Quantum-fluctuation-induced collisions and subsequent excitation gap of an elastic string between walls

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An elastic string embedded between rigid walls is simulated by means of the density-matrix renormalization group. The string collides against the walls owing to the quantum-mechanical zero-point fluctuations. Such a "quantum entropic" interaction has come under thorough theoretical investigation in the context of the stripe phase observed experimentally in doped cuprates. We found that the excitation gap opens in the form of an exponential singularity $\Delta E \sim \exp(-Ad^{\sigma})$ (d=wall spacing) with the exponent $\sigma=0.6(3)$, which is substantially smaller than the mean-field value $\sigma=2$. That is, the excitation gap is much larger than that anticipated from mean field, suggesting that the string is subjected to a robust pinning potential due to the quantum collisions. This feature supports Zaanen's "order out of disorder" mechanism, which would be responsible for the stabilization of the stripe phase.

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I. INTRODUCTION

Recently, Zaanen brought up the problem of a "quantum string," which is a linelike object subjected to line tension, and it wanders owing to quantum zero-point fluctuations.[1,2] The central concern is to estimate the interaction among strings as it wanders quantum mechanically and undergoes entropy-reducing collisions with adjacent neighbors. The statistical mechanics of quantum-string gas would be responsible for the low-energy physics of the stripe phase observed experimentally in doped cuprates.[3–5] In particular, one is motivated to gain insight into how the stripe pattern acquires stability. Actually, a good deal of theoretical analyses had predicted a tendency toward stripe-pattern formation.[6–9] However, *ab initio* simulations on the t-J model still remain controversial about that issue.[10–14]

In a series of papers,[1,2] the authors pointed out that the "quantum entropic" interaction lies out of the conventional picture, and it would rather give rise to solidification of the gas of strings; namely, the stripe phase is stabilized by mutual collisions. (In a different context, the entropic interaction was explored in Refs. 15 and 16.) Their analysis[1,2] is based on the Helfrich approximation,[17] which has been very successful in the course of studies of stacked membranes under *thermal* undulations. Based on this approximation, they revealed the significance of *long*-wavelength fluctuations. Note that in the conventional picture, on the contrary, the string is "disordered" as in the Einstein-like view of crystal, and only short-wavelength fluctuations contribute to collisions.

To be specific, the key relation in their theory is

$$f = C\frac{B}{\Sigma d^2}\left[\ln\left(\frac{\Sigma d}{B}\right)+C'\right], \tag{1}$$

with collision-induced energy cost f (per unit volume) and elasticity modulus (with respect to the compression of string intervals) $B=d^2\partial^2 f/\partial d^2$; see the Hamiltonian (2) as well. The logarithmic term signals the significance of long-wavelength fluctuations. The relation (1) yields remarkable consequences. For instance, the elastic modulus is given by the *stretched* exponential form $B\sim\exp(-Ad^{2/3})$.[1,2] It is noteworthy that the elasticity modulus B is much larger than that of the mean field $B\sim\exp(-Ad^2)$. Hence, the result indicates that contrary to our naive expectations, short-wavelength modes are suppressed owing to collisions, and the collisions rather contribute to solidification of the string gas; namely, the stripe phase is stabilized by the "order out of disorder" mechanism.[1,2]

In our preceding paper,[18] we have verified the above relation (1) and demonstrated that the elastic modulus is actually governed by the stretched exponential form $B\sim\exp(-Ad^{0.808(1)})$. We have carried out the first-principles simulation by means of the density-matrix renormalization group[19–21]: We put a quantum string between rigid walls with spacing d and measured its repelling interaction. (This technique has been utilized in the course of studies of the fluctuation pressure of stacked membranes.)[22–24] The Hamiltonian is given by

$$\mathcal{H}=\sum_{i=1}^{L}\left(\frac{p_i^2}{2m}+V(x_i)\right)+\sum_{i=1}^{L-1}\frac{\Sigma}{2}(x_i-x_{i+1})^2. \tag{2}$$

Here, x_i denotes the operator of the transverse displacement of a particle at the ith site, and p_i is its conjugate momentum. They satisfy the canonical commutation relations $[x_i,p_j]=i\hbar\delta_{ij}$, $[x_i,x_j]=0$ and $[p_i,p_j]=0$. Here $V(x)$ is the rigid-wall potential with spacing d;

$$V(x)=\begin{cases}0 & \text{for} \quad 0\leq x\leq d,\\ \infty & \text{otherwise.}\end{cases} \tag{3}$$

Σ denotes the line tension which puts particles into line. The classical version of this Hamiltonian has been used as a model for line dislocations and steps on (vicinal) surfaces.[25–27] Note that for sufficiently large Σ, one can take a continuum limit, with which one arrives at a field-theoretical version of quantum string.[28]

In the present paper, we are concerned in the excitation (mass) gap due to the collisions. We postulate the exponential singularity

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$$\Delta E \sim \exp(-Ad^{\sigma}) \tag{4}$$

for sufficiently large d. In Ref. 2, the gap (crossover temperature) T_0 is calculated in the form $T_0 \propto \sqrt{B}$; namely, one should obtain $\sigma = 2/3$. This result cannot be understood in terms of the mean-field picture, yielding a much smaller mass gap $\sigma = 2$. (We will outline this picture in the next section.) The purpose of this paper is to judge the validity of those scenarios by performing first-principles simulations. Our result is $\sigma \approx 0.6(3)$ for $\Sigma = 0.5$–4.

The rest of this paper is organized as follows. In the next section, we argue the physical implications of the singularity exponent σ. We introduce the viewpoint of critical phenomena in order to interpret the gap formula (4). The mean-field argument is also explicated. In Sec. III, we perform numerical simulations and show evidence of the breakdown of the mean field. In the last section, we give a summary and discussion.

II. INTERPRETATION OF THE SINGULARITY EXPONENT σ: A STATISTICAL-MECHANICAL OVERVIEW

In the Introduction, we have overviewed the quantum string in the context of the stripe phase. In this section, we will survey different aspects of the quantum string in terms of statistical mechanics. This viewpoint is utilized in the simulation-data analyses in the succeeding section III.

In the path-integral picture, a quantum string spans a "world sheet" as time evolves.[29] Therefore, a quantum string is equivalent to the random surface under *thermal* undulations. The random surface is in the critical phase of Kosterlitz and Thouless (KT). [In our model (2), however, there appears no "flat phase," because the "height" variables $\{x_i\}$ are continuous.] The presence of rigid walls is supposed to destroy the KT criticality. Therefore, the collision-induced mass gap (4) reflects the universality class of the phase transition at $1/d \to 0$. In that sense, our aim is to determine the universality class.

The phase transition has not been studied very extensively so far. The rigid-wall potential is, by nature, nonanalytic, and hence, it is quite cumbersome to carry out perturbative analyses such as loop expansions. Moreover, the confinement due to walls destroys the applicability of the duality transformation, with which one could establish an elucidating equivalence between the random surface and two-dimensional XY model.

Even in computer simulations, verification of the gap formula (4) is rather troublesome. Note that the gap opens very slowly. That is, the correlation length is kept exceedingly large in the vicinity of the critical point. The correlation length would exceed the system sizes. Note that the conventional criticality exhibits the *power-law* singularity

$$\Delta E \sim \xi^{-1} \sim (1/d)^{\nu}, \tag{5}$$

which would be much easier to cope with. We will overcome the difficulty through resorting to the density-matrix renormalization group[19–21]; with this technique, we treat system sizes up to $L = 42$.

Now, we are in a position to discuss the meaning of the singularity exponent σ. The correlation length is proportional to the inverse of the excitation (mass) gap: namely, $\xi \sim \exp(Ad^{\sigma})$. Here ξ sets the characteristic length scale of the collision intervals. Therefore, in the length scale $l = \xi$, the random surface fluctuates freely. And so, the mean fluctuation deviation is calculated,

$$\sqrt{\langle x_i^2 \rangle} \sim (\ln l)^{1/2} \sim d^{\sigma/2}. \tag{6}$$

From this relation, we see that σ reflects an amount of fluctuation amplitudes. In the meantime, the mean-field picture insists $\sqrt{\langle x_i^2 \rangle} \propto d$. (More precisely, an artificial mass term is included so as to enforce the condition; see Refs. 16 and 22.) Hence, one should obtain

$$\sigma = 2 \tag{7}$$

in the mean-field picture.

On the contrary, as mentioned in the Introduction, recent theory[1,2] predicts a much smaller singularity exponent $\sigma = 2/3$, from which one obtains a counterintuitive result $\sqrt{\langle x_i^2 \rangle} \sim d^{1/3} \ll d$. The result indicates that the string is straightened macroscopically by collisions: This is quite reminiscent of the aforementioned claim that the infrared modes are still active, withstanding the collisions.[1,2] A similar, but slightly modest, exponent $\sigma = 1$ was reported (in a different context) with analytical calculations.[15,16]

III. NUMERICAL RESULTS AND DISCUSSIONS

In this section, we perform first-principles simulations so as to estimate the singularity exponent σ. First, we will explicate the simulation algorithm.

A. Details of the density-matrix renormalization group

The density-matrix renormalization group has been utilized for the purpose of treating very large system sizes.[19,20] The technique is based on an elaborate reduction of the Hilbert-space bases, and it has been applied to various spin and electron systems very successfully.[21] Meanwhile, the technique had become applicable to bosonic systems such as phonons and oscillators.[30–33] (Note that the full exact diagonalization does not apply, because even a single oscillator spans infinite-dimensional Fock space. The huge dimensionality overwhelms the computer memory space.) Here, we employ the density-matrix-renormalization technique in order to diagonalize the quantum string (2). A full account of the technical details is presented in our preceding paper.[18] In this paper, we will outline the simulation algorithm with an emphasis on the modification to calculate the excitation gap precisely.

To begin with, we need to set up local (on-site) Hilbert-space bases: Provided that the line tension Σ is turned off, oscillators are independent, and each of them reduces to the textbook problem of a "particle in a box." Hence, the full set of eigensystems is calculated easily. In this way, we set up the intrasite Hilbert space with use of the low-lying $M = 12$ states and discarded the others.

Second, provided that those intrasite bases are at hand, we are able to apply the density-matrix renormalization group. The total system consists of block, site, site, and block. The left-half part (block and site) is renormalized into a new block with reduced dimensionality m; we set, at most, $m=50$. More precisely, those m bases are chosen from the eigenvectors of the density matrix for the left-half part,

$$\rho = \mathrm{Tr}_{\mathrm{R}} |\Psi\rangle\langle\Psi|, \tag{8}$$

with the largest m eigenvalues. Tr_{R} denotes the partial trace with respect to the right-half part and $|\Psi\rangle = |0\rangle + |1\rangle$ with the ground state $|0\rangle$ and the first excitation state $|1\rangle$ of the total system. (Note that in our previous simulation,[18] we simply set $|\Psi\rangle = |0\rangle$, because we were just concerned in the ground-state properties.) The ground state $|0\rangle$ has even parity with respect to the reflection $x_i \to -x_i$, whereas the first excitation state $|1\rangle$ belongs to the odd-parity sector. In other words, each of them is the ground state of the respective subspaces. Therefore, we set $|\Psi\rangle = |0\rangle + |1\rangle$ in order to cover both subspaces. (This choice is suitable as for calculating the first excitation gap. However, in order to calculate the spectral function, one should prepare a much larger series of target states.[21]) Note that the change of sign $|\Psi\rangle = |0\rangle - |1\rangle$ does not make any difference; the phase of the wave function should not affect the physics. In fact, from the definition of the density matrix (8), we see that the density-matrix eigenvalues are kept invariant under that change.

To summarize, we have carried out truncations of bases through two steps: One is the truncation of the intrasite bases M, and the other is the truncation of the ''block'' states m through the density-matrix renormalization. Each of these procedures is monitored carefully, and the relative error of low-lying energy levels is kept within 10^{-7}; see Ref. 18 for details.

We have repeated renormalizations 20 times. The system size reaches $L=42$.

B. Excitation energy gap

We have plotted the energy gap against the inverse of wall spacing $1/d$ for several values of line tension Σ; see Fig. 1. From the plot, we see that the gap opens extremely slowly; namely, in the range $1/d \lesssim 0.3$, the mass gap ΔE is maintained to be very small. This is a typical signature of the exponential singularity (4) rather than the power law (5). For $1/d < 0.2$, the simulation does not continue, because the numerical diagonalization fails in resolving the nearly degenerate low-lying levels.

In the inset, we have presented the logarithmic plot. The data exhibit convex curves. Hence, we see that the singularity exponent σ would not exceed $\sigma=1$. As is mentioned in Sec. II, the mean-field argument predicts $\sigma=2$. Therefore, we found that the collision-induced gap cannot be understood in terms of the mean-field picture.

C. β-function analyses

The criticality is best analyzed by the β function. The β function describes the flow of a certain controllable parameter (in our case, $\delta = 1/d$) with respect to the infinitesimal rescaling of the unit of length: namely,

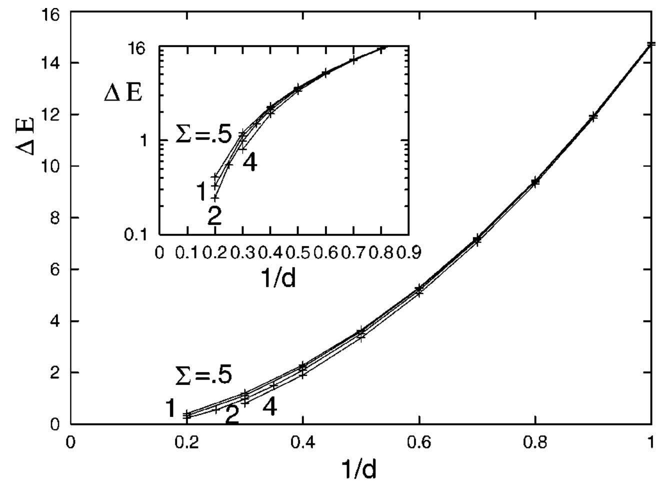

FIG. 1. Excitation gap ΔE is plotted for $1/d$ (d = wall spacing). The excitation gap ΔE opens extremely slowly: This feature is characteristic of the universality class of exponential singularity (4) rather than the power law (5). The inset shows the logarithmic plot. The curves bend convexly. Therefore, the singularity exponent would not exceed $\sigma=1$.

$$\beta(1/d) = \frac{\xi(1/d)}{\xi'(1/d)} = \left(\frac{\mathrm{d}}{\mathrm{d}(1/d)} \ln \xi \right)^{-1}, \tag{9}$$

with correlation length ξ. Because the mass gap is the inverse of the correlation length, we obtain

$$\beta(1/d) = -\left(\frac{\mathrm{d}}{\mathrm{d}(1/d)} \ln \Delta E \right)^{-1}, \tag{10}$$

with excitation gap ΔE.

As is emphasized in Sec. II, the gap formula (4) is deeply concerned with the criticality at $\delta = 1/d \to 0$. The β function reflects the universality class of the phase transition. For instance, as for the exponential singularity such as Eq. (4), it behaves like

$$\beta(1/d) \sim 1/(A\sigma)(1/d)^{\sigma+1}. \tag{11}$$

On the other hand, the conventional second-order transition (5) is characterized by the behavior

$$\beta(1/d) = (1/d)/\nu. \tag{12}$$

In this way, we can read off the critical exponents such as σ and ν.

As is presented in the previous subsection, the excitation-gap data ΔE are readily available. The remaining task is to perform the numerical derivatives of $\Delta E'$. We adopted the ''Richardson's deferred approach to the limit'' algorithm in the textbook of Ref. 34. In this algorithm, one takes an extrapolation after calculating various finite-difference differentiations. We monitored the relative error and checked that the error is kept within 10^{-8}. From these preparations, we can calculate the β function from our simulation data.

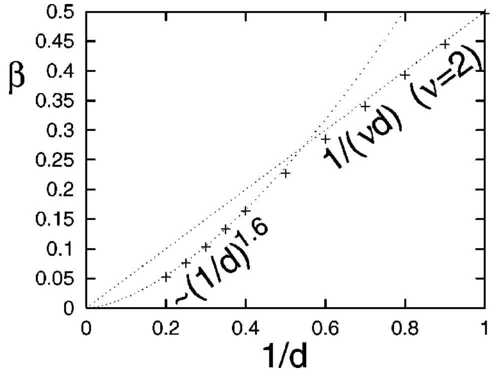

FIG. 2. β function (10) is plotted for $\Sigma=2$. There appear two regimes with respective asymptotic forms; see text. The small-$1/d$ behavior indicates that the transition belongs to the universality class of exponential singularity with $\sigma\approx0.6$; see Eqs. (11) and (12).

We have plotted the β function $\beta(1/d)$ in Fig. 2 for $\Sigma=2$. We see that there appear two regimes: As is indicated in the plot, in the region $1/d\lesssim0.3$, the β function is best fitted by a power law $(1/d)^{1.6}$. Hence, the universality would belong to the exponential singularity (11) with exponent $\sigma=0.6$. Note that such stretched-exponential behavior is suggested in the previous subsection. On the contrary, the β function falls in the simple behavior $1/\nu(1/d)$ with the index $\nu=2$ for large $1/d$; see Eq. (12). That result tells us that for large $1/d$, the gap formula enters the regime of power law (5). That is quite convincing, because for large $1/d$, Σ becomes irrelevant and the system reduces[18] to the textbook problem of a "particle in a box." Hence, the excitation gap is simply given by the power law (5) with the index $\nu=2$. To summarize, we found that for large $1/d$, the physics changes so that we must look into the behavior in the vicinity of $1/d=0$.

In order to estimate σ, we have presented the log-log plot in Fig. 3 for various Σ. From the slopes, we obtain an estimate $\sigma=0.6(3)$. This estimate is far less than the mean-field value $\sigma=2$. It clearly supports Zaanen's claim $\sigma=2/3$ (Refs. 1 and 2) that the collision-induced mass gap is governed by the stretched-exponential singularity. That is, the collision-

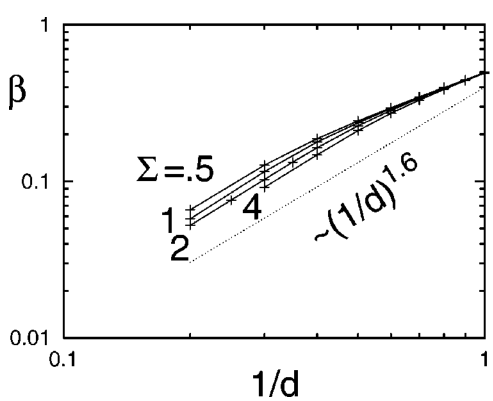

FIG. 3. Logarithmic plot of the β function for various Σ. From the slopes, we read off the singularity exponent $\sigma=0.6(3)$; see Eq. (11). Our result indicates the breakdown of the mean-field picture $\sigma=2$.

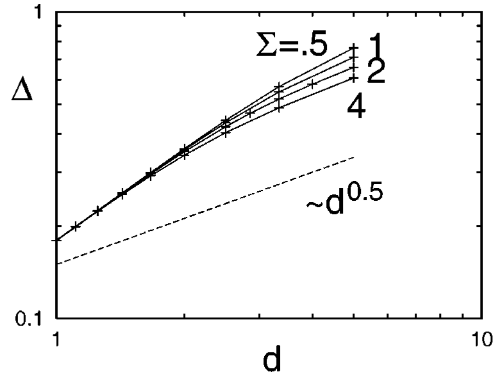

FIG. 4. Mean fluctuation width Δ, Eq. (14), is plotted for wall spacing d. A naive argument postulates $\Delta\propto d$. However, the simulation data exhibit $\Delta\sim d^{0.5}$. We see that the string is straightened macroscopically. Our result supports the "order out of disorder" mechanism proposed by Refs. 1 and 2.

induced mass gap is far larger than that anticipated from the mean field, and hence, the string is subjected to robust pinning potential due to quantum collisions; see Sec. II.

Meanwhile, we also calculated the Roomany-Wyld approximant of the β function,[35]

$$\beta=-\frac{1+\ln(\Delta E_l/\Delta E_{l'})/\ln(l/l')}{(\Delta E_l'\Delta E_{l'}'/\Delta E_l\Delta E_{l'})^{1/2}}, \tag{13}$$

where l and l' denote a pair of system sizes. This approximant, in general, exhibits smaller finite-size collections. In fact, we found that it converges rapidly to the thermodynamic limit. However, the resultant data are identical to those with the aforementioned formula (10) for sufficiently large L. Because we take advantage of very large system sizes owing to the density-matrix renormalization group, the approximant formula (13) is not particularly necessary.

D. Mean-fluctuation deviation

So far, we have extracted the singularity exponent directly from the excitation-gap data. However, as is mentioned in Sec. II, the mean deviation of the string undulations contains information about the exponent:

$$\Delta=\sqrt{\langle x_i^2\rangle-\langle x_i\rangle^2}\sim d^{\sigma/2}. \tag{14}$$

In Fig. 4, we plotted the mean fluctuation width Δ for various d and $\Sigma=0.5$–4. From the plot, we see that there appear two distinctive regimes as in Fig. 2. For small d, Δ is proportional to d, as is anticipated from a naive argument; see Sec. II. However, for large d, Δ starts to bend down, indicating that the string undulation becomes suppressed. Hence, for large d, the conventional picture does not apply. From the slopes, we read off the exponent $\sigma/2\approx0.5$. [This result supports our estimate $\sigma=0.6(3)$ rather than the mean-field value $\sigma=2$.] Hence, we see $\Delta/d\ll1$ as for $d\to\infty$. As a consequence, we found fairly definitely that the string is straightened macroscopically due to quantum collisions. This feature is reminiscent of the infrared divergences encountered in the theory by Zaanen.[1]

IV. SUMMARY AND DISCUSSIONS

We have investigated the quantum entropic (collision-induced) interaction of an elastic string confined between walls (2). We performed a first-principles simulation by means of the density-matrix renormalization group. Our aim is to estimate the singularity exponent σ in the excitation-gap formula (4). The exponent contains a number of significant pieces of information which are overviewed in Sec. II.

In order to estimate σ, we utilized the β function (10), which is readily accessible from our simulation data. From the asymptotic form of large d, we obtained the estimate $\sigma = 0.6(3)$ for $\Sigma = 0.5–4$; see Fig. 3. Our estimate supports the recent proposal[1,2] that ΔE is described by the stretched-exponential form with $\sigma = 2/3$, whereas it might conflict with the mean-field value $\sigma = 2$. It would be noteworthy that the elastic modulus also obeys the stretched exponential, as is shown in our previous study.[18] Hence, it is established fairly definitely that the excitation gap is also described by the stretched-exponential singularity. Namely, the excitation gap is much larger than that anticipated from the mean-field. Moreover, we found that the mean fluctuation width Δ is far less than the wall spacing d: namely, $\Delta \sim d^{0.5}$. This again supports our conclusion rather than the mean field; see Eq. (6).

From those observations, we are led to the conclusion that the string is confined by an extremely robust effective pinning potential due to the quantum collisions; subsequently, a large mass gap opens and Δ gets bounded. Those features are also quite consistent with the findings of the series of works Refs. 1 and 2, validating their ‘‘order out of disorder’’ mechanism responsible for the stabilization of the stripe phase.

Provided that plural strings are concerned, does the value σ get affected? As a matter of fact, the exponent σ is not necessarily universal, but it does exhibit continuous variation[36,37] for a certain class of extended models. More specifically, in Refs. 38 and 39, the authors claim that extended models with high central charges (that is, many random surfaces) exhibit various types of criticalities. Therefore, it is likely that σ would acquire corrections for the multistring case. An extended simulation directed to this issue remains for future study.

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