Physical properties of condensed matters have always been clarified in experiments by measuring their responses to applied fields, e.g. phase transition as a divergence of susceptibility under gradually varying conjugate fields, charge gaps by pumping up the electrons with varying frequencies in spectroscopies. Such "measurement", when applied to theories, requires an extra prescription; setting the system size, \( L \), and quantizing it with the virtual boundaries, which discitizes the energy levels by \( \sim h/L \). By taking \( L \to \infty \), the observables are extrapolated to their bulk values. This size scaling was practically indispensable from the early milestone numerical calculation by Bonner and Fisher on the magnetic susceptibility of spin chains\([1]\). Ever since then, how to reach larger \( L \) and to find an appropriate scaling function was the standard direction of pursuing bulk results. However, even far developed numerics at present are still unable to clarify numerous quantum many body problems, particularly in two dimensions, where the size scaling is extremely difficult. Thid Communication develops a first-step-prescription to overcome this fundamental quantum mechanical problem in theories. The highlight is that one could directly observe physical quantities mimicking their thermodynamic limit at small fixed \( L \). The observables and quantum numbers are continuous functions of applied fields, which enables the determination of the response functions to arbitrary small variation of fields, e.g. the differential susceptibility. In our setup, the continuity of the observables is guaranteed by using the system edges as virtual "particle bath" which is connected to the main part of the system by the small fluctuations. The numerical accuracy of the observables are insensitive to the particle number given on the whole cluster, since the excess particles from the required bulk value is absorbed by the edge "particle bath".

For simplicity, we confine ourselves to one-dimensional (1D) quantum many body lattice models, and test the applicability of our scheme by comparing its demonstration by density-matrix renormalization group(DMRG) \([2, 3]\) with the exact results. However, the present scheme could be extended to higher dimensional systems or applied to any other numerical methods. Let us start from the general Hamiltonian on a 1D lattice consisting of \( L \) sites and with two open ends, 
\[
H = \sum_{i=1}^{L} u(i) + \sum_{i} \sum_{l=1}^{L-1} h_{l}(i), \quad \text{where } u(i) \text{ includes the on-site interaction and potential, and } h_{l}(i) \text{ is the interaction between } i\text{-th and } (i + l)\text{-th sites.}
\]

The major point of our setup is to deform the Hamiltonian as,
\[
H_{\text{deform}} = \sum_{i=1}^{L} f_{0}(i)u(i) + \sum_{i} \sum_{l=1}^{L-1} f_{l}(i)h_{l}(i),
\]

by externally given function, \( f_{l}(i) \), which should smoothly vary from the maximum value near the center to zero at both ends, so as to gradually scale down the energy. The smooth boundary condition is first introduced to realize the flat translationally invariant wave function by getting rid of the boundary effects\([5, 6]\). Such a flat wave function is recently realized systematically by another function called sine-square deformation (SSD) with \( f_{l}(i) = \sin^{2}\left(\frac{\pi(i+(L-l)/2)}{L}\right) \), which turned out to suppress the finite-size effects. Indeed, in the critical system, this SSD Hamiltonian, \( H_{\text{SSD}} \), realizes a wave function of PBC \([7, 9]\), whose reason is partially clarified\([10, 11]\).

In our framework, we mainly adopt this SSD as a representative \( f_{l}(i) \), since it is an established boundary and does not include adjustable parameters. However, notice that \( f_{l}(i) \) is not limited to SSD, since the translational invariance/flattness of the wave function is not required in our scheme. We confirmed that any function as far as it is convex downward at the edges, could be applied(see the results in Fig.2(e)), We took full advantage regarding \( f_{l}(i) \) that the energy and quantum fluctuation are all scaled down to nearly zero at the edges, and use these edges as buffers to absorb the deviation of energies and particle numbers from the thermodynamic value in the main part of the system. Using this setup, we develop an unprecedented method to calculate the static "bulk" responses to applied field.

In the following, the on-site field, \( u(i) \) in Eq.(1), plays an important role; the Zeeman term, \(-\hbar f_{0}(i) S_{l}^{z} \), where \( \hbar \) is the external magnetic field and \( S_{l}^{z} \) is the \( z\)-component of
Fig. 1(a), the magnetization curve of the analyses no longer requires such fine tuning. In contrast, the present was indispensable to recover the translational invariance in the number operator. In the SSD Hamiltonian, the fine tuning of the spin operator on site \( -\Delta = 1 \) with \( \Delta = 1 \) and XXZ (\( \Delta = 2 \)) spin chain as a function of magnetic field \( h \), with \( J = 1 \). The results are obtained by the DMRG with \( m \leq 200 \) on \( \mathcal{H}_{\text{SSD}} \) by our analyses. The solid line is the exact solution. The inset shows the magnified curve near the cusp at \( h \sim 1.8 \) for \( J_2/J_1 = 0.5 \) for several system sizes.

The analyses to obtain the above results are extremely simple. We fix the value of \( h \), give appropriate but not necessarily precise total number of the \( z \)-component of spins, \( M_{\text{given}} \), and perform a usual DMRG on \( \mathcal{H}_{\text{deform}} \) (here we take \( \mathcal{H}_{\text{SSD}} \)) to calculate the expectation value of the local operator, \( \langle S_i^z \rangle \). The representative behavior of the spacial dependence of \( \langle S_i^z \rangle \) is shown in Fig. 2(a) for the Heisenberg chain under magnetic field. There arises two types of spacial oscillations with short and long periods with a particularly large peak at the edge. The center line of the oscillation near \( i - L/2 \) is almost flat, which is expected to reproduce the value of \( \langle S_i^z \rangle \) realized in the bulk limit, \( \langle S_z \rangle_{L=\infty} \). One could extract systematically the value of \( \langle S^z \rangle_{L=\infty} \) as in the following. We first take the average of \( \langle S_i^z \rangle \) from the center of the system toward the edge over \( 2r \) sites as,

\[
O(r) = \frac{1}{2r} \sum_{i=-r}^{r-1} \langle S_{i+r}^z \rangle, \tag{2}
\]

as shown in Fig. 2(b). Reflecting the non-uniform structure of \( \langle S_i^z \rangle \) throughout the system, \( O(r) \) oscillates from \( r = 1 \), with coexisting large and small periods. One could safely fit \( O(r) \) by setting the fitting range from one node of the large oscillation to another. The broken line in Fig. 2(b) is the result fitted in powers of \( r \) as, \( O(r) = m_0 + c r^2 \). The resultant \( m_0 \) give the magnetization density, \( M/L \), shown in Fig. 1(b) in almost perfect coincidence with the exact solution even for system size as small as \( L = 32 \), a relatively small size which could be calculated even by the exact diagonalization. The obtained results are thus arbitrary continuous real numbers, and are free from finite size discreteness.

Let us discuss the implication of the success in taking \( m_0 = \langle S_z \rangle_{L=\infty} \). Figure 2(c) shows the expectation value of the nearest neighbor spin-spin interaction, \( \langle S_i^z S_{i+1}^z \rangle \). The results for \( M_{\text{given}} = 13 \) is almost uniform, whereas for \( M_{\text{given}} = 16 \) a large oscillation amplitude is found near the edges. However, the bond energy, \( e(i) = J f_1(i) \langle S_i^z S_{i+1}^z \rangle \), which is scaled down smoothly from the center toward the edge, are al-
most equivalently smooth for both cases (see Fig. 2(c)). This is because the energy of extra spins, $\Delta M = M_{\text{given}} - m_0 L$ ($\sim 3$ for $M_{\text{given}} = 16$), which concentrate near the edge sites, remains almost zero, so that they can be approximately excluded from the main part of the system. Thus, one could effectively get rid of the excess $\Delta M > 0$ by concentrating them near the edge sites, or supply the deficient $\Delta M < 0$ from the edge site to the center of the system (see the lower panel of Fig. 2(c)). The variational determination of a wave function in standard DMRG automatically carries out this procedure. In other words, the edge site serves as a small particle bath which is connected smoothly with the main part of the system, and the distribution of the spins/particles are automatically optimized by the variational principle. One may regard this as a “grand canonical” setup, in analogy with the grand canonical ensemble used for convenience in quantum mechanical problems when it is not easily solved by fixing the number of particles in the system for technical reason. Here, the finite $L$ requires smooth variation of non-integer particle number under applied field, which cannot be given by hand as a conserved number. Instead, by loosely dividing the system into energetically inequivalent center and the edges by the scaling function $f_1(i)$, and allowing for a small quantum fluctuation of energy and particle numbers between them via $-f_1(j)\delta_1(j)$ ($j$: near the edges), one could obtain a non-integer expectation number as a quantum ensemble. The range of the ensemble required to adjust the particle density within the order of $1/L$ near the system center, does not need to be large. Namely, a small bath connected with the small fluctuation is enough.

One thus expects that $m_0$ does not depend on the choice of $M_{\text{given}}$ owing to the buffer edges. Figure 2(d) shows $m_0$ at fixed $h$ as a function of $M_{\text{given}}$. There exists an inflection point in the very vicinity of the exact solution $m_{\text{exact}}$, which remains almost unchanged with $L$. This point, giving with most precise result, can be detected practically as $M_{\text{given}}$ having the minimum of the total energy. This fact also verifies the variational principle we discussed earlier. We also perform the same analysis under the OBC without deformation. Notice that the scale of the vertical axis is ten times larger than the deformed results, and that $m_0$ is a linearly increasing function of $M_{\text{given}}/L$, i.e. with no inflection point. This comparison guarantees that not the translational symmetry breaking itself, but the spatial scaling down of the Hamiltonian, is important to endow the edge site a role of particle bath.

We further examined the accuracy of the evaluated $m_0$ as a function of $h$ for various $M_{\text{given}}/L$, as shown in Fig. 2(e). Regardless of the value of $M_{\text{given}}$, $m_0$ is a smooth function of $h$, and the deviation from the exact results remains less then
the center of the system as,
\[ O(r) = \frac{1}{2\rho} \sum_{i=-r}^{r-1} (n_{i+} + n_{i-}) = \rho + cr^2, \]  
(3)
will give the electron density in the bulk limit, \( \rho \), for any value of \( \mu \). Figure 3 shows the \( \mu-\rho \) curve at \( U/t = 4 \) for \( L = 64 \), which clearly indicates kinks at \( \mu = \pm \Delta_c(L = \infty)/2 \), where \( \Delta_c(L = \infty) = 1.2867(2) \) is the charge gap evaluated from the exact solution[13]. Again, the curve is continuous and the typical finite size effect remains less than the order of \( 10^{-4} \) (see the comparison of \( L = 32, 64 \) and 80 in the inset). We also calculated the charge gap, \( \Delta_c^{\text{(OBC)}}(L) \), under usual OBC without deformation, and plotted them together in the inset of Fig.3 by sharing the two axes, \( \rho \) and \( -\mu \), with \( 1 + L^{-1} \) and \( \Delta_c^{\text{(OBC)}}(L)/2 \), respectively, due to the following context; the states at \( |\mu| \geq \Delta_c/2 \) off the gap are the Tomonaga-Luttinger liquid, where the low energy excitation is dominated by the bosonic quasi-particles which can be approximated by the non-interacting fermions in a 1D chain in the dilute limit. In calculating \( \Delta_c(L) \) with electron number, \( N_e^{\text{given}} = L + 1 \), the density of the doped quasi-particle corresponds to \( 1/L \), and \( \Delta_c(L) \) as a function of \( 1/L \) will approximately give its low energy dispersion, namely the bulk \( \mu-\rho \) curve. Indeed, as shown in the inset of Fig.3, \( \Delta_c(L) \) as a function of \( 1/L \) show good correspondence with the \( \mu-\rho \) curve by our analyses, which means that our grand canonical analysis on small systems well reproduce the bulk properties.

To summarize, we elucidated a way to directly obtain bulk physical quantities against continuously varying field in a small finite size cluster. We find that scaling down the energy of the Hamiltonian from the system center toward the edges endows to the edge state a role as a small particle bath. The particles trapped at the edges have negligibly small energy, and are connected to the bulk part by an ideally small fluctuation. The variational optimization of the wave function actually uses the edge sites as particle bath, and one obtains continuously varying conserved numbers \( S_z^2 \) or \( N_e \) in the main part of the system. The results obtained are almost free from finite size effect and reproduces the exact solution within the accuracy of \( \sim 10^{-4} \) even for the system as small as \( L \sim O(10) \). The present analyses is applied to methods other than DMRG, such as exact diagonalization, quantum Monte Carlo method, or other variational methods, as far as the optimized wave function is used, and thus will open a new path toward solving numerous still unknown problems in low-energy many body physics.

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