Generalized Moment Method for Gap Estimation and Quantum Monte Carlo Level Spectroscopy

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We formulate a convergent sequence for the energy gap estimation in the worldline quantum Monte Carlo method. The ambiguity left in the conventional gap calculation for quantum systems is eliminated. Our estimation will be unbiased in the low-temperature limit, and also the error bar is reliably estimated. The level spectroscopy from quantum Monte Carlo data is developed as an application of the unbiased gap estimation. From the spectral analysis, we precisely determine the Kosterlitz-Thouless quantum phase-transition point of the spin-Peierls model. It is established that the quantum phonon with a finite frequency is essential to the critical theory governed by the antiadiabatic limit, i.e., the $k = 1$ SU(2) Wess-Zumino-Witten model.

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The excitation gap is one of the most fundamental physical quantities in quantum systems. The Haldane phase and the Z_2 topological phase are characterized by the topologically protected gap [1]. Recently, the existence of gapful or gapless quantum spin-liquid phases has been discussed in frustrated spin systems [2]. Not only in the gapful but also critical phases, the system-size dependence of the excitation gap is useful for the analysis of the quantum phase transition [3]. Particularly, the energy gap Δ in the conformal quantum phases scales as $\Delta \propto xv/L$, apart from possible logarithmic correction, where L is the system size, x is the scaling dimension, and v is the velocity appearing in the conformal field theory [4]. An unbiased gap calculation, thus, allows for extracting the universal properties of the critical phases from finite-size data.

The gap estimation for large systems is not trivial. For small systems, it is possible to calculate the gap by the exact diagonalization method. The reachable system size is, however, strongly limited because of the explosion of required memory size and computation time. The density matrix renormalization group (DMRG) method [5] works well for many one-dimensional systems, but it becomes less effective in gapless or degenerated phases. In the meantime, the quantum Monte Carlo (QMC) method based on the worldline representation is a powerful method for various strongly correlated systems without dimensional restriction [6]. In previous QMC calculations [7], the gap is extracted by the fitting of the correlation function; the tail of the exponential function is estimated as a fitting parameter [see Eq. (1) below]. Here we encounter a trade-off between the systematic error and the statistical error. The lower the temperature is in a QMC simulation, the smaller the systematic error becomes, but the statistical error becomes larger. It is because the correlation in long imaginary time has an exponentially small absolute value. Since in practice we do not have prior knowledge of the optimal temperature and the range of imaginary time where the correlation function follows the asymptotic form, a choice of data necessarily introduces some bias in the fitting procedure. Our purpose in the present Letter is to establish a versatile and unbiased gap-estimation procedure free from an ambiguous fitting.

In the meantime, the recently advanced technology has allowed for quantum simulators that can realize ideal quantum many-body systems [8]. In particular, the quantum phonon effect of trapped ions has caught a great deal of attention, which provides rich physics and engineering, e.g., spin frustration [9], long-range spin interaction [10], phonon superfluids [11], quantum gates [12], etc. As an application of the present gap-estimation method, we will elucidate the quantum phase transition of the spin system coupled with quantum phonons, which is called the spin-Peierls transition [13–19] and is accessible in the ion system [20]. The level spectroscopy [3] from Monte Carlo data is developed to overcome the difficulty of the [Kosterlitz-Thouless (KT)] transition that makes the conventional approaches ineffective. We establish that the quantum phonon effect is essential to the spin-Peierls system and its critical phenomena.

The spectral information of a quantum system described by a Hamiltonian H is encoded in the imaginary time (dynamical) correlation function:

$$\begin{aligned} C(\tau) &= \langle \hat{O}(\tau)\hat{O}^\dagger \rangle = \frac{1}{Z}\mathrm{tr}[e^{\tau H}\hat{O}e^{-\tau H}\hat{O}^\dagger e^{-\beta H}] \\ &= \frac{1}{Z}\sum_{\ell,\ell'} b_{\ell,\ell'} e^{-\tau(E_\ell - E_{\ell'})} e^{-\beta E_{\ell'}} \\ &\to \sum_{\ell\geq 1} b_\ell e^{-\tau(E_\ell - E_0)} \quad (\beta\to\infty), \end{aligned} \tag{1}$$

where $\hat{\mathcal{O}}$ is a chosen operator, Z is the partition function, and $\beta = 1/T$ is the inverse temperature. Also, $\{|\ell\rangle\}$ is the complete orthogonal set of eigenstates, E_ℓ is the associated eigenenergy, $b_{\ell,\ell'} = |\langle \ell'|\hat{O}|\ell\rangle|^2$, and $b_\ell = b_{\ell,0}$, where the ground state is $|0\rangle$, the first excited state is $|1\rangle$, and so are the higher excited states, respectively. We assume $\hat{\mathcal{O}}|0\rangle \neq 0$, $\langle 0|\hat{\mathcal{O}}|0\rangle = 0$, and $E_\ell > E_0$ $(\ell \geq 1)$; i.e., the ground state is certainly excited by the operator, and the gap is finite. The latter is the case for finite-size systems even if the ground state is degenerated in the thermodynamic limit.

Here, let us consider the moment of the imaginary time correlation function [21]:

$$I_k = \frac{1}{k!}\int_0^\infty \tau^k C(\tau)d\tau = \sum_{\ell\geq 1}\frac{b_\ell}{\Delta_\ell^{k+1}} \quad (k\geq 0), \tag{2}$$

where $\Delta_\ell \equiv \Delta_{\ell,0}$ and $\Delta_{\ell,\ell'} = E_\ell - E_{\ell'}$. The higher moment will be dominated by the contribution from the first excitation gap as $I_k \sim b_1/\Delta_1^{k+1}$ because $\Delta_1 < \Delta_2 < \Delta_3 < \cdots$. Then we can see a useful limit, $(I_k/I_{k+m})^{1/m} \to \Delta_1$ $(k\to\infty)$ $\forall\, m \in \mathbf{N}$. However, we cannot use the moment directly in finite-temperature simulations. It is because the correlation function is periodic for bosons or antiperiodic for fermions, and the moment is not well defined. Then the Fourier series can be exploited instead. Let us think of the bosonic case because we will investigate spin excitation. The Fourier component of the correlation function at a Matsubara frequency $\omega_j = 2\pi j/\beta$ $(j\in\mathbf{Z})$ is expressed as

$$\tilde{C}(\omega_j) = \int_0^\beta C(\tau)e^{i\tau\omega_j}d\tau = \begin{cases} \dfrac{1}{Z}\displaystyle\sum_{\ell,\ell'}\frac{g_{\ell,\ell'}\Delta_{\ell,\ell'}}{\Delta_{\ell,\ell'}^2+\omega_j^2} & (\omega_j\neq 0) \\ \dfrac{1}{Z}\left\{\displaystyle\sum_{E_\ell\neq E_{\ell'}}\frac{g_{\ell,\ell'}}{\Delta_{\ell,\ell'}} + \sum_{E_\ell = E_{\ell'}} b_{\ell,\ell'}e^{-\beta E_\ell}\beta\right\} & (\omega_j = 0), \end{cases} \tag{3}$$

where $g_{\ell,\ell'} = b_{\ell,\ell'}(e^{-\beta E_{\ell'}} - e^{-\beta E_\ell})$. In many simulations, the so-called *second moment* [22] is used as the lowest-order gap estimator:

$$\hat{\Delta}_{(1,\beta)} = \omega_1\sqrt{\frac{\tilde{C}(\omega_1)}{\tilde{C}(\omega_0)-\tilde{C}(\omega_1)}} \to \sqrt{\frac{I_0}{I_2}} \quad (\beta\to\infty). \tag{4}$$

Interestingly, this estimator will be the ratio of the zeroth and the second moment in the low-temperature limit. We have to take notice of the systematic error carefully. The error remains even in $\beta\to\infty$ as

$$\frac{\hat{\Delta}_{(1,\beta)}}{\Delta_1} \to 1+\frac{1}{2}\sum_{\ell>1}\left[\frac{b_\ell}{b_1}\frac{\Delta_1}{\Delta_\ell} + O\left(\left(\frac{\Delta_1}{\Delta_\ell}\right)^2\right)\right], \tag{5}$$

which is typically a few percent of Δ_1 [23]. This correction hampers proper identification of the universality class in the level spectroscopy analysis as we will see below.

Our main idea in the present Letter is to construct a sequence of gap estimators that converges to a ratio of higher-order moments in the low-temperature limit. We will consider an estimator that has a correction of $O((\Delta_1/\Delta_\ell)^{2n-1})$. Let us expand Eq. (3) in powers of $(1/\beta\Delta_{\ell,\ell'})$ and make a linear combination of Fourier components so that the lowest orders cancel: $(-1)^n\sum_{k=0}^n x_{n,k}\tilde{C}(\omega_k) = \sum_{\ell,\ell'} g_{\ell,\ell'}\omega_1^{2n}\Delta_{\ell,\ell'}^{-(2n+1)}/Z + O(\beta^{-(2n+2)}\Delta_{\ell,\ell'}^{-(2n+3)})$ with coefficients $x_{n,k}$. It will be dominated by the smallest gap Δ_1 in $\beta\to\infty$ and $n\to\infty$. The coefficients $x_{n,k}$ satisfy the following equations: $\sum_{k=0}^n x_{n,k}k^{2m} = \delta_{m,n}$ $(0\leq m\leq n)$, where δ_{mn} is the Kronecker delta. They are exactly solved for by the formula of the inverse of Vandermonde's matrix [24]. We can also show $(-1)^{n-1}\sum_{k=0}^n k^2 x_{n,k}\tilde{C}(\omega_k) = \sum_{\ell,\ell'} g_{\ell,\ell'}\omega_1^{2(n-1)}\Delta_{\ell,\ell'}^{-(2n-1)}/Z + O(\beta^{-2n}\Delta_{\ell,\ell'}^{-(2n+1)})$ by using the same $x_{n,k}$. Then, a sequence of the higher-order estimators is derived as

$$\hat{\Delta}_{(n,\beta)} = \omega_1\sqrt{-\sum_{k=0}^n k^2 x_{n,k}\tilde{C}(\omega_k)\bigg/\sum_{k=0}^n x_{n,k}\tilde{C}(\omega_k)} \tag{6}$$

with $x_{n,k} = 1/\prod_{j=0,j\neq k}^n (k+j)(k-j)$. Importantly, $\hat{\Delta}_{(n,\beta)} \to \sqrt{I_{2(n-1)}/I_{2n}}$ $(\beta\to\infty)$, and the systematic error is expressed as

$$\frac{\hat{\Delta}_{(n,\beta)}}{\Delta_1} \to 1+\frac{1}{2}\sum_{\ell>1}\left[\frac{b_\ell}{b_1}\left(\frac{\Delta_1}{\Delta_\ell}\right)^{2n-1} + O\left(\left(\frac{\Delta_1}{\Delta_\ell}\right)^{2n}\right)\right]. \tag{7}$$

Note that I_k can be achieved only for even-numbered k since $\tilde{C}(\omega_j)$ is real. As examples, $(x_{2,0}, x_{2,1}, x_{2,2}) = (\frac{1}{4}, -\frac{1}{3}, \frac{1}{12})$ for $n=2$ [23] and $(x_{3,0}, x_{3,1}, x_{3,2}, x_{3,3}) = (-\frac{1}{36}, \frac{1}{24}, -\frac{1}{60}, \frac{1}{360})$ for $n=3$. We have analytically written down the bias of the gap estimator (6) and shown the following remarkable property:

$$\lim_{n\to\infty}\lim_{\beta\to\infty}\hat{\Delta}_{(n,\beta)} = \lim_{\beta\to\infty}\lim_{n\to\infty}\hat{\Delta}_{(n,\beta)} = \Delta_1. \tag{8}$$

That is, these two limits are interchangeable (see the Supplemental Material [25] for details). This important property makes our gap estimation greatly robust. Note that the present approach works also in the stochastic series expansion QMC method by the time generation [27].

Our generalized gap estimator is applicable to any quantum system. As an example, we will show an application with the level spectroscopy to the following one-dimensional $S = 1/2$ spin-Peierls model:

$$H = \sum_r \left[1 + \sqrt{\frac{\omega\lambda}{2}}(a_r + a_r^\dagger)\right] S_{r+1} \cdot S_r + \sum_r \omega a_r^\dagger a_r, \quad (9)$$

where ω is a dispersionless phonon frequency, λ is a spin-phonon coupling constant, S_r is the spin-$\frac{1}{2}$ operator, and a_r and $a_r^\dagger$ are the annihilation and creation operator of the soft-core bosons (phonons) at site r, respectively. This spin-Peierls model has been investigated in the adiabatic limit ($\omega \to 0$) [13], from the antiadiabatic limit ($\omega \to \infty$) [14–18,28,29], and in its crossover [19]. The relevance of the present model to real materials, such as $CuGeO_3$ [30], has been discussed [31]. The model is expected to exhibit a KT-type quantum phase transition between the Tomonaga-Luttinger (TL) liquid phase and the dimer phase at a finite spin-phonon coupling [15,19], which is absent when either the spin or phonon is classically treated [13]. The realization of the quantum phase transition was recently proposed in the trapped ion system [20].

It is difficult to precisely locate the transition point by the conventional analyses. The huge Hilbert space with the soft-core bosons hinders the sufficient-size calculation by the diagonalization method [16]. The effective spin-model approach by the perturbation [14] or the unitary transformation [17] does not take into account all marginal terms, e.g., the four-spin and six-spin interactions examined in Ref. [32]. As for the DMRG method, it needs an additional symmetry breaking term, which blurs the phase-transition point, in the degenerated phase [28]. In addition, the method has difficulty in precise calculation of the relevant quantities, such as the central charge, around an essential singularity [33]. Also, the previous QMC approach [29] suffers from the exponential divergence of the correlation length and the logarithmic correction around the KT transition point. These difficulties mentioned above can be overcome by employing the level spectroscopy method [3,34] combined with our precise gap estimation. In the TL liquid phase, both the triplet and singlet excitations are gapless in the thermodynamic limit, but the lowest excited state of finite-size systems is the triplet because of the logarithmic correction [35]. In the dimer phase, on the other hand, the first excited state is the singlet for finite-size systems. It forms the degenerated ground states eventually in the thermodynamic limit. Thus, the excitation gaps of the triplet and singlet excitation intersect at a spin-phonon coupling for finite-size systems. The transition point can be efficiently extrapolated from the gap-crossing points [3].

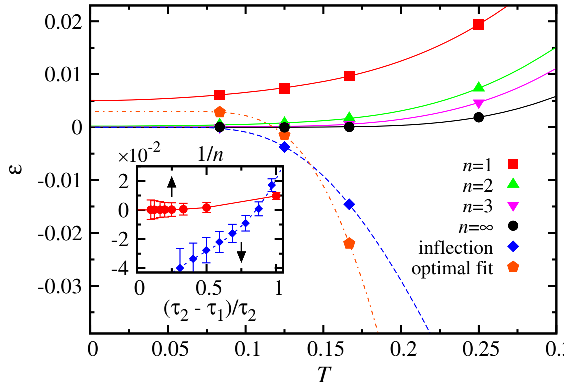

FIG. 1 (color online). Triplet-gap-estimation (relative) error of our estimators (6) ($n = 1, 2, 3, \infty$), the inflection-point value of $-d \log C(\tau)/d\tau$, and the optimal fit (defined in the main text) for the spin-Peierls model (9) with $L = 4$, $\omega = 4$, $\lambda = 1/2$, $D = 4$, which has $\Delta_1 \simeq 1.111\,388$. The inset shows the n dependence of the gap estimate (circles) for $1 \le n \le 10$ and the τ_1 dependence of the $\log C(\tau)$ linear-fit result (diamonds) for $\tau_1 \le \tau \le \tau_2$ with $\tau_2 = \beta/4$, calculated from $2^{20}(\sim 10^6)$ Monte Carlo steps at $\beta = 6$.

We used the continuous-time worldline representation [27,36] and the worm (directed-loop) algorithm [37] in the QMC method. Thanks to the exponential form of the diagonal operators, our simulation is free from an occupation-number cutoff of the soft-core bosons. The Fourier components of the correlation function (3) are directly calculated during the simulation. The worm-scattering probability is optimized in rejection (bounce) rate by breaking the detailed balance [38]. The boundary condition was periodic in the space and time directions. More than $2^{25}(\simeq 3.4 \times 10^7)$ Monte Carlo samples were taken in total after $2^{18}(\simeq 2.6 \times 10^5)$ thermalization steps. The error bar of the gap estimates is calculated by the jackknife analysis [39].

First, the convergence of our gap estimate was tested for $L = 4$, $\omega = 4$, $\lambda = 1/2$, where L is the system size. We set ω here fairly larger than the actual spin gap because this condition is satisfied for large systems in the relevant spin-phonon coupling region. The boson occupation-number cutoff D was set to 4 only in this test for comparing with the diagonalization result. Figure 1 shows the calculated triplet-gap-estimation errors, where $\hat{\mathcal{O}} = \sum_r S_r^z e^{i\pi r}$ is used in the dynamical correlation function. We compared the gap estimators (6) to the previous approach [7] where the first gap is estimated as $-d \log C(\tau)/d\tau$ from the asymptotic form (1). The derivative will show a plateau at the gap value in an appropriate τ region. When $\beta(= 1/T)$ is not large enough, however, the plateau is indistinct. Then the inflection point could be used, but it is hard to estimate in practice (here we calculated it by longer QMC simulation for comparison). As another practical and reasonable gap estimation, we test a linear fit of $\log C(\tau)$ for $\tau_1 \le \tau \le \tau_2$, where we fix $\tau_2 = \beta/4$. The inset of Fig. 1 shows the feasible convergence of the gap estimate in n and the

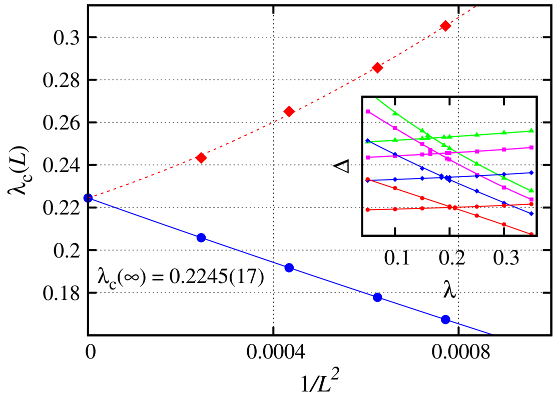

FIG. 2 (color online). Convergence of the gap-crossing point (circles) between the triplet and the singlet excitation for $L = 36, 40, 48, 64$, together with the crossing point of the spin susceptibility (diamonds) between $\chi_s(L)/L$ and $\chi_s(L/2)/(L/2)$. The spin-phonon coupling dependence of the gaps is shown in the inset for each L. The dashed line is the fitting curve with $\lambda_c(\infty)$ fixed, which results in large χ^2/d.o.f. ≈ 5.0. The statistical errors are smaller than the symbol size.

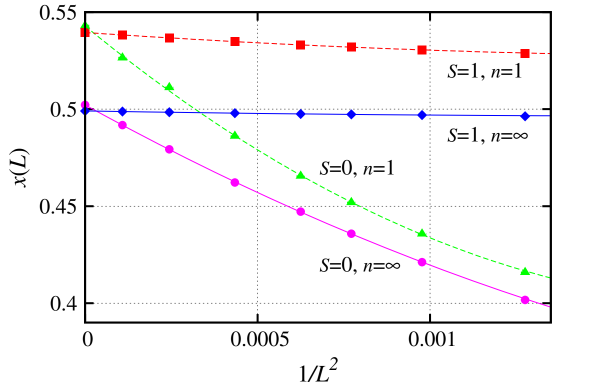

FIG. 3 (color online). System-size dependence of the scaling dimension corresponding to the triplet or the singlet excitation at the transition point ($\lambda = 0.2245$), calculated from the second-moment ($n = 1$) or the $n = \infty$ gap estimate.

difficulty of finding appropriate τ_1 for the linear fit. The function $\log C(\tau)$ is poorly fitted to a linear form at small τ_1, while it has larger statistical error at large τ_1. Then the gap error resulting from the linear regression takes a minimum value at optimal τ_1^*, which we call "optimal fit." Even though it seems reasonable, the optimal fit underestimates the gap at $\beta = 6, 8$ and overestimates it at $\beta = 12$ as shown in the main panel of the figure. Meanwhile, the second-moment estimator ($n = 1$) has a non-negligible bias even in $T \to 0$ as expected from Eq. (5). The estimate with large enough n (we call it the $n = \infty$ estimate hereafter), on the other hand, exponentially converges to the exact value as the temperature decreases [25]. The bias convergence is much faster than that of the inflection point (one of the best estimates from the fitting approach). Moreover, the higher-order estimator provides a reliable error bar, while the optimal fit significantly underestimates it [25]. Therefore, our approach is more precise and straightforward than the fitting approach. In the present study, we have used a simple recipe to optimize n and β, minimizing both the systematic and the statistical error [25].

The scaling of the gap-crossing point for the spin-Peierls model between the triplet and singlet excitation is shown in Fig. 2. For the singlet excitation gap, we used $\hat{O} = \sum_r S_r \cdot S_{r+1} e^{i\pi r}$. The bare excitation phonon gap was set to $\omega = 1/4$ for the comparison with the previous result [29]. The transition point $\lambda_c = 0.2245(17)$ in the thermodynamic limit was extrapolated without logarithmic correction, which is much more precise than the previous estimate, $0.176 < \lambda_c < 0.23$ [29] in our notation. Also, the spin susceptibility $\chi_s = \int_0^\beta \sum_r \langle S_r^z(\tau) S_0^z \rangle e^{i\pi r} d\tau$ could be used for finding the transition point (Fig. 2). Nevertheless, the gap-crossing point provides the much more reliable extrapolation with the $1/L^2$ correction from irrelevant fields [3], while the susceptibility is likely to have some more complicated corrections.

We have also calculated the velocity, the central charge, and the scaling dimensions at the transition point, fixing $\lambda = 0.2245$. The velocity $v = 1.485(8)$ was calculated from the scaling form $v(L) = \Delta_{k_1}/k_1 = v + a/L^2 + b/L^4 + o(1/L^4)$, where Δ_{k_1} is the triplet gap at $k_1 = 2\pi/L$, a and b are nonuniversal constants. The central charge $c = 0.987(13)$ was obtained from the finite-size correction [35], $E_0(L) = E_0 - \pi v c/6L + o(1/L)$. The scaling dimension corresponding to the triplet or singlet excitation was calculated from the relation $x(L) = L\Delta_\pi/2\pi v$, where Δ_π is the lowest (triplet or singlet) excitation gap at $k = \pi$. As shown in Fig. 3, the $n = \infty$ estimates converged to $x_{S=1} = 0.502(3)$ and $x_{S=0} = 0.499(3)$ without logarithmic correction as expected only at the transition point [3]. Hence, we conclude that this transition point is described by the $k = 1$ SU(2) Wess-Zumino-Witten model [40] with $c = 1$ and $x = 1/2$. On the other hand, the second-moment estimates ($n = 1$) failed to approach $1/2$ as seen in Fig. 3. This identification of the critical theory clearly demonstrates the importance of the higher-order estimator. The present study nontrivially clarified that the critical theory at the transition point of the spin-Peierls model with a finite phonon frequency coincides with that in the antiadiabatic limit ($\omega \to \infty$) where the effective spin model is the frustrated J_1-J_2 chain [3]. Our result strongly indicates that the quantum phonon effect is *relevant* to the spin-Peierls system in the sense that it necessarily triggers the universal KT phase transition.

In conclusion, we have presented the generalized moment method for the gap estimation. The advantages of our method over the previous approaches are as follows: the unbiased estimation [Eq. (8)], the absence of ambiguous procedure, the faster convergence with respect to the temperature, and the reliable error-bar estimation. We emphasize that our approach is generally applicable to any quantum system. The QMC level spectroscopy was demonstrated, for the first time, for the KT transition in the spin-Peierls model. This spectral analysis will likely work in various systems including most conformal phases. We elucidated that the quantum phonon effect is relevant to the critical theory of the spin-phonon system, which is expected to be universal in many kinds of one-dimensional systems, e.g., (spinless) fermion-phonon systems, by virtue of the well-established transformations. The clarified quantum phase transition and the criticality would be directly observed in the quantum simulator [20].

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