrite the first-order correction as

$$E^{(1)} = \frac{1}{2L}\sum_{k_1,k_2}[f(k,k)-f(-k,k)]\,N(k_1)\,N(k_2) - \frac{1}{2L^2}\sum_{k_1,k_2,k'}\frac{[V(k-k')-V(-k-k')]\,f(k',k)}{\hbar^2(k^2-k'^2+i0)/m}N(k_1)\,N(k_2)\,. \tag{S.18}$$

In the second term of Eq. (S.18) we represent $f(k',k)$ according to Eq. (S.1) and keep only the odd-wave part $f_{odd}(k',k)$, because the quantity $[V(k-k')-V(-k-k')]$ is odd in k', and the terms containing $f_{even}(k',k)$ vanish after the integration over dk'. Then, we replace the Fourier components by the exact scattering amplitudes, which gives $[V(k-k')-V(-k-k')] = [f(k,k')-f(-k,k')] = 2f_{odd}(k,k')$, and the first-order correction becomes:

$$E^{(1)} = \frac{1}{L}\sum_{k_1,k_2} f_{odd}(k)N(k_1)\,N(k_2) - \frac{1}{L}\sum_{k_1,k_2}N(k_1)\,N(k_2)\int_{-\infty}^{\infty}\frac{dk'}{2\pi}\frac{m}{\hbar^2}\frac{f_{odd}(k',k)f_{odd}(k,k')}{k^2-k'^2+i0}. \tag{S.19}$$

The contribution of the pole at $k'=k$ to the integral in Eq. (S.19) gives $-imf_{odd}^2(k)/2\hbar^2 k$ for each term in the sum over k_1, k_2, and we can use here $\tilde{f}_{odd}(k)$ instead of $f_{odd}(k)$. At the same time, the second term of the right hand side of Eq. (S.11), being substituted into the first term of Eq. (S.19), cancels the contribution of the pole in the second term of Eq. (S.19). Therefore, we use the amplitude $\tilde{f}_{odd}(k)$ in the first term of Eq. (S.19) and take the principal value of the integral in the second term. This leads to the following expression for the first-order correction:

$$E^{(1)} = \frac{1}{L}\sum_{k_1,k_2}\tilde{f}_{odd}(k)N(k_1)\,N(k_2) - \frac{1}{L^2}\sum_{k_1,k_2,k_1'}\frac{2m}{\hbar^2}\frac{\tilde{f}_{odd}(k',k)\tilde{f}_{odd}(k,k')}{k_1^2+k_2^2-k_1'^2-k_2'^2}N(k_1)\,N(k_2)\,. \tag{S.20}$$

The second-order correction can also be expressed in terms of the scattering amplitude. Taking into account that $V(k_1'-k_1) = V(k'-k)$ and $V(k_2'-k_1) = V(-k-k')$, we write

$$[V(k_1'-k_1)-V(k_2'-k_1)][V(k_1-k_1')-V(k_1-k_2')] = [V(k-k')-V(k')]\,[V(k'-k)-V(-k-k')] = 4f_{odd}(k',k)f_{odd}(k,k').$$

Then for the second-order correction we obtain:

$$E^{(2)} = \frac{1}{L^2}\sum_{k_1,k_2,k_1'}\frac{2m}{\hbar^2}\frac{f_{odd}(k',k)f_{odd}(k,k')}{k_1^2+k_2^2-k_1'^2-k_2'^2}N(k_1)\,N(k_2)\left(1-N(k_1')\right)\left(1-N(k_2')\right), \tag{S.21}$$

where we may use the amplitudes $\tilde{f}_{odd}(k',k)$ and $\tilde{f}_{odd}(k,k')$ because the contribution of $\tan\delta_{odd}(k)$ in the denominator of Eq. (S.9) is negligible. Then, the divergent term proportional to $N(k_1)\,N(k_2)$ in Eq. (S.21) and the (divergent) second term of Eq. (S.20) exactly cancel each other. Note that in Eq. (S.21) the term proportional to the product of four occupation numbers vanishes, since its numerator is symmetrical and the denominator is antisymmetrical with respect to an interchange of k_1, k_2 and k_1', k_2'. Two terms containing the product of three occupation numbers are equal to each other, because the expression (S.21) for $E^{(2)}$ is symmetrical with respect to an interchange of k_1' and k_2'. Therefore, the sum of the first- and second-order corrections can be written as $E^{(1)}+E^{(2)} = \tilde{E}^{(1)}+\tilde{E}^{(2)}$, where $\tilde{E}^{(1)}$ and $\tilde{E}^{(2)}$ are given by

$$\tilde{E}^{(1)} = \frac{1}{L}\sum_{k_1,k_2}\tilde{f}_{odd}(k)N(k_1)\,N(k_2) = \frac{2\hbar^2}{mL}\sum_{k_1,k_2}\frac{l_p k^2}{1+l_p\xi_p k^2}N(k_1)\,N(k_2)\,, \tag{S.22}$$

$$
\begin{aligned}
\tilde{E}^{(2)} &= -\frac{1}{L^2}\sum_{k_1,k_2,k'_1}\frac{4m}{\hbar^2}\frac{\tilde{f}_{odd}(k',k)\tilde{f}_{odd}(k,k')}{k_1^2+k_2^2-k_1'^2-k_2'^2}N(k_1)\,N(k_2)\,N(k'_1)\\
&= -\frac{16\hbar^2}{mL^2}\sum_{k_1,k_2,k'_1}\frac{l_p^2\,k'^2k^2}{k_1^2+k_2^2-k_1'^2-k_2'^2}\,\frac{N(k_1)\,N(k_2)\,N(k'_1)}{(1+l_p\xi_p k'^2)(1+l_p\xi_p k^2)}.
\end{aligned}
\tag{S.23}
$$

We then reduce Eqs. (S.22) and (S.23) to equations (6)-(9) of the main text.

Momentum distributions for the antiferro- and paramagnetic states. The momentum distribution functions $N_\uparrow(k)$ and $N_\downarrow(k)$ for the antiferro- and paramagnetic states can be calculated from the Bethe Ansatz wave functions of the Yang-Gaudin model with an infinite repulsion. To this end, we will use the method proposed by Ogata and Shiba [S3]. The one-dimensional two-component Fermi gas with contact interactions is described by the Hamiltonian [S4, S5] $\hat{H}=-\sum_{i=1}^N\partial^2/\partial x_i^2+2c\sum_{i<j}\delta(x_i-x_j)$, where $c=mg_{1\mathrm{D}}/\hbar^2$ is the interaction strength for the even-wave scattering. The Bethe Ansatz wavefunction for this model is given by [S5]

$$
\Psi_{\boldsymbol{\sigma}}(\boldsymbol{x})=\sum_{\mathcal{QP}}\Theta(\mathcal{Q})\boldsymbol{A}(\mathcal{Q},\mathcal{P})\mathrm{e}^{\mathrm{i}\sum_j k_{\mathcal{P}_j}x_{\mathcal{Q}_j}},
\tag{S.24}
$$

where $\mathcal{Q}=(Q1,Q2,\ldots,QN)$ and $\mathcal{P}=(P1,P2,\ldots,PN)$ are two permutations of integers $\{1,2,\cdots,N\}$ and $\Theta(\mathcal{Q})$ denotes the step function, i.e. $\Theta(\mathcal{Q})=\theta(x_{\mathcal{Q}_2}-x_{\mathcal{Q}_1})\theta(x_{\mathcal{Q}_3}-x_{\mathcal{Q}_2})\cdots\theta(x_{\mathcal{Q}_N}-x_{\mathcal{Q}_{N-1}})$ with $\theta(x)=1$ for $x>0$ whereas $\theta(x)=0$ for $x<0$. In the above equations, we denoted $\boldsymbol{x}=\{x_1,x_2,\cdots,x_N\}$, $\boldsymbol{\sigma}=\{\sigma_1,\sigma_2,\cdots,\sigma_N\}$, and $\boldsymbol{A}=A_{\sigma_1\cdots\sigma_N}(\mathcal{Q},\mathcal{P})$ are superposition coefficients. Here $\sigma_j=\pm1/2$ stand for the spin projection of the j-th particle.

For periodic boundary conditions the wavenumbers $\{k_j\}$ with $j=1,2\ldots,N$ are subject to the following Bethe Ansatz equations (BAE):

$$
\begin{aligned}
\mathrm{e}^{\mathrm{i}k_jL} &= \prod_{i=1}^{M}\frac{k_j-\mu_i+\mathrm{i}c/2}{k_j-\mu_i-\mathrm{i}c/2},\\
\prod_{j=1}^{N}\frac{\mu_i-k_j-\mathrm{i}c/2}{\mu_i-k_j+\mathrm{i}c/2} &= -\prod_{i'=1}^{M}\frac{\mu_i-\mu_{i'}-\mathrm{i}c}{\mu_i-\mu_{i'}+\mathrm{i}c}.
\end{aligned}
\tag{S.25}
$$

Here M is the number of down-spin fermions, and μ_i with $i=1,\ldots,M$ are spin rapidities.

We observe that the BAE (S.25) decouple into two parts in terms of charge and spin degrees of freedom as $c\to\infty$. The second set of equations in the BAE (S.25) reduces to the BAE for the spin-1/2 Heisenberg XXX model with the scaling $\mu_\alpha\to\mu_\alpha c$. In this limit, the wavefunction (S.24) can be simplified as

$$
\Psi_{\boldsymbol{\sigma}}(\boldsymbol{x})=\sum_{\mathcal{QP}}(-1)^{\mathcal{Q}+\mathcal{P}}\Phi\left(y_1,\ldots,y_M\right)\mathrm{e}^{\mathrm{i}\sum_j k_{\mathcal{P}_j}x_{\mathcal{Q}_j}}.
\tag{S.26}
$$

Here $\Phi\left(y_1,\ldots,y_M\right)$ is the eigenstate of the spin XXX model with M down-spins in the N-site lattice [S3, S5].

Using the wavefunction (S.26), we first calculate the momentum distribution in an analytical fashion. Then the final momentum distributions can be obtained by further numerical calculation. The momentum distribution is defined as $\mathcal{N}_\sigma(k)=\langle\hat{\psi}^\dagger_\sigma(k)\hat{\psi}_\sigma(k)\rangle$, which is the Fourier transform of the density matrix $\mathcal{N}_\sigma(k)=\iint\mathrm{d}y\mathrm{d}y'\mathcal{N}_\sigma(y',y)\mathrm{e}^{\mathrm{i}k(y-y')}$. The density matrix is given by

$$
\mathcal{N}_\sigma(y',y)=\langle\psi^\dagger_\sigma(y')\psi_\sigma(y)\rangle=N!\int_0^{x_3}\mathrm{d}x_2\int_0^{x_4}\mathrm{d}x_3\cdots\int_0^{x_N}\mathrm{d}x_{N-1}\int_0^{L}\mathrm{d}x_N\sum_{\sigma_2\cdots\sigma_N}\Psi^*_{\boldsymbol{\sigma}}(\boldsymbol{x}^{(l)})\Psi_{\boldsymbol{\sigma}}(\boldsymbol{x}^{(r)}),
\tag{S.27}
$$

where we used the following notations:

$$
\boldsymbol{x}^{(l)}=\{y',x_2,x_3,\cdots,x_N\},\;\;\boldsymbol{x}^{(r)}=\{y,x_2,x_3,\cdots,x_N\},\;\;\boldsymbol{\sigma}=\{\sigma,\sigma_2,\sigma_3,\cdots,\sigma_N\}.
\tag{S.28}
$$

In the limit $c\to\infty$, the superposition coefficients satisfy the relations [S3]:

$$
\vec{\boldsymbol{A}}(\mathcal{Q}^{(ab)},\mathcal{P}^{(ab)})=\hat{P}_{ab}\vec{\boldsymbol{A}}(\mathcal{Q}^{(ba)},\mathcal{P}^{(ba)}),\;\;\vec{\boldsymbol{A}}(\mathcal{Q}^{(ab)},\mathcal{P}^{(ab)})=-\vec{\boldsymbol{A}}(\mathcal{Q}^{(ab)},\mathcal{P}^{(ba)}),
$$

where

$$
\mathcal{Q}^{(ab)}=\{\mathcal{Q}_1,\mathcal{Q}_2,\cdots,\mathcal{Q}_a,\mathcal{Q}_b,\cdots,\mathcal{Q}_N\},\;\;\mathcal{Q}^{(ba)}=\{\mathcal{Q}_1,\mathcal{Q}_2,\cdots,\mathcal{Q}_b,\mathcal{Q}_a,\cdots,\mathcal{Q}_N\}.
$$

Substituting the wave function (S.26) into (S.27), the density matrix is thus rewritten as

$$\mathcal{N}_\sigma(y',y) = N!\int_0^{x_3}\mathrm{d}x_2\int_0^{x_4}\mathrm{d}x_3\cdots\int_0^{L}\mathrm{d}x_N\sum_{\mathcal{P},\mathcal{P}'}(-1)^{\mathcal{P}'+\mathcal{P}+\mathcal{Q}+\mathcal{Q}'}\mathrm{e}^{-\mathrm{i}\sum_{j=1}^{N}k_{\mathcal{P}'_j}x^{(l)}_{\mathcal{Q}'}}\mathrm{e}^{\mathrm{i}\sum_{j=1}^{N}k_{\mathcal{P}_j}x^{(l)}_{\mathcal{Q}}}$$
$$\times\sum_{\sigma_2,\cdots,\sigma_N}\left[\boldsymbol{A}^\dagger\boldsymbol{\beta}^\dagger(\mathcal{Q}')\right]_{\sigma,\sigma_2,\cdots,\sigma_N}\left[\boldsymbol{\beta}(\mathcal{Q})\boldsymbol{A}\right]_{\sigma,\sigma_2,\cdots,\sigma_N}. \tag{S.29}$$

Here the positions y and y' in the domain $x_2<\cdots<x_N$ satisfy two inequalities:

$$x_2<x_3<\cdots<x_\eta<y'<x_{\eta+1}<\cdots<x_N,$$
$$x_2<x_3<\cdots<x_\xi<y<x_{\xi+1}<\cdots<x_N.$$

Accordingly, the permutations $\mathcal{Q}$ and $\mathcal{Q}'$ are given by

$$\mathcal{Q}'=\{2,3,\cdots,\eta,1,\eta+1,\cdots,N\},\ \ \mathcal{Q}=\{2,3,\cdots,\xi,1,\xi+1,\cdots N\}. \tag{S.30}$$

The values of η and ξ are fixed by the values of y and y' in the set of $\{x_j\}$ with $j=2,3,\cdots,N$. In equation (S.29) we define the operator $\boldsymbol{\beta}$ as

$$\boldsymbol{\beta}(\mathcal{Q}')=\hat{P}_{\eta,1}\hat{P}_{\eta-1,1}\cdots\hat{P}_{3,1}\hat{P}_{2,1}, \tag{S.31}$$
$$\boldsymbol{\beta}(\mathcal{Q})=\hat{P}_{\xi,1}\hat{P}_{\xi-1,1}\cdots\hat{P}_{3,1}\hat{P}_{2,1}. \tag{S.32}$$

Where $\hat{P}_{i,j}$ is the permutation operator.

Defining an identity order $\mathbb{1}=\{1,2,\cdots,N\}$ for the permutation operator, we find that $\boldsymbol{\beta}(\mathcal{Q}')\mathbb{1}=\mathcal{Q}'$ and $\boldsymbol{\beta}(\mathcal{Q})\mathbb{1}=\mathcal{Q}$. In Eq. (S.29) the superposition coefficient $\boldsymbol{A}\equiv\boldsymbol{A}(\mathbb{1},\mathbb{1})$ is an eigenstate of the XXX Heisenberg spin chain, i.e. $H_{\rm xxx}\boldsymbol{A}=E_{\rm xxx}\boldsymbol{A}$. It has C_N^M components of spin wavefunction for each $\mathcal{Q}$. Each of them is characterized by the coordinates of M down-spins. In the following, we use the eigenstate of the Heisenberg spin chain to evaluate the integral in Eq. (S.29). For convenience, we denote that

$$w^\sigma_{\eta,\xi}=\boldsymbol{A}^\dagger\hat{\boldsymbol{W}}_\sigma\boldsymbol{A}=\sum_{\sigma_2,\cdots,\sigma_N}\left[\boldsymbol{A}^\dagger\boldsymbol{\beta}^\dagger(\mathcal{Q}')\right]_{\sigma,\sigma_2,\cdots,\sigma_N}\left[\boldsymbol{\beta}(\mathcal{Q})\boldsymbol{A}\right]_{\sigma,\sigma_2,\cdots,\sigma_N},$$

with

$$\hat{\boldsymbol{W}}_\sigma=\hat{n}^\sigma_\xi\hat{P}_{\xi,\xi+1}\hat{P}_{\xi+1,\xi+2}\cdots\hat{P}_{\eta-1,\eta}. \tag{S.33}$$

Thus $w^\sigma_{\eta,\xi}$ can be regarded as the expectation value of the operator $\hat{\boldsymbol{W}}_\sigma$ of the XXX spin chain. In the above equation we also denoted the operators $\hat{n}^\uparrow=\hat{\sigma}_+\hat{\sigma}_-$, $\hat{n}^\downarrow=\hat{\sigma}_-\hat{\sigma}_+$. By using the above notations, the density matrix is rewritten as

$$\mathcal{N}_\sigma(y',y)=N!\int_0^{x_3}\mathrm{d}x_2\int_0^{x_4}\mathrm{d}x_3\cdots\int_0^{L}\mathrm{d}x_N\,w^\sigma_{\eta,\xi}\sum_{\mathcal{P},\mathcal{P}'}(-1)^{\mathcal{P}'+\mathcal{P}+\mathcal{Q}+\mathcal{Q}'}\,\mathrm{e}^{-\mathrm{i}\sum_{j=1}^{N}k_{\mathcal{P}'_j}x^{(l)}_{\mathcal{Q}'}}\mathrm{e}^{\mathrm{i}\sum_{j=1}^{N}k_{\mathcal{P}_j}x^{(l)}_{\mathcal{Q}}}. \tag{S.34}$$

Due to the translational symmetry of the system, it is convenient to introduce $x=y-y',\ \tau=|\eta-\xi|$ and $w^\sigma_{\eta,\xi}=w^\sigma_\tau$. Then the density matrix is simplified as

$$\mathcal{N}_\sigma(x)=N!\,\mathrm{e}^{\mathrm{i}k_0x}\sum_{i,j}^{N}(-1)^{i+j}\mathrm{e}^{\mathrm{i}\Delta kI_jx}\sum_{Q}(-1)^{Q}f_m(x)\prod_{i=1}^{n}\frac{1-\mathrm{e}^{-\mathrm{i}d_i\Delta kx}}{-\mathrm{i}d_i\Delta k}, \tag{S.35}$$

The quantities f_m, d_i, and Δk used in (S.35) are explained below.

In the ground state the quasi-momenta take the following values [S3]:

$$k_j=I_j\Delta k+k_0,\quad \Delta k=\frac{2\pi}{L},$$
$$I_j=-\frac{N-1}{2},-\frac{N-3}{2},\cdots,\frac{N-1}{2}. \tag{S.36}$$

It is worth noting that the quantum numbers I_j are different form the quantum numbers defined in the usual Bethe Ansatz equations [S3]. This notation is convenient for our calculation. The index i (j) in Eq. (S.35) indicates the quasi-momentum of the i-th (j-th) particle which is separated from other k's, i.e.

$$\{k_1,k_2,\cdots,k_{i-1},k_{i+1},\cdots,k_N\},\ \ \{k_1,k_2,\cdots,k_{j-1},k_{j+1},\cdots,k_N\}. \tag{S.37}$$

The corresponding quantum numbers of these two sets of k's read

$$\mathcal{I} = \{I_1, I_2, \cdots, I_{i-1}, I_{i+1}, \cdots, I_N\}, \;\; \mathcal{J} = \{J_1, J_2, \cdots, J_{j-1}, J_{j+1}, \cdots, J_N\}. \tag{S.38}$$

For fixing the first set of quantum numbers $\mathcal{I}$, there are $(N-1)!$ permutations Q for the second set $\mathcal{J}$. The summation of Q in Eq. (S.35) is carried out for $(N-1)!$ permutations. Each of these permutations gives a set of d's

$$\{d'_1, \cdots, d'_{N-1}\} = \mathcal{I} - Q\mathcal{J}. \tag{S.39}$$

Assuming that there are m zero elements in the set $\{d'_1, \cdots\}$ we have $n = N - 1 - m$ nonzero d's. We denote the nonzero ones as $\{d_1, d_2, \cdots, d_n\}$. The function $f_m(x)$ introduced in (S.35) is derived explicitly:

$$f_m(x) = \sum_{\tau=0}^{N-1} w_\tau^\sigma (-1)^\tau \sum_{t=0}^{\tau} C_m^j C_n^{\tau-t} (L-x)^t (-x)^{m-t}, \tag{S.40}$$

where C_b^a stands for the combinatory. This is the key simplification of the momentum distribution (S.34).

In the main text, we presented the interaction energy of the ferro- and non-ferromagnetic states, calculated through the corresponding momentum distribution functions. For the antiferromagnetic state, the momentum distribution function (S.35) can be calculated by using the corresponding ground state wave function of the XXX spin chain model, denoted as $\boldsymbol{A}_{\rm anti}$. We performed our calculation from the Bethe Ansatz roots of the XXX spin chain with a finite size and finite number of down-spins.

The paramagnetic state is more peculiar. It is a mixed state which consists of all possible spin states classified by the total spin of the system [S6, S7]. We denote the ferromagnetic state of the XXX spin chain as $\boldsymbol{A}_{\rm ferro}^{(m)} \propto (\hat{\boldsymbol{S}}^-)^m|0\rangle$ with $m = 0, 1, \cdots N$. Here the state $|0\rangle = |\uparrow, \uparrow, \cdots, \uparrow\rangle$ is the highest state and the total spin operator is given by $\hat{\boldsymbol{S}}^- = \hat{\boldsymbol{S}}_1^- + \hat{\boldsymbol{S}}_2^- + \cdots + \hat{\boldsymbol{S}}_N^-$. Each state $\boldsymbol{A}_{\rm ferro}^{(m)}$ gives rise to the density matrix $n_{\rm ferro}^{(m)}(x)$. Here we chose the state with zero spin projection, i.e., $S_z = 0$, as the ferromagnetic state. In the main text, the momentum distribution of the ferromagnetic state refers to $n_{\rm ferro}^{(N/2)}(x)$. For the paramagnetic state, we have to consider a mixed state that contains all possible spin configurations for the spin chain, i.e. using all the eigenstates $\boldsymbol{A}_m$ with $m = 1, 2, \cdots 2^N$. The corresponding density matrix is denoted as $n_m(x)$. Then the density matrix for the paramagnetic state is equally weighted as $n_{\rm para}(x) = \sum_m n_m(x)/2^N$.

The kinetic energy obtained by using the calculated non-ferromagnetic distributions directly in Eq. (1) of the main text differs from E_{kin} by less than 0.3% in the antiferromagnetic phase and by approximately 0.5% in the paramagnetic phase.

[S1] L. Pricoupenko, Phys. Rev. Lett. **100**, 170404 (2008).
[S2] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics, Non-Relativistic Theory* (Butterworth-Heinemann, Oxford, 1999).
[S3] M. Ogata and H. Shiba, Phys. Rev. B **41**, 2326 (1990).
[S4] M. Gaudin, Phys. Lett. A **24**, 55 (1967).
[S5] C.-N.Yang, Phys. Rev. Lett. **19**, 1312 (1967).
[S6] E. Eisenberg and E. H. Lieb, Phys. Rev. Lett. **89**, 220403 (2002).
[S7] X.-W. Guan, M. T. Batchelor, and M. Takahashi, Phys. Rev. A **76**, 043617 (2007).