Spectral-edge mode in interacting one-dimensional systems

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Spectral-edge mode in interacting one-dimensional systems

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A continuum of excitations in interacting one-dimensional systems is bounded from below by a spectral edge that marks the lowest possible excitation energy for a given momentum. We analyze short-range interactions between Fermi particles and between Bose particles (with and without spin) using Bethe-ansatz techniques and find that the dispersions of the corresponding spectral edge modes are close to a parabola in all cases. Based on this emergent phenomenon we propose an empirical model of a free, nonrelativistic particle with an effective mass identified at low energies as the bare electron mass renormalized by the dimensionless Luttinger parameter K (or K_σ for particles with spin). The relevance of the Luttinger parameters beyond the low-energy limit provides a more robust method for extracting them experimentally using a much wider range of data from the bottom of the one-dimensional band to the Fermi energy. The empirical model of the spectral edge mode complements the mobile impurity model to give a description of the excitations in proximity of the edge at arbitrary momenta in terms of only the low-energy parameters and the bare electron mass. Within such a framework, for example, exponents of the spectral function are expressed explicitly in terms of only a few Luttinger parameters.

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I. INTRODUCTION

The low-energy properties of interacting particles in one dimension are well described by the Tomonaga-Luttinger model [1] based on the linear approximation to the spectrum of the excitation at the Fermi energy. In this framework various correlation functions that involve a continuum of many-body excitations can be evaluated explicitly resulting in a common power-law behavior—in contrast to higher dimensions where the Fermi gas approximation with renormalized parameters (the Fermi liquid model) [2] remains robust. In the last few decades different experimental realizations of one-dimensional geometries were developed: carbon nanotubes [3], cleaved edge [4] or gated [5] one-dimensional channels in semiconductor heterostructures, and cold atomic gases in cigar-shaped optical lattices [6] where the predictions of the low-energy theory [7] have already been observed and measurements of high-energy effects are already possible.

Recently, a new theoretical understanding of the behavior at high energies was achieved by making a connection between the features of the dynamical response of the one-dimensional systems and the Fermi edge singularity in x-ray scattering in metals [8]. Application of the mobile impurity model [9] to the Tomonaga-Luttinger model gives a description of excitations at high energies incorporating dispersion of the spectral edge as an input parameter; the edge marks the smallest excitation energy at a fixed momentum. Within the resulting theory correlation functions exhibit a common power-law behavior where exponents are related to the curvature of the spectral edge and the Luttinger parameters [10–13]. However, the theory for the edge mode itself remains an open problem.

In this paper we analyze fundamental models of Fermi and Bose particles with short-range interactions (with and without spin) in one dimension using the available diagonalization methods based on Bethe ansatz. We investigate the edge mode of the spectral function—a dynamical response function that generalizes the single-particle spectrum to the many-particle systems—and find that its dispersion is close to a parabola for all cases in the thermodynamic limit [14]. It is exactly parabolic for fermions without spin and the biggest deviation ($\lesssim$20%) occurs for fermions with spin and a very large interaction potential. Based on this result we propose an empirical model of a free, nonrelativistic particle for the spectral edge mode, which describes a charge wave in the spinless case and a spin wave in the spinful case (see a graphical representation of the spectral function in Fig. 1). The effective mass m^* is identified at low energies as the bare electron mass m strongly renormalized by the dimensionless Luttinger parameter; $m^*/m = K$ and $m^*/m = K_\sigma$ in the spinless and the spinful case, respectively. The position of the edge of the spectral function in terms of this empirical model can

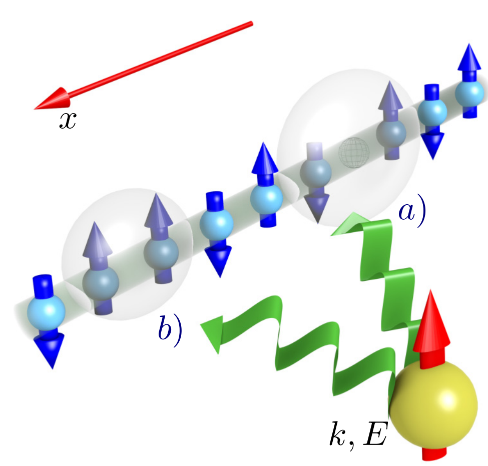

FIG. 1. (Color online) A schematic representation of a tunneling process into a one-dimensional system for a particle with fixed momentum k and energy E that is described by the spectral function. Excitations of the system are (a) density waves or [(a) and (b)] spin wave for particles with spin.

be expressed as

$$\varepsilon_{\text{edge}}(k) = \mu + \frac{k_F^2}{2m^*} - \frac{(k-k_0)^2}{2m^*}, \quad (1)$$

where μ is the chemical potential, k_F is the Fermi momentum, and $k_0 = 0$ (k_F) for Fermi (Bose) particles.

The empirical model in Eq. (1) breaks down when the effective mass becomes infinite. At low energies $m^* = \infty$ is equivalent to zero sound velocity of the collective modes $v(v_\sigma)$. The characteristic threshold is given by the quantum of the momentum $v_1 = 2\pi/(mL)$ in a system of a finite size L. For slower velocities $v(v_\sigma) \lesssim v_1$ the dispersion of the spectral edge mode is not parabolalike and is not universal.

The parabolic shape of the spectral edge mode, which we obtain in microscopic calculations for different models, can be interpreted as emergence of "translational invariance." The kinetic energy of a single free particle is a parabolic function of its momentum, enforced by the translational symmetry. Finite system size discretizes the boosts for changing inertial frames of reference in quanta of $2\pi/L$. For a system consisting of N particles the minimal boost of $2\pi N/L$ corresponds to the $2k_F$ periodicity in the momentum space; note that interaction potentials are also Galilean invariant. However, the total momentum of the whole many-particle system is still quantized in the units of $2\pi/L$ that can be facilitated by giving a boost to only a fraction of the particles $j < N$. The state on the spectral edge with the momentum $k = 2\pi j/L$ corresponds to a hole left between $N - j$ particles in the rest frame and j particles which have received the minimal boost (see Sec. III for details). The effective mass of the holelike quasiparticle is strongly renormalized by interactions since a partial boost is not a Galilean invariant transformation. However, the parabolic dependence of the hole energy on momentum—which is analogous to the kinetic energy of a free particle—is common for different microscopic models thus it is an emergent phenomenon.

Excitations above the spectral edge are well described at high energies by the application of the mobile impurity model to the Tomonaga-Luttinger theory which incorporates the curvature of the spectral edge as an input parameter [15]. The result in Eq. (1) removes this arbitrary input complementing the model above. Within such a framework, for example, the edge exponents of the spectral function are expressed explicitly in terms of only a few Luttinger parameters and the bare electron mass that provides a systematic way to classify them for a wide range of microscopic parameters.

The rest of the paper is organized as follows. Section II describes the model of one-dimensional particles interacting via short-range potentials, the corresponding spectral function, and discusses their general properties. In Sec. III we evaluate momentum dependence of the spectral edge mode using the Bethe-ansatz approach for Fermi particles in the fundamental region. Section IV contains the effective field theory for excitations above the spectral edge and calculates the edge exponents of the spectral functions using the dispersion of the spectral edge mode itself obtained in Sec. III. In Sec. V we show that Bose particles have the same parabolic dispersion, with the mass renormalized by the same Luttinger parameter K of the spectral edge mode as the Fermi particles. In Sec. VI we summarize the results and discuss experimental implications.

II. MODEL

We consider particles in one dimension interacting via a contact two-body potential U as

$$H = \int_{-L/2}^{L/2} dx \left(-\frac{1}{2m} \psi_\alpha^\dagger(x) \Delta \psi_\alpha(x) - U L \rho(x)^2 \right), \quad (2)$$

where $\psi_\alpha(x)$ are the field operators of Fermi or Bose particles at point x (with a spin $\alpha = \uparrow, \downarrow$ for spinful particles), $\rho(x) = \psi_\alpha^\dagger(x)\psi_\alpha(x)$ is the particle density operator, L is the size of the system, and m is the bare mass of a single particle. Below we consider periodic boundary conditions, $\psi_\alpha(x+L) = \psi_\alpha(x)$, to maintain the translational symmetry of the finite length system, restricting ourselves to repulsive interaction only, $U > 0$, and we assume $\hbar = 1$.

The spectrum of excitations in the many-body case is given by the spectral function which describes the response of a strongly correlated system to a single-particle excitation at energy ε and momentum k, $A_\alpha(k,\varepsilon) = -\text{Im}\, G_{\alpha\alpha}(k,\varepsilon)\text{sgn}(\varepsilon - \mu)/\pi$, where μ is a chemical potential and $G_{\alpha\beta}(k,\varepsilon) = -i \int dx\, dt e^{i(kx-\varepsilon t)} \langle T(e^{-iHt}\psi_\alpha(x)e^{iHt}\psi_\beta(0))\rangle$ is a Fourier transform of Green function at zero temperature. To be specific, we discuss particlelike excitations, $\varepsilon > \mu$. The spectral function in this domain reads [16]

$$A_\alpha(k,\varepsilon) = \sum_f |\langle f|\psi_\alpha^\dagger(0)|0\rangle|^2 \delta(\varepsilon - E_f + E_0)\delta(k - P_f), \quad (3)$$

where E_0 is the energy of the ground state $|0\rangle$, and P_f and E_f are the momenta and the eigenenergies of the eigenstate $|f\rangle$; all eigenstates are assumed normalized.

Galilean invariance defines a fundamental region for the spectrum of excitations on the momentum axis. A minimal boost for changing an inertial frame of reference for N particles is $2\pi N/L$ which is twice the Fermi momentum $k_F = \pi N/L$. In momentum space this boost corresponds to $2k_F$ periodicity. We choose the fundamental region as $-k_F < k < k_F$ for the Fermi and as $0 < k < 2k_F$ for Bose particles.

Under a $2k_F$ translation, the form factors in Eq. (3) do not change and the energies acquire simple shifts. The interaction term in Eq. (2) is invariant under the transformation $x \to x + 2\pi t j/(mL)$, where j is the number of the translation quanta, since the latter can be absorbed into a change of the integration variable. The transformation of the momentum operator, $-i\nabla \to -i\nabla + 2\pi j/L$, in the the kinetic term results in a constant energy shift, $E \to E + 2\pi j P/(mL) + 2\pi^2 j^2 N/(mL^2)$, of the Hamiltonian but keeps its matrix structure, and therefore, eigenstates unaltered. Thus the spectral function can be extended to arbitrary momenta by simultaneous translation of the momentum and of the energy variables starting from the fundamental region.

Here, we are concerned with a distinctive feature of the spectral function—the edge that marks the lowest possible excitation energy for a given momentum. To identify its location we need to obtain only the many-body spectrum of the model due to a singularity [15] that guarantees large values of the form factors in the proximity of the spectral edge. The two δ functions in Eq. (3) directly map the total momenta P_f

and the eigenenergies E_f of all many-body states $|f\rangle$ into the points of the spectral function k and ε. We are going to identify the states that have the smallest energy for each momentum and study how the dispersion of the spectral edge mode, which they form, depends on the interaction strength.

III. FERMIONS

A. Spinless

The zero range profile of two-body interaction potential in the model in Eq. (2) has zero matrix elements for the Fermi particles without spin due to the Pauli exclusion principle. A model of interactions in this case requires a finite range of interactions which is usually introduced by the point-splitting technique [17] developed to address the problem in the low-energy limit. Here we will use a different approach of introducing a lattice with the next-neighbor interaction between particles. The lattice counterpart of the model in Eq. (2) is the Hamiltonian $H = -\sum_{j=-L/2}^{L/2}(\psi_j^\dagger\psi_{j+1} + \psi_j^\dagger\psi_{j-1})/(2m) - U\sum_{j=-L/2}^{L/2}\psi_j^\dagger\psi_j\psi_{j+1}^\dagger\psi_{j+1}$, where j is the site index on the lattice and the operators ψ_j obey the Fermi commutation relations $\{\psi_i,\psi_j^\dagger\} = \delta_{ij}$.

The model above can be diagonalized using the Bethe-ansatz approach [18]. In the coordinate basis a superposition of N plane waves, $\Psi = \sum_{P,j_1<\dots<j_N} e^{i\sum_{l=1}^N k_{P_l} j_l + i\sum_{l<l'=1}^N \varphi_{P_l,P_{l'}}}\psi_{j_1}^\dagger\cdots\psi_{j_N}^\dagger|\mathrm{vac}\rangle$, is an eigenstate, $H\Psi = E\Psi$, with the corresponding eigenenergy

$$E = \frac{1}{m}\sum_{j=1}^{N}[1-\cos(k_j)]. \tag{4}$$

Here $|\mathrm{vac}\rangle$ is the vacuum state, the scattering phases are fixed by the two-body scattering problem

$$e^{i2\varphi_{ll'}} = -\frac{e^{i(k_l+k_{l'})}+1-2mUe^{ik_l}}{e^{i(k_l+k_{l'})}+1-2mUe^{ik_{l'}}}, \tag{5}$$

and $\sum_P$ is a sum over all permutations of N quasimomenta. The periodic boundary condition quantizes the set of N quasimomenta simultaneously,

$$Lk_j - 2\sum_{l\neq j}\varphi_{jl} = 2\pi I_j, \tag{6}$$

where I_j is a set of nonequal integer numbers. The total momentum of N particles, $P = \sum_j k_j$, is a conserved quantity.

The continuum model in Eq. (2) corresponds to the low-density (long-wavelength) limit of the lattice model. In this limit the scattering phases in Eq. (5) are linear functions of quasimomenta, $2\varphi_{ll'} = (k_l - k_{l'})/[1+(mU)^{-1}] + \pi$, and the nonlinear system of equations in Eq. (6) becomes linear. In the thermodynamic limit we solve it using perturbation theory and obtain an independent quantization condition for each quasimomentum as solutions of the Bethe equations in the leading $1/N$ order,

$$k_j = \frac{2\pi I_j}{L - \frac{N}{1+\frac{1}{mU}}}. \tag{7}$$

Thus all N-particle eigenstates can be labeled by all possible sets of integers I_j similarly to Slater determinants for free fermions. The latter is possible as long as no bound states exist, which is the case for any value of interaction strength $U \geqslant 0$ in this limit [18].

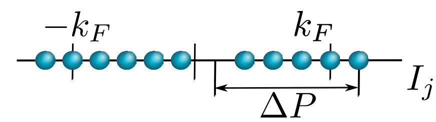

FIG. 2. (Color online) A set of quasimomenta from Eq. (7) that corresponds to the edge mode of the spectral function for Fermi particles without spin. The momentum of each many-particle state is given by $k = -k_F + \Delta P$.

The eigenstates contributing to the spectral function satisfy the number of particle constraints, i.e., fixed to be $N+1$. The lowest energy state for a fixed momentum $-k_F + \Delta P$ is given by the set of integers in Fig. 2. At low energies the system is in the universality class of Luttinger liquids. Its properties are fully determined by the linear slope of the spectrum of excitations at $\pm k_F$. Using the parametrization in Fig. 2, the first Luttinger parameter (the sound velocity of the collective modes) is a discrete derivative $v = L(E_2 - E_1)/(2\pi)$, where E_2 and E_1 are the energies of the states with $\Delta P = 2\pi/L$ and $\Delta P = 0$.

For Galilean invariant systems the product of the first and the second (dimensionless K) Luttinger parameters gives the Fermi velocity of the noninteracting system [19], $vK = v_F$ where $v_F = \pi N/(mL)$. By a straightforward calculation of the eigenenergies in Eq. (4) using Eq. (7) for a pair of states in Fig. 2 with $\Delta P = 0, 2\pi/L$ we directly obtain the second Luttinger parameter,

$$K = \left(1 - \frac{N}{L\left(1+\frac{1}{mU}\right)}\right)^2. \tag{8}$$

The dispersion of the spectral edge mode is given by the energies and the momenta of all states in Fig. 2. Starting from the solutions for quasimomenta in Eq. (7) and repeating the same calculation as before, we directly obtain the parabolic function of momentum [20] in Eq. (1), where $m^*/m = K$ from Eq. (8) [21]. This calculation also gives the chemical potential in Eq. (1) as the bare electron mass renormalized by the Luttinger parameter K, $\mu = k_F^2/(2mK)$.

B. Spinful

When Fermi particles have spin 1/2, the Pauli exclusion principle suppresses only the interaction between the particles with the same spin orientation in the model in Eq. (2). The remaining part of the density-density interaction term consists of a coupling between particles with opposite spin orientations.

This model can be diagonalized using the Bethe-ansatz approach but the Bethe hypothesis has to be applied twice [22]. In the coordinate basis, a superposition of plane waves is an eigenstate, $H\Psi = E\Psi$, of the model in Eq. (2),

$$\Psi = \int\cdots\int_{-L/2}^{L/2} dx_1\cdots dx_N \sum_{P,Q} A^{PQ} e^{i(P\mathbf{k})\cdot(Q\mathbf{x})}\psi_{Q_1}^\dagger(x_1)\cdots \times \psi_{Q_N}^\dagger(x_N)|\mathrm{vac}\rangle, \tag{9}$$

where the operators $\psi_\alpha(x)$ obey the Fermi commutation rules $\{\psi_\alpha(x),\psi_\beta^\dagger(x')\}=\delta(x-x')\delta_{\alpha\beta}$, k_j are N quasimomenta, $\sum_{P,Q}$ is a sum over all permutations of two independent sets of N integer numbers (P and Q), and the coefficients A^{PQ} are chosen by a secondary use of the Bethe hypothesis,

$$A^{PQ}=\text{sgn}(PQ)\sum_R\left(\prod_{1\leqslant l<l'\leqslant M}\frac{\lambda_{R_l}-\lambda_{R_{l'}}-imU}{\lambda_{R_l}-\lambda_{R_{l'}}}\right)\prod_{l=1}^M \times\frac{imU}{\lambda_{R_l}-k_{P_{z_l}}+\frac{imU}{2}}\prod_{j=1}^{z_l-1}\frac{\lambda_{R_l}-k_{P_j}-\frac{imU}{2}}{\lambda_{R_l}-k_{P_j}+\frac{imU}{2}}. \quad (10)$$

Here λ_l are spin degrees of freedom of M "up" spins with respect to the reference ferromagnetic state of N "down" spins, $\sum_R$ is a sum over all permutations of M integer numbers, and z_l is the position of the lth spin ↑ in permutation Q. The eigenenergy corresponding to the eigenstate in Eq. (9) is

$$E=\sum_{j=1}^N\frac{k_j^2}{2m}. \quad (11)$$

The periodic boundary condition quantizes the set of N quasimomenta k_j (charge degrees of freedom) simultaneously,

$$Lk_j-\sum_{l=1}^M\varphi_{jl}=2\pi I_j, \quad (12)$$

where scattering phases $\varphi_{jl}=\log[(\lambda_l-k_j-\frac{imU}{2})/(\lambda_l-k_j+\frac{imU}{2})]/i$ depend on the quasimomenta of both kinds (k_j and λ_l), I_j is a set of N nonequal integer numbers, and M quasimomenta λ_l (spin degrees of freedom) satisfy another set of nonlinear equations,

$$\prod_{j=1}^N\frac{\lambda_l-k_j-\frac{imU}{2}}{\lambda_l-k_j+\frac{imU}{2}}=\prod_{l'=1\neq l}^M\frac{\lambda_{l'}-\lambda_m-imU}{\lambda_{l'}-\lambda_m+imU}. \quad (13)$$

The sum $P=\sum_{j=1}^N k_j$ is a conserved quantity—the total momentum of N particles.

The system of nonlinear equations, Eqs. (12) and (13), can be solved explicitly in the limit of infinite repulsion $U=\infty$ [23]. The quasimomenta λ_l diverge in this limit. Under the substitution of $\lambda_l=mU\tan y_l/2$, the second system of equations, Eq. (13), becomes independent of the first system of equations, Eq. (12), in leading $1/U$ order,

$$e^{iNy_l}=(-1)^{N+M-1}\prod_{l'=1\neq l}^M\frac{e^{i(y_l+y_{l'})}+1+2e^{iy_l}}{e^{i(y_l+y_{l'})}+1+2e^{iy_{l'}}}. \quad (14)$$

The above Bethe equations are identical to that of a Heisenberg antiferromagnet [18] where the number of particles N plays the role of the system size. In one dimension a spin chain is mapped into the model of interacting Fermi particles by the Jordan-Wigner transformation [18]; Eq. (14) is identical to Eqs. (5) and (6) where the interaction strength is set to $mU=-1$. Thus all solutions of Eq. (14) can be labeled by all sets of M nonequal integer numbers J_l similarly to the case of Fermi particles without spin (see Fig. 2). The system of equations for the quasimomenta k_j in Eq. (12) in the $U=\infty$ limit decouples

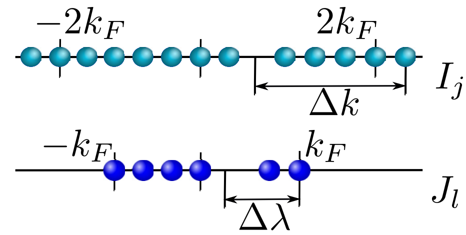

FIG. 3. (Color online) Parametrization of many-body states for fermions with spin using the $U=\infty$ limit in Eqs. (14) and (15). Chargelike excitations correspond to different sets of I_j and spinlike excitations correspond to different sets of J_j.

into a set of single-particle quantization conditions,

$$Lk_j=2\pi I_j+\frac{1-(-1)^M}{2}\pi+\sum_{l=1}^M y_l. \quad (15)$$

Note that the independent magnetic subsystem, where quasimomenta y_l satisfy Eq. (14), is translationally invariant, thus $\sum_{l=1}^M y_l=2\pi\sum_{l=1}^M J_l/N$ [as can be checked explicitly by multiplying Eq. (14) for all y_l]. Therefore, the quantization condition in Eq. (17) depends only on two sets of integer numbers, I_j and J_l.

All solutions of the original system of equations, Eqs. (12) and (13) can be labeled by all sets of $N+M$ integer numbers I_j and J_l (see Fig. 3). The values of k_j and λ_l that correspond to these integers can be obtained in two steps. First, the spin degrees of freedom y_l that correspond to a set of J_l are adiabatically continued under a smooth deformation of Eq. (6) from $U=0$, which is the free particle limit, to $U=-1/m$, which coincides with Eq. (14). Note that the long-wavelength solution in Eq. (7) cannot be used here because the most interesting case of zero polarization for spinful fermions corresponds to half-filling of the band for the model in Eqs. (12) and (13) which is outside of the limits of applicability of the low-density regime. The values k_j that correspond to a set of I_j and J_l are obtained directly from Eq. (15). Secondly, the known values of k_j and λ_l in the $U=\infty$ limit are adiabatically continued under a smooth deformation of Eqs. (12) and (13) to arbitrary value of the interaction strength U.

The interaction effects are controlled by a single dimensionless parameter that can be defined using the $1/U$ corrections in the large U limit. Power series expansion of Eqs. (12) and (13) up to the first subleading $1/U$ order, $\lambda_l=mU\tan y_l/2+y_l^{(1)}$ and $k_j=k_j^{(0)}+2k_j^{(1)}/(mU)$, where y_l and $k_j^{(0)}$ are the solutions of Eqs. (14) and (15), yields

$$\sum_{j=1}^N\left(k_j^{(0)}-y_l^{(1)}\right)\cos^2 y_l=-2\sum_{l'=1\neq l}^M\frac{y_{l'}^{(1)}-y_l^{(1)}}{(\tan y_l-\tan y_{l'})^2+4} \quad (16)$$

and

$$k_j^{(1)}=\frac{2}{L}\sum_{l=1}^M\left(k_j^{(0)}-y_l^{(1)}\right)\cos^2 y_l. \quad (17)$$

The first-order coefficients $y_l^{(1)}$ can be expressed from Eq. (16) in terms of zeroth-order coefficients $k_j^{(0)}$ and y_l. Then, in the

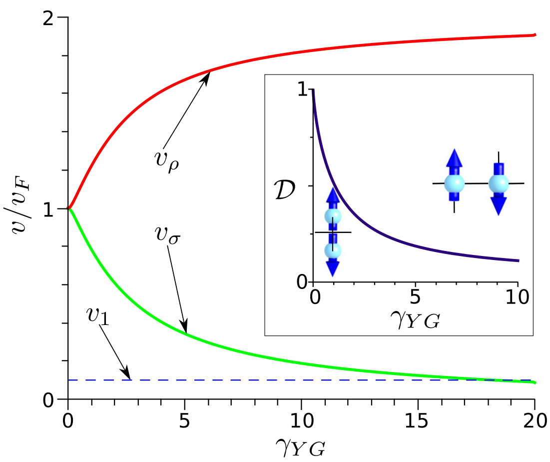

FIG. 4. (Color online) Velocities of the collective modes for fermions with spins at low energies as a function of the interaction parameters γ_{YG} from Eq. (18). The red line corresponds to the holon branch, the green line corresponds to the spinon branch, and the blue dashed line marks a quantum of momentum $v_1 = 2\pi/(mL)$; $L = 400$, $N = 40$, $\gamma_{YG} = 3.44mU$. Inset: Degree of double degeneracy [see the definition in Eq. (19)] for the ground state in Fig. 3 with $\Delta k = \Delta\lambda = 0$ as a function of the interaction parameter γ_{YG}.

thermodynamic limit, the first-order corrections to the quasi-momenta k_j in Eq. (17) become $k_j^{(1)} = 2k_j^{(0)} \sum_{m=1}^{M} \cos^2 y_l/L$. This gives a condition of validity for the $1/U$ expansion of the Bethe equations, $2k_j^{(1)}/(mUk_j^{(0)})$, which is independent of both indices j and l.

We use the latter to define a single parameter,

$$\gamma_{YG} = \frac{mL}{2N} \frac{U}{\left(1 + \frac{1}{N}\sum_{l=1}^{M} \cos\, y_l\right)}, \qquad (18)$$

that characterizes the degree of repulsion between fermions. When $\gamma_{YG} \gg 1$ the particles with opposite spin orientations scatter strongly off each other and when $\gamma_{YG} \ll 1$ they interact weakly with each other. For example, this is manifested in a change of degeneracy of the quasimomenta k_j that correspond to the ground state of unpolarized Fermi particles, $M = N/2$. We account for the degree of double degeneracy with respect to spin 1/2 using

$$\mathcal{D} = 2 - \frac{L\sum_{j=1}^{N-1}(k_{j+1} - k_j)}{\pi N}. \qquad (19)$$

This quantity is $\mathcal{D} = 1$ when each momentum state of free fermions is doubly occupied ($U = 0$) and is $\mathcal{D} = 0$ when each momentum state is occupied by a single particle ($U = \infty$). The crossover from one regime to another occurs at $\gamma_{YG} = 1$ where $\mathcal{D}$ crosses the value of 1/2 (see inset in Fig. 4).

The ground state of the model in Eq. (2) has zero spin polarization when the external magnetic field is absent, $M = N/2$. To be specific we consider the ground states with even values of N and M. Excited states contributing to the spectral function satisfy the number of particles being constrained to be $N + 1$. In the $U = \infty$ limit the lowest-energy eigenstates for a fixed momentum $P = -k_F + \Delta P$ are given by a set of integers in Fig. 3 with $\Delta k = 0$ and $\Delta P = \Delta\lambda$ [24]. In the opposite limit of free fermions, the lowest-energy eigenstates for a fixed momentum $P = -k_F + \Delta P$ are doubly degenerate with respect to spin 1/2 and are given by the set of integers in Fig. 3 for each spin orientation. The quasimomenta in both limits are smoothly connected under adiabatic deformation of Eqs. (12) and (13) from $U = \infty$ to $U = 0$ marking the edge of the spectral function in Eq. (3) for arbitrary U.

At low energies the eigenstates are strongly mixed in the spin sector due to spin-charge separation [7] implying that $A_\uparrow(k,\varepsilon) = A_\downarrow(k,\varepsilon)$. The excitations of the system are spinons and holons which are well approximated by the spinful generalization of the Tomonaga-Luttinger model with only four free parameters $v_{\rho,\sigma}$ and $K_{\rho,\sigma}$. The pair of velocities is the slopes of the linearized dispersions of the charge and spin excitations at $\pm k_F$. Using the representation of the eigenstates in Fig. 3 they are

$$v_\rho = \frac{L(E_2 - E_1)}{2\pi}, \quad v_\sigma = \frac{L(E_3 - E_1)}{2\pi}, \qquad (20)$$

where E_1, E_2, and E_3 correspond to the energies of the states with ($\Delta k = 0$, $\Delta\lambda = 0$), ($\Delta k = 2\pi/L$, $\Delta\lambda = 0$), and ($\Delta k = 0$, $\Delta\lambda = 2\pi/L$), respectively [25]. The numerical evaluation of $v_{\rho,\sigma}$ as a function of the interaction parameter γ_{YG} [26] is presented in Fig. 4. For $\gamma_{YG} = 0$ both velocities coincide, $v_\rho = v_s = v_F$. For large $\gamma_{YG} \gg 1$ the holon velocity doubles, $v_\rho = 2v_F$, due to strong repulsion between particles with opposite spin orientations [27], and the spinon velocity becomes zero, $v_\sigma = 0$, since it vanishes as $\sim 1/(m^2U)$ in this limit [18]. The other pair of Luttinger parameters can be obtained directly for Galilean invariant systems using $v_{\rho,\sigma}$ and the Fermi velocity $K_{\rho,\sigma} = v_F/v_{\rho,\sigma}$ where $v_F = \pi M/L$, without the need of a second observable such as compressibility [7].

Beyond the linear regime the position of the edge of the spectral function is given by following of the low-energy spinon mode. Numerical evaluation shows that $\varepsilon_{\text{edge}}(k) = E_k - E_0$, where E_k corresponds to the states in Fig. 3 with $\Delta k = 0$ and $k = -k_F + \Delta\lambda$, is close to a parabola for all values of γ_{YG} (see Fig. 5). For $\gamma_{YG} = 0$ the shape of the spectral edge mode is exactly parabolic following the dispersion of free Fermi particles. For $\gamma_H \gg 1$ deviations from a parabola are largest. We quantify them by comparing the effective mass m^*, obtained by the best fit of Eq. (1) at all energies, with the spinon velocity v_σ from Eq. (20), obtained at low energy [28]. The deviation $(v_\sigma - k_F/m^*)/v_\sigma$ decreases as the number of particles N grows but it saturates at a finite value of ~ 0.2 in the limit $N \to \infty$ [29] (see the inset in Fig. 5).

The edge of the spectral function in the complementary part of the fundamental range, $k_F < k < 3k_F$, also has a parabolic shape. The eigenstates with the smallest eigenenergies for a fixed momentum k in this range are connected with their counterparts in the $-k_F < k < k_F$ range by a shift of the spin variables $\lambda_j \to \lambda_j + 2\pi/L$. Repeating the same numerical procedure as before for $\varepsilon_{\text{edge}}(k) = E_k - E_0$, where E_k corresponds to the states in Fig. 3 with $\Delta k = 0$ and $k = k_F + \Delta\lambda$, we obtain the result in Eq. (1) with $k_0 = 2k_F$. In the "hole region" $\varepsilon < \mu$, the position of the edge of the spectral function is obtained by reflection of $\varepsilon_{\text{edge}}(k)$ with respect to the line $\varepsilon = \mu$.

The parabolalike behavior of the edge mode breaks down in finite-sized systems in the ultrastrong interaction regime when the spinon velocity v_σ becomes smaller than its own

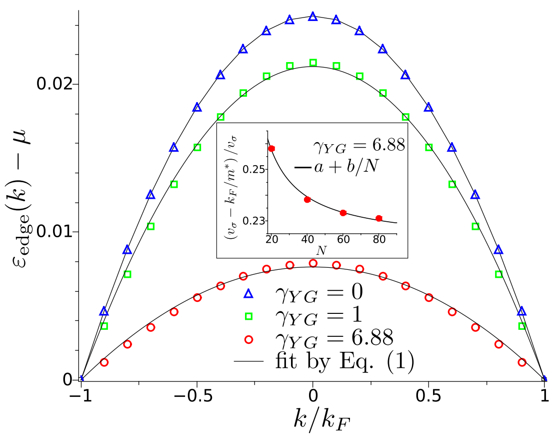

FIG. 5. (Color online) Dispersion of the spectral edge mode (extension of the spinon branch to high energies) for fermions with spins for different values of the interaction parameter $\gamma_{YG}=0,1,6.88$; $L=400$, $N=40$. The blue triangles, green squares, and red ellipses are the numerical solutions of Eqs. (12) and (13); the solid black lines are the best parabolic fits by Eq. (1). Inset: Difference between the slope of the parabolic dispersion at E_F, which is given by the effective mass m^*, and the velocity of spin waves at low energies, which is obtained directly from Eq. (20) $[(v_\sigma - k_F/m^*)/v_\sigma]$ as a function of the number of particles N for $\gamma_{YG}=6.88$. The solid black line is the $1/N$ fit, $a+b/N$, that gives $a=0.22$ [29].

quantum set by the finite size of the system $v_1 = 2\pi/(mL)$ (see the dashed line in Fig. 4). Correspondingly, the threshold for entering this regime becomes $\gamma_{YG}\to\infty$ in the thermodynamic limit, as observed in Fig. 4 when $v_1\to 0$. When $v_\sigma < v_1$, the behavior of the system is dominated by doubling of the period in the momentum space from $2k_F$ to $4k_F$, which can be seen explicitly from Eqs. (11) and (15) in the $U=\infty$ limit. The doubling in the spinful case is a direct consequence of Galilean invariance of the model in Eq. (2). However, it does not manifest itself in the thermodynamic limit for finite spinon velocities $v_\sigma > v_1$, for which the edge of the spectral function is still $2k_F$ periodic.

IV. EFFECTIVE FIELD THEORY

Eigenmodes above the spectral edge can be described by "the mobile impurity model" [15] with two different types of fields that account for all possible low-energy excitations with respect to a state on the spectral edge with a given momentum k in Figs. 2 and 3. One field is responsible for bosonic excitations around $\pm k_F$ whose behavior is well approximated by the Tomonaga-Luttinger model. Another field models the dynamics of the holelike degree of freedom, as observed in Fig. 2 for a large ΔP. For a k away from $\pm k_F$ creation of a second or removal of the existing holelike excitation is associated with a significant energy cost, thus the corresponding field describes a single Fermi particle.

The interaction between the deep hole and the excitations at $\pm k_F$ is of the density-density type since their corresponding energy bands are separated by a large barrier. Bosonization of the excitations at $\pm k_F$ leaves two unknown coupling constants between a pair of the canonically conjugated variables of the Tomonaga-Luttinger model and a fermionic field of the deep hole that can be identified by considering two different physical properties [10,30]. One is translation invariance of the hybrid system that can be represented as a motion of a fermionic excitation in a bosonic fluid with the velocity $u=\langle\nabla\theta\rangle/m$. Another is an observable that corresponds to the change of the total energy with respect to long-range variations of the density, which for the hybrid systems is given by $\delta\rho = -\langle\nabla\varphi\rangle/\pi$. Here φ and $\nabla\theta$ are the canonically conjugated variables of the Tomonaga-Luttinger model that correspond to the density and the current of the hydrodynamic modes, respectively.

For a fixed value of k, the dynamics of the free Bose-like and the free Fermi-like fields can be linearized for states close to the spectral edge. Using the dispersion in Eq. (1) for the Fermi-like field and the Luttinger parameters for the Bose-like field, the mobile impurity model reads

$$H = \int dx \left[\frac{v}{2\pi}\left(K(\nabla\theta)^2 + \frac{(\nabla\varphi)^2}{K}\right) + \left(\frac{k(K-1)}{m^*}\nabla\theta + \frac{v(K+1)}{K}\nabla\varphi\right)d^\dagger d + d^\dagger\left(\frac{k^2}{2m^*} - \frac{ik\nabla}{m^*}\right)d\right], \tag{21}$$

where $-k_F < k < k_F$ is the total momentum of the system—an input parameter of the model, $m^* = mK$ is the effective mass of the deep hole, v and K are the Luttinger parameters defined at $\pm k_F$, the fields θ and φ are the canonically conjugated variables $[\varphi(x),\nabla\theta(y)] = i\pi\delta(x-y)$ of the Tomonaga-Luttinger model, and the field d obeys the Fermi commutation rules $\{d(x),d^\dagger(y)\} = \delta(x-y)$.

The Hamiltonian in Eq. (21) can be diagonalized by a unitary transformation [8,10]. The rotation $e^{-iU}He^{iU}$, where $U=\int dy[C_+(\sqrt{K}\theta+\varphi/\sqrt{K}) + C_-(\sqrt{K}\theta-\varphi/\sqrt{K})]d^\dagger d$ and $C_\pm = (2\sqrt{K})^{-1}[k(K-1)\pm k_F(K+1)]/(k\pm k_F)$, eliminates the coupling term between the fields turning Eq. (21) into a pair of free harmonic models. Then, the observables can be calculated in a straightforward way as averages over free fields only.

The spectral function in Eq. (3) can be calculated using the effective field model [8]. The original operators $\psi^\dagger(x)$ of Fermi particles of the model in Eq. (2) correspond to a composite excitation consisting of two bosons and one fermion in the field language of the model in Eq. (21) (see the state in Fig. 2). The fermionic excitation gives a dominant contribution to the spectral weight $|\langle f|\psi^\dagger(0)|0\rangle|^2$, thus at leading order in $|\varepsilon - \varepsilon_{\rm edge}(k)|$ close to the spectral edge the spectral function reads $A(k,\varepsilon) = \int dt\, dx\, e^{-i\varepsilon t}\langle d^\dagger(x,t)d(0,0)\rangle$ where $d(x,t) = e^{-iHt}d(x)e^{iHt}$ and $\langle\cdots\rangle$ is the zero temperature expectation value with respect to the model in Eq. (21). In the diagonal basis the average is evaluated over free fields by standard means. Following the steps of Ref. [10] we obtain $A(\varepsilon,k)\sim\theta[\varepsilon-\varepsilon_{\rm edge}(k)]/|\varepsilon-\varepsilon_{\rm edge}(k)|^\alpha$, where the exponent depends only on the Luttinger parameter K,

$$\alpha = 1 - \frac{K}{2}\left(1-\frac{1}{K}\right)^2. \tag{22}$$

This result is the same for the particle and the hole parts of the spectrum. Here K is given by the analytic result in Eq. (8).

Excitations above the spectral edge for Fermi particles with spin can be described using the mobile impurity model in an analogous way [13,24]. The number of bosonic fields doubles due to the two spin orientations. Bosonization of the modes at $\pm k_F$ gives a diagonal Tomonaga-Luttinger model in the basis of spin and charge fields. Here there are four unknown coupling constants between two pairs of the canonically conjugated variables of the Tomonaga-Luttinger model and the Fermi-like field of the deep hole. One pair of constants that corresponds to the coupling to spinon modes is zero due to the symmetry with respect to the spin orientation in the original microscopic model in Eq. (2), where the external magnetic field is zero. Another pair of the constants that correspond to the coupling to holon modes can be identified by considering the same physical properties as for the Fermi particles without spin.

Using the result in Eq. (1) and the Luttinger parameters, the mobile impurity model reads

$$H = \int dx \left[\sum_{\alpha=\rho,\sigma} \frac{v_\alpha}{2\pi} \left(K_\alpha (\nabla\theta_\alpha)^2 + \frac{(\nabla\varphi_\alpha)^2}{K_\alpha} \right) + \frac{v_\sigma - \frac{k}{m^*}}{\sqrt{2}} (K_\sigma \nabla\theta_\rho + \nabla\varphi_\rho) d^\dagger d + d^\dagger \left(\frac{k^2}{2m^*} - \frac{ik\nabla}{m^*} \right) d \right], \quad (23)$$

where k is the total momentum of the system—an input parameter of the model; $m^* = mK_\sigma$ is the effective mass of the deep hole; v_ρ, K_ρ, v_σ, and K_σ are the four Luttinger parameters for the spin and the charge modes; the bosonic fields θ_ρ,φ_ρ,θ_σ,φ_σ are canonically conjugated variables $[\varphi_\alpha(x), \nabla\theta_\beta(y)] = i\pi\delta_{\alpha\beta}\delta(x-y)$ of the Tomonaga-Luttinger model; and the field d obeys the Fermi commutation rules $\{d(x), d^\dagger(y)\} = \delta(x-y)$.

The diagonalization of the Hamiltonian in Eq. (23) can be done by a unitary transformation in a very similar fashion to the spinless case [13,24]. The rotation $e^{-iU} H e^{iU}$, where $U = \int dx [C_+(\sqrt{K_\rho}\theta + \varphi/\sqrt{K_\rho}) + C_-(\sqrt{K_\rho}\theta - \varphi/\sqrt{K_\rho})] d^\dagger d$ and $C_\pm = \mp\sqrt{K_\rho} 8^{-5/2} (k - k_F)(K_\rho^{-1} \mp K_\sigma^{-1})/(k/K_\sigma \pm k_F/K_\rho)$, removes the coupling term in the Hamiltonian in Eq. (23) allowing straightforward calculations of the observables.

The spectral function in Eq. (3) can be evaluated within the framework of the effective field model in the same way. The original Fermi operators $\psi_\alpha^\dagger(x)$ in the form factor $|\langle f|\psi_\alpha^\dagger(0)|0\rangle|^2$ correspond to composite excitation consisting of two bosons (one for spin and one for charge) and one fermion in the field language of the model in Eq. (23) (see the state in Fig. 3). The fermionic part gives the dominant contribution to the spectral weight, thus the spectral function reads $A(k,\varepsilon) = \int dt\, dx\, e^{-i\varepsilon t} \langle d^\dagger(x,t) d(0,0)\rangle$ where $d(x,t) = e^{-iHt} d(x) e^{iHt}$ and $\langle \cdots \rangle$ is the zero temperature expectation value with respect to the model in Eq. (23). In the diagonal basis the average is evaluated over free fields by standard means. Following the steps of Ref. [13] we obtain in proximity of the edge $A(\varepsilon,k) \sim \theta[\varepsilon - \varepsilon_{\rm edge}(k)]/|\varepsilon - \varepsilon_{\rm edge}(k)|^\alpha$ where the exponent depends only on a pair of the dimensionless Luttinger parameters and the momentum along the spectral edge,

$$\alpha = \frac{1}{2} \pm \frac{1}{2} - \frac{K_\rho}{4} \left(1 - \frac{(k-k_F)\left(\frac{k_F}{K_\rho^2} + \frac{k}{K_\sigma^2}\right)}{\left(\frac{k}{K_\sigma}\right)^2 - \left(\frac{k_F}{K_\rho}\right)^2} \right)^2 - \frac{K_\rho}{4} \left(\frac{1}{K_\rho} \pm \frac{(k-k_F)\left(\frac{k_F}{K_\rho K_\sigma} + \frac{k}{K_\rho K_\sigma}\right)}{\left(\frac{k}{K_\sigma}\right)^2 - \left(\frac{k_F}{K_\rho}\right)^2} \right)^2. \quad (24)$$

The result is different for the particle (+) and the hole (−) sectors. The values of the Luttinger parameters obtained numerically using Eq. (20) (see Fig. 4) give divergent values of $0 < \alpha < 1$ in the particle sector and cusplike positive powers $-1 < \alpha < 0$ in the hole sector.

V. BOSONS

While our primary interest lies in Fermi particles, for completeness and to test the generality of our result we consider Bose particles without spin [31]. In this case the application of the Bethe-ansatz approach is very similar to the case of Fermi particles without spin [18]. Our approach of solving a discrete model is complementary to previous approaches to this problem based around numerical solution of the continuum form of the Bethe-ansatz equations and a comparison with a mean-field-like result from the Gross-Pitaevskii equation [32].

We closely follow the original approach of Lieb and Liniger in Ref. [33]. In the coordinate basis a superposition of N plane waves, $\Psi = \int \cdots \int_{-L/2}^{L/2} dx_1 \cdots dx_N \sum_P e^{i\sum_j k_{P_j} x_j} e^{i\sum_{l<l'} \varphi_{P_l P_{l'}}} \psi^\dagger(x_1) \cdots \psi^\dagger(x_N) |{\rm vac}\rangle$, is an eigenstate, $H\Psi = E\Psi$, of the model in Eq. (2) with the corresponding eigenenergy $E = \sum_{j=1}^N k_j^2/(2m)$. Here the operators $\psi(x)$ obey the Bose commutation rules $[\psi(x), \psi^\dagger(y)] = \delta(x-y)$, $\sum_P$ is a sum over all permutations of N quasimomenta k_j, and the scattering phases $2\varphi_{ll'} = \log[(k_l - k_{l'} + i2mU)/(k_l - k_{l'} - i2mU)]/i$ are fixed by the two-body scattering problem.

The periodic boundary condition quantizes a set of N quasimomenta simultaneously,

$$k_j L - \sum_{l=1\neq j}^{N} 2\varphi_{jl} = 2\pi I_j, \quad (25)$$

where I_j is a set of nonequal integer numbers. The total momentum of N particles, $P = \sum_j k_j$, is a conserved quantity.

The nonlinear system of equations, Eq. (25), can be solved explicitly in the limit of infinite repulsion. The hard-core bosons in this limit are identical to free fermions [34] which decouples Eq. (25) into a set of plane wave quantization conditions, $k_j = 2\pi I_j/L$. The corresponding eigenstates are Slater determinants whose classification is identical to that of free fermions—all many-body states correspond to all sets of N nonequal integer numbers. These values of quasimomenta k_j can be adiabatically continued under a smooth deformation of Eq. (25) by varying the interaction strength from $U = \infty$ to an arbitrary value of U.

The single parameter that controls the behavior of interacting bosons can be obtained from the Bogoliubov theory in the weak interaction regime [35]. This theory is valid when

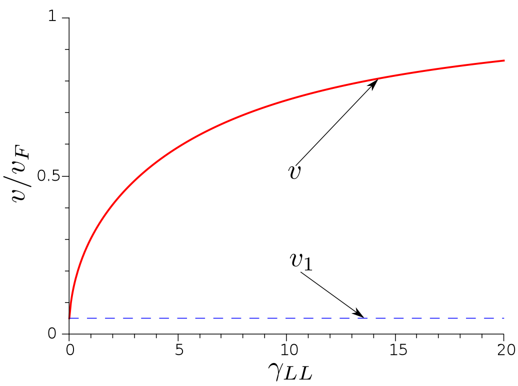

FIG. 6. (Color online) The sound velocity of the collective modes for spinless bosons v at low energies as a function of the interaction parameter γ_{LL} from Eq. (26) (red line) and the quantum of momentum $v_1 = 2\pi/(mL)$ (blue dashed line); $L = 200$, $N = 20$, and $\gamma_L = 0.2mU$.

the interaction length is smaller than the kinetic energy of particles, e.g., the high-density limit. The same parameter can be generalized to arbitrary interaction strengths [33],

$$\gamma_{LL} = \frac{2mUL}{N}. \tag{26}$$

When $\gamma_{LL} \ll 1$ the interacting particles are like bosons and when $\gamma_{LL} \gg 1$ the system is almost a free Fermi (Tonks-Girardeau) gas.

The eigenstates contributing to the spectral function in Eq. (3) satisfy the number of particles being constrained to be $N + 1$. The lowest energy state for a fixed momentum $-k_F + \Delta P$, where $k_F = \pi N/L$, is given by the sets of integer numbers in Fig. 2. At low energies the system is well approximated by the Tomonaga-Luttinger model with only two free parameters [7,32]. Using the parametrization in Fig. 2, the first Luttinger parameter (the sound velocity of the collective modes) is a discrete derivative $v = L(E_2 - E_1)/(2\pi)$, where E_1 and E_2 are the energies of the states in Fig. 2 with $\Delta P = 0$ and $\Delta P = 2\pi/L$. For Galilean invariant systems the second (dimensionless K) Luttinger parameter can be obtained from the relation $vK = v_F$ where $v_F = \pi N/(mL)$ [19]. Numerical evaluation of v as a function of the interaction parameters γ_{LL} is given in Fig. 6.

Beyond the linear regime the position of the edge of the spectral function is given by the momentum dependence of the states in Fig. 6, $\varepsilon_{\text{edge}}(k) = E_k - E_0$ where E_k corresponds to the states with $k = \Delta P$. Numerical evaluation shows that the shape of $\varepsilon_{\text{edge}}(k)$ is close to a parabola for all values of γ_{LL} (see Fig. 7). The biggest deviation from a parabola occurs when $\gamma_{LL} \ll 1$. We quantify it by comparing the effective mass m^*, obtained by the best fit of Eq. (1), with v in Fig. 6, obtained at low energies. The deviation $(v - k_F/m^*)/v$ increases as the number of particles N grows but it saturates at a finite value of ~ 0.1 in the limit $N \to \infty$ (see inset in Fig. 7).

As with Fermi particles with spin, for finite systems the parabolalike behavior of the spectral edge mode breaks down in the ultraweak interaction regime when the sound velocity of collective modes at low energies mode becomes comparable with its own quantum set by the finite size of the system $v_1 = 2\pi/(mL)$ (see the dashed line in Fig. 6). Correspondingly, the threshold for entering this regime becomes $\gamma_{LL} \to 0$ in the thermodynamic limit, as observed in Fig. 6 when $v_1 \to 0$. When $v \sim v_1$ the edge of the spectral function is linear at all energies, including the high-energy domain, with the slope that is governed by the kinetic energy of a single free Bose particle. These findings are consistent with the work in Ref. [32] where, within their methodology, the authors find a breakdown in parabolicity in the region of small γ_{LL} and a result consistent with GPE.

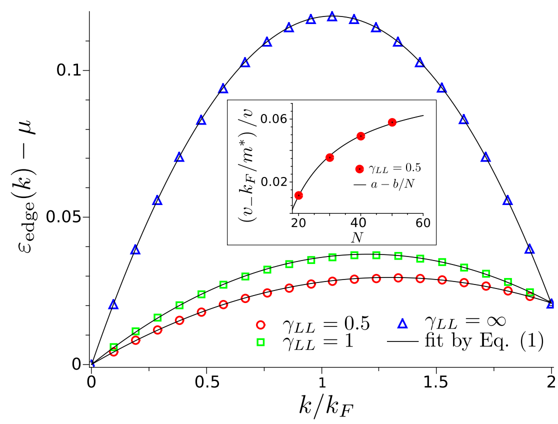

FIG. 7. (Color online) Dispersion of the spectral edge mode for spinless bosons for different values of the interaction parameter $\gamma_L = 0.5, 1, \infty$; $L = 200$, $N = 20$. The blue triangles, green squares, and red ellipses are the numerical solutions of Eq. (25), the solid black lines are the best parabolic fits by Eq. (1). Inset: Difference between the slope of the parabolic dispersion at E_F, which is given by the effective mass m^*, and the velocity of the sound modes, which is obtained by direct evaluation of the energy of the first excited state above the Fermi energy $[(v - k_F/m^*)/v]$ as a function of the number of particles N for $\gamma_{LL} = 0.5$. The solid black line is the $1/N$ fit, $a - b/N$, that gives $a = 0.09$.

VI. CONCLUSIONS

In this work, we have analyzed the spectral edge mode for a variety of one-dimensional models with short-range interactions that bounds from below a continuum of many-body excitations. Explicit diagonalization by means of Bethe-ansatz techniques shows this mode to have an almost perfect parabola dispersion in all cases. Based on this emergent phenomenon, the spectral edge mode can be described empirically by a free, nonrelativistic particle with effective mass identified from the low-energy theory as a free electron mass strongly renormalized by interactions via the dimensionless Luttinger parameter K (K_σ for particles with spin). However, unlike a free particle, the spectral edge mode is not protected by a symmetry, thus deviations from the quadratic dispersion may develop—the biggest discrepancy ($\lesssim 20\%$) occurs for Fermi particles with spin and a very large interaction strength. The empirical model remains robust for finite sound velocities of the collective modes at low energies $v(v_\sigma) > v_1$, where $v_1 = 2\pi/(mL)$ is the quantum of momentum.

The relevance of the Luttinger (low-energy) parameters beyond the low-energy limit implies that they can be extracted using a much wider range of experimental data using the whole energy window from the bottom of the band to the Fermi energy. However, the dispersion of the spectral edge mode itself cannot be used as a qualitative feature to rule out interaction effects since the interactions between particles do not change the parabolic shape of the single-particle dispersion. The biggest deviations could be observed for strongly interacting spinful fermions ($K_\sigma \gtrsim 10$), e.g., electrons in semiconductors at low densities or cold Fermi atoms in a 1D trap that would require a good resolution of the experiment.

The main result of this paper, Eq. (1), complements the mobile impurity model which was developed by Glazman and co-workers as a description of one-dimensional systems above the spectral edge at high energies. Our explicit expression for the dispersion of the edge mode removes an arbitrary input parameter (curvature of the dispersion) that leaves only the few Luttinger parameters and the bare electron mass as a minimal set of necessary ingredients to model excitations above the spectral edge at arbitrary energies. Within such a framework, for example, exponents of the spectral functions are expressed explicitly in terms of only a few Luttinger parameters. The results in Eqs. (22) and (24) provide a systematic way to classify the edge exponents for a wide range of microscopic parameters.

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