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Smooth Boundary Conditions for Quantum Lattice Systems

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We introduce a new type of boundary conditions, *smooth boundary conditions*, for numerical studies of quantum lattice systems. In a number of circumstances, these boundary conditions have substantially smaller finite-size effects than periodic or open boundary conditions. They can be applied to nearly any short-ranged Hamiltonian system in any dimensionality and within almost any type of numerical approach.

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In most numerical calculations for quantum systems, periodic boundary conditions (PBC's) are the accepted standard. There are a number of situations, however, where PBC's are inadequate. In systems with some form of incommensurate order, for example, very large system sizes are needed to approximate the incommensurate behavior of the infinite system, and in mean-field methods, where a number of iterations are required to achieve convergence, the system can get stuck in a commensurate state far from the desired incommensurate order. Another example, which forms the primary motivation for this work, stems from the density-matrix renormalization group (RG) method [1]. This new real-space numerical method has proven to be extremely accurate for Heisenberg spin chains [2], but for greatest accuracy requirements are that the chain *not* form a closed loop, as in PBC's. This poses no great inconvenience for the $S=1$ chain, where there is a finite correlation length, but is quite inconvenient for half-integer spin chains (and most 1D fermion systems), where boundary effects decay as a power law.

Recently, new types of boundary conditions, such as self-determined boundary conditions [3] and nebula boundary conditions [4], have been studied in conjunction with quantum Monte Carlo simulations, but cannot be generalized in an easy manner to any arbitrary system or to other types of numerical techniques. In this paper we introduce a new type of boundary conditions, *smooth boundary conditions* (SBC's), which in the circumstances listed above perform better than PBC's and open boundary conditions (OBC's). The main idea of these new boundary conditions is to smoothly "turn off" (set to zero) the parameters of the Hamiltonian near the edges of the system. Surprisingly, in many cases where PBC's or OBC's perform very well, SBC's perform better. They can be applied to numerical calculations for nearly any system with local interactions in any number of dimensions.

After introducing the ideas of SBC's, we will illustrate their use in several systems. The ideas behind SBC's are closely related to the summation of infinite series and the Borel transform, and we will motivate their development by first discussing accelerated convergence of numerical series.

Let $s_n=\sum_{m=0}^{n}a_m$ be a slowly converging alternating series, with $s=\lim_{n\to\infty}s_n$. For example, we can consider the series

$$a_m=(-1)^m/\ln[\ln(m+3)]\,. \tag{1}$$

The summation of such a series can be viewed as a termination problem; if we stop with an odd number of terms, we get a positive result, while stopping with an even number gives a negative result. We would like to find some way of terminating the series in a way that does not bias between an odd and even number of terms. We can do this by constructing a smoothing function, c_m, and taking

$$s\approx\sum_{m=0}^{M}a_m c_m\,. \tag{2}$$

The smoothing function is conveniently described as a continuous function $y(x)$, $0\le x\le 1$, with $y(0)=1$ and $y(1)=0$, samples at a discrete set of M points,

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$$c_m = y(m/M)\,, \tag{3}$$

with $0 < m < M$. An effective choice for $y(x)$ is

$$y(x) = \frac{1}{2}\left[1 - \tanh\frac{x-1/2}{x(1-x)}\right]. \tag{4}$$

This approach is remarkably successful at summing a wide variety of common, slowly converging, alternating series, such as those for π, ln2, etc., attaining results accurate to 10 or 12 digits with 100 terms. Convergence is roughly exponential with M. For the series in Eq. (1), we obtain the result $s = 8.749\,551\,241(2)$ with $M = 100$. The same c_m's are used for each series, and the total numerical work is extremely small. Note that all derivatives of y are zero at 0 and 1; in fact, the function has essential singularities at 0 and 1. These properties are crucial for effective termination of a series; for example, if the function $y(x) = (1-x^2)^2$ is used, for which $y'' \neq 0$ at 0 and 1, convergence is only quadratic in $1/M$.

This procedure is closely related to the Borel transform [5], which is usually applied to *divergent* series. The Borel transform of the series s is defined as

$$a(x) = \sum_{m=0}^{\infty} \frac{a_m}{m!} x^m. \tag{5}$$

From the definition of $a(x)$ it follows trivially that

$$s = \int_0^{\infty} dx\, e^{-x} a(x)\,. \tag{6}$$

The standard use of the Borel transform is to calculate $a(x)$ and then perform the integration; however, here we will not calculate $a(x)$. We will only assume that $a(x)e^{-x}$ is negligible for x greater than a cutoff M'. We take M' as the upper limit of the integral in Eq. (6), then replace $a(x)$ by its definition Eq. (5), and exchange the sum and integral. We obtain

$$s \approx \sum_{m=0}^{\infty} a_m c_m(M')\,, \tag{7}$$

where

$$c_m(M') = e^{-M'} \sum_{n=m+1}^{\infty} \frac{M'^n}{n!}\,. \tag{8}$$

For $m > M \approx 2M'$, $c_m(M')$ is completely negligible, and the sum in Eq. (7) can be terminated, yielding Eq. (2). In Fig. 1 we show both c_m as defined in Eq. (8) with $M' = 20$, and $y(m/M)$ as defined in Eq. (4) with $M = 40$. The Borel approach and the approach using Eq. (4) are roughly equally effective at summing common series. However, the Borel form is slightly less convenient, since one must chose both M and M'.

This approach to numerical series is largely pedagogical; there are probably even more efficient ways to sum such series. To apply these ideas to reduce finite-size effects in a general Hamiltonian system, we consider first a trivial example, a one-dimensional tight-binding chain.

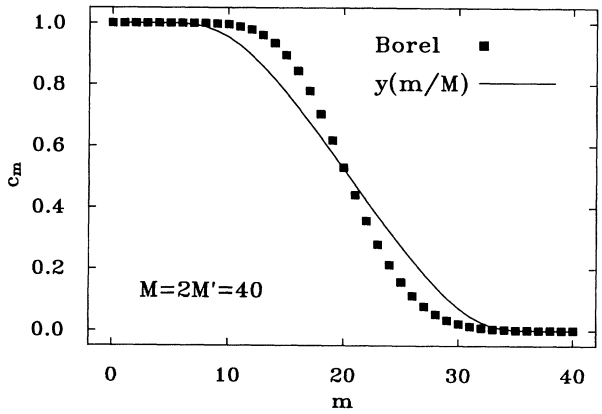

FIG. 1. The smoothing function, c_m, as a function of the lattice site, m. The solid line corresponds to Eq. (4) in the text, and the squares correspond to the smoothing function derived from the Borel transform defined through Eq. (8).

We consider an L-site lattice with hopping matrix element t_i, centered at $E = 0$, with Fermi level ϵ_F, and Hamiltonian matrix

$$H_{ij} = -t_i \delta_{j,i+1} - t_j \delta_{i,j+1}\,. \tag{9}$$

Ordinarily t_i (which gives the hopping between sites i and $i+1$) is a constant t. To apply SBC's we set

$$t_i/t = \begin{cases} c_{M-i}, & 1 \le i \le M, \\ 1, & M < i \le L-M, \\ c_{i-L+M}, & L-M < i < L. \end{cases} \tag{10}$$

Here c_i is the smoothing function defined by Eq. (4) or Eq. (8).

We also need to adjust the diagonal elements of H. A general rule for applying SBC's is that in the limit that the width of the smoothing region $M \to \infty$, the local properties of the system should be constant with i. In this case the Fermi level ϵ_F is constant across the system, so that, as we vary the local bandwidth, we must shift the band center so that ϵ_F strikes the band in the same *relative* position. Thus, Eq. (9) becomes

$$H_{i,j} = -t_i \delta_{j,i+1} - t_j \delta_{i,j+1} + \delta_{i,j}\epsilon_F \left[1 - \frac{t_{i-1}+t_i}{2t}\right]. \tag{11}$$

Note that Eq. (11) explicitly depends on ϵ_F, whereas Eq. (9) does not. This Hamiltonian reproduces the properties of the infinite system extremely well, even on a relatively small lattice.

If OBC's are used on this system, edge effects produce slowly decaying Friedel-type oscillations in local properties, such as the density. PBC's work much better, but still, the typical energy level spacing decays only as $1/L$. SBC's concentrate more states at ϵ_F than elsewhere. The advantages of this are apparent in Fig. 2, where we plot

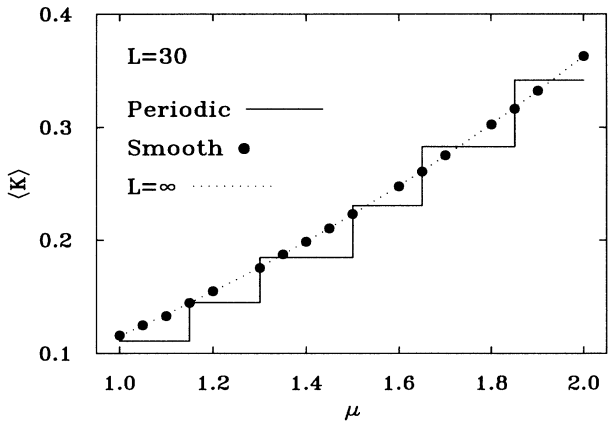

FIG. 2. The average kinetic energy, $\langle K\rangle$, as a function of the chemical potential, μ, for the noninteracting one-dimensional tight-binding chain with $L=30$ sites. For SBC's the smoothing occurs on the leftmost and rightmost 10 sites.

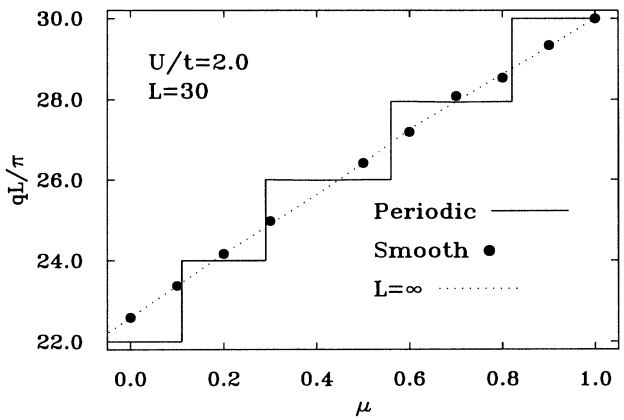

FIG. 3. The incommensurate spin-density-wave vector, q, on a Hubbard chain as a function of the chemical potential, μ. The chain has $L=30$ sites, the on-site repulsion is $U/t=2.0$, and for the SBC's the smoothing occurs on the leftmost and rightmost 10 sites. Here q is rescaled by L/π in order to show that with PBC's the spin density wave is commensurate with the lattice.

the average kinetic energy per site, $\langle K\rangle$, as a function of the chemical potential, $\mu=\epsilon_F$. The choice of PBC's shows the presence of discontinuous jumps, typical of a finite-size system. On the other hand, the use of SBC's eliminates the discontinuities in $\langle K\rangle$ already on a system as small as $L=30$ sites, and agrees extremely well with the infinite system results. The Friedel-like edge effects are also absent (not shown).

We next consider incommensurate spin-density-wave order in the positive-U 1D Hubbard Hamiltonian [6] within a mean-field approximation. The Hubbard Hamiltonian is

$$H=-\sum_{i,\sigma} t_i(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i,\sigma}) +\sum_i U_i n_{i,\uparrow}n_{i,\downarrow}-\sum_{i,\sigma}\mu_i n_{i,\sigma}, \tag{12}$$

which consists of a system of electrons with an on-site interaction with coupling constant U_i. Here t_i is the nearest-neighbor hopping parameter between sites i and $i+1$, and μ_i is the chemical potential. The $c_{i,\sigma}^{\dagger}$ are fermion creation operators at site i with spin σ, and $n_{i,\sigma}=c_{i,\sigma}^{\dagger}c_{i,\sigma}$. Here t_i/t is scaled according to the left-hand side of Eq. (10) when we use SBC's and $U_i/U=\mu_i/\mu=(1/2t)(t_{i-1}+t_i)$, where t, U, and μ are the bulk values.

Applying the Hartree-Fock approximation, we rewrite the density operators as

$$n_{i,\sigma}=\langle n_{i,\sigma}\rangle+\delta n_{i,\sigma}=\langle n_{i,\sigma}\rangle+(n_{i,\sigma}-\langle n_{i,\sigma}\rangle)\,. \tag{13}$$

We then insert Eq. (13) in the Hamiltonian of Eq. (12), ignore terms quadratic in the density fluctuations, $\delta n_{i,\sigma}$, and obtain the effective Hartree-Fock Hamiltonian

$$H_{\mathrm{HF}}=-\sum_{i,\sigma} t_i(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}^{\dagger}c_{i,\sigma}) +\sum_{i,\sigma}(U_i\langle n_{i,-\sigma}\rangle-\mu_i)n_{i,\sigma}, \tag{14}$$

where we have dropped all constant terms. This Hamiltonian can be easily diagonalized, and solutions can be found self-consistently by iteration. Previous studies using PBC's and OBC's have shown that the Hamiltonian in Eq. (14) has both spin and charge incommensurate density waves [7,8]. Here we will show that the incommensurate wavelength for the bulk can be already determined to high accuracy on a small lattice using SBC's but not with standard boundary conditions.

In Fig. 3 we show the incommensurate spin-density-wave vector q as a function of the chemical potential, $\mu=\epsilon_F$, on a lattice with $L=30$ sites. We find that when applying PBC's to the system, q takes only commensurate, discrete values. On the other hand, when considering SBC's with all energy scales (t_i/t and U_i/U) decreasing on the rightmost and leftmost 10 sites according to the smooth function defined in Eq. (10), we see that q increases smoothly with μ in agreement with the infinite lattice results, which were derived from solving the system on larger lattices ($L=120,180$ sites) with OBC's and SBC's and finding no changes in the results upon increasing L or changing types of boundary conditions. It is clear from Fig. 3 that, even on a small lattice ($L=30$), SBC's give results that are in good agreement with the results in the bulk.

To show that the application of SBC's is not only effective for noninteracting systems or within mean-field theories, we studied the Heisenberg chain using the density-matrix RG approach [1,2]. Here, we consider an antiferromagnetic $S=\frac{1}{2}$ Heisenberg chain described by the Hamiltonian

$$H=\sum_{i=1}^{L} J_i\mathbf{S}_i\cdot\mathbf{S}_{i+1}\,. \tag{15}$$

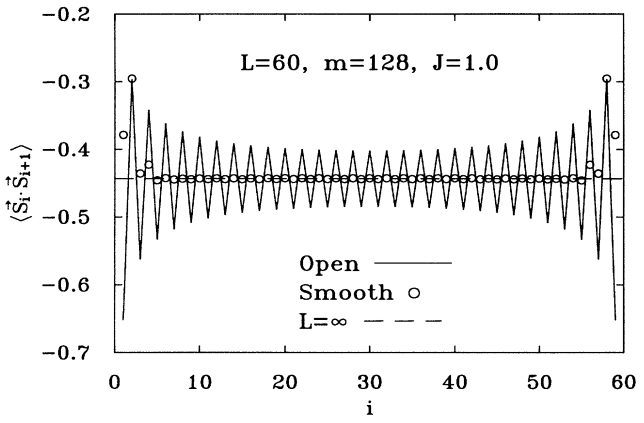

FIG. 4. The bond strength, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$, as a function of the site index, i, for an $S = \frac{1}{2}$ Heisenberg chain with $L = 60$ sites and $m = 128$ states kept. For SBC's the smoothing occurs on the leftmost and rightmost 10 sites.

The Bethe ansatz exact solution to the model for the infinite system predicts a ground state energy, $E_0 = \frac{1}{4} - \ln 2$, with $S_z^T = 0$, where S_z^T is the z component of the total spin [9]. As expected from the valence bond picture of the $S = \frac{1}{2}$ chain [2], the density-matrix RG calculations show that the effect of OBC's causes a strong alternation in the bond strength, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$, as a function of the site index, i. This alternation decays very slowly as the size of the system is increased [2].

We apply SBC's in order to eliminate, even on a relatively small chain, the bond-strength alternation which is absent in the infinite system. For this purpose, we choose J_i/J according to the function on the left-hand side of Eq. (10). In Fig. 4 we show the bond energy per site, $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ as a function of the site index, i, with OBC's and SBC's on a chain with $L = 60$ sites. It is clear that the strong-bond alternation present in the system with OBC's is strongly suppressed when we apply SBC's.

In summary, we have studied the effect of SBC's on one-dimensional systems of interacting particles. For all systems under consideration (noninteracting Fermi gas, Hubbard model, and Heisenberg chain) and within all numerical techniques used (exact diagonalization, mean-field self-consistent calculations, numerical renormalization group), the use of SBC's allows one to greatly reduce finite-size effects (such as spatial fluctuations and frustration) and extrapolate to the thermodynamic limit on relatively small systems. The use of SBC's can easily be extended to quantum Monte Carlo techniques, and to systems of higher dimensionality, where work is still in progress.

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