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Supersymmetric quantum mechanics on the lattice: I. Loop formulation

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Abstract

Simulations of supersymmetric field theories on the lattice with (spontaneously) broken supersymmetry suffer from a fermion sign problem related to the vanishing of the Witten index. We propose a novel approach which solves this problem in low dimensions by formulating the path integral on the lattice in terms of fermion loops. For $\mathcal{N} = 2$ supersymmetric quantum mechanics the loop formulation becomes particularly simple and in this paper – the first in a series of three – we discuss in detail the reformulation of this model in terms of fermionic and bosonic bonds for various lattice discretisations including one which is Q-exact.

1. Introduction

Independently of whether or not supersymmetry is realised in high energy particle physics, supersymmetric quantum field theories remain to be interesting and fascinating on their own. One intriguing feature of supersymmetric theories is for example the emergence of a Goldstino mode when the supersymmetry is broken, or the appearance of mass degenerate multiplets of fermionic and bosonic particles if the ground state of the theory is invariant under the supersym-

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metry transformation. In nature though, such degeneracies among elementary particles have so far not been observed, and as a consequence the supersymmetry must be spontaneously broken at some scale [1] if supersymmetry is indeed a true symmetry of nature. In fact, the spontaneous breaking of supersymmetry is a generic phenomenon which is relevant for many physical systems beyond particle physics and quantum field theories. The question of spontaneous supersymmetry breaking, however, cannot be addressed in perturbation theory and nonperturbative methods are therefore desirable and even crucial. In the past, numerical simulations of quantum field theories on Euclidean lattices have proven to be a very successful tool for studying nonperturbative phenomena. Consequently, a lot of effort has been put into the lattice formulation of supersymmetric field theories, e.g. [2–8], see [9] for a comprehensive review. Finding an appropriate formulation, however, turns out to be far from trivial due to the explicit breaking of symmetries in connection with the discretisation. The Poincaré group for example is broken down to the subgroups of discrete rotations and finite translations by multiples of the lattice spacing. Since supersymmetry is an extension of the Poincaré algebra, a complete realisation of the continuum supersymmetry algebra on the lattice is therefore not possible. For lattice regularised theories which are composed of local lattice operators, however, the remnant subgroups guarantee that the Poincaré symmetry is fully restored in the continuum. Unfortunately, in contrast to the Poincaré symmetry, for supersymmetry there is in general no subgroup left on the lattice which could play the role of the discrete subgroups above. It is therefore a priori not clear at all how a lattice formulation can be found for which supersymmetry is restored in the continuum [10], a problem which can eventually be traced back to the failure of the Leibniz rule on the lattice [11–13].

Apart from the explicit breaking of supersymmetry by the finite lattice spacing, additional complications for the investigation of supersymmetric theories on the lattice arise from the finite extent of the lattice. One problem concerns for example supersymmetry breaking due to finite temperature, or the tunnelling between separate ground states on finite volumes. While the former problem can be circumvented by assigning periodic boundary conditions to the fermionic variables in (imaginary-)time direction (at the price of losing the concept of temperature), the latter problem requires an explicit extrapolation to the thermodynamic infinite volume limit. Whether and how such an extrapolation interferes with the extrapolation to the continuum limit, where the lattice spacing goes to zero, is obviously an interesting question. It is hence important to understand all the systematics of the lattice regularisation in detail, in particular the interplay between the infrared and ultraviolet regulators, and a thorough comprehension of these problems and the corresponding solutions is crucial for any investigation of spontaneous supersymmetry breaking.

It turns out that even a simple system such as $\mathcal{N} = 2$ supersymmetric quantum mechanics subsumes all the complications discussed above [14,15]. In addition, it also provides a testing ground for any new approach to regularise, and possibly simulate, supersymmetric field theories on the lattice [16–18]. Therefore, besides being worth studying in its own right, supersymmetric quantum mechanics provides an ideal set up for nonperturbative investigations of supersymmetric field theories on the lattice. Consequently, supersymmetric quantum mechanics on the lattice has been the subject of intensive studies. Over time, different discretisation schemes have been developed in order to meet the requirement of the correct continuum limit of the theory [9,19,20]. In the context of unbroken supersymmetry, these schemes have well established numerical support [21–24]. For broken supersymmetry, however, the model reveals a severe fermion sign problem affecting simulations with standard Monte Carlo methods [25,26]. Because of this additional obstruction, first results in the context of broken supersymmetry were published only very recently [27].

In a series of three papers we introduce and exploit a novel approach with which it is possible to study, and in fact solve, supersymmetric quantum mechanics on the lattice for both broken and unbroken supersymmetry. In particular, we reformulate the system and its degrees of freedom in terms of fermionic and bosonic bond variables. This reformulation – the subject matter of the present paper – is based on the exact hopping expansion of the bosonic and fermionic actions on the lattice and allows the explicit decomposition of the partition function into bosonic and fermionic contributions. This explicit separation of the system paves the way for circumventing the fermion sign problem which appears for broken supersymmetry due to the vanishing of the Witten index. Furthermore, the formulation in terms of bond variables enables the construction of explicit transfer matrices which in turn allow to solve the lattice system exactly. As a consequence we are then able to study in extenso the continuum and infinite volume limit of systems both with broken or unbroken supersymmetry. In particular, by means of Ward identities one can precisely illustrate how supersymmetry is restored. Furthermore, in the context of broken supersymmetry the emergence of the Goldstino mode in the thermodynamic limit and at zero temperature can be studied in detail. In summary, all the problems and issues appearing in the context of realising supersymmetry on the lattice can be addressed and studied by means of the exact results from the loop formulation. This investigation will be the subject matter of the second paper in the series. Finally, the formulation also forms the basis for a highly efficient fermion string algorithm [28,29] which may be employed in numerical Monte Carlo simulations. Thus in the third paper of the series we eventually describe the details and properties of the algorithm which can be validated using the exact results from the transfer matrices. While the exact solution of the lattice system is specific to the low dimensionality and the subsequent simplicity of the supersymmetric quantum mechanics system, the bond formulation and the fermion string algorithm is applicable also to more complicated systems, e.g. in higher dimensions, or involving gauge fields. In particular it can be applied to supersymmetric Yang–Mills quantum mechanics [30] and certain two-dimensional supersymmetric field theories, such as the $\mathcal{N} = 1$ Wess–Zumino model [31–34] and the supersymmetric nonlinear O(N) sigma model [35].

The present paper concerns the reformulation of supersymmetric quantum mechanics on the lattice in terms of bosonic and fermionic bonds. Starting from the formulation of supersymmetric quantum mechanics as an Euclidean quantum field theory, we discuss its lattice formulation using different variants of Wilson fermions including a Q-exact discretisation in Section 2. There we also emphasise the generic fermion sign problem which arises for numerical simulations of systems with broken supersymmetry due to the vanishing of the Witten index. In Section 3 we derive the loop formulation for both the fermionic and the bosonic degrees of freedom, while in Section 4 we discuss in detail how observables such as the fermionic and bosonic two-point functions are calculated for generic boundary conditions in the loop formulation. Finally, in Appendix A we summarise the explicit actions emerging for the various discretisations from the different superpotentials which we employ throughout this and the following papers of the series.

2. Supersymmetric quantum mechanics on the lattice

We start our discussion with the partition function of a zero dimensional supersymmetric quantum mechanical system with temporal extent L in the path integral formalism [36],

$$Z = \int \mathcal{D}\phi \mathcal{D}\overline{\psi} \mathcal{D}\psi \; \mathrm{e}^{-S(\phi,\overline{\psi},\psi)} \tag{1}$$

with the Euclidean action

$$S(\phi, \overline{\psi}, \psi) = \int_0^\beta dt \Big\{ \frac{1}{2} \left(\frac{d\phi(t)}{dt} \right)^2 + \frac{1}{2} P'(\phi(t))^2 + \overline{\psi}(t) \left(\partial_t + P''(\phi(t)) \right) \psi(t) \Big\}. \tag{2}$$

Here, $\phi(t)$ is a commuting bosonic coordinate while the two (independent) anticommuting fermionic coordinates are denoted by $\overline{\psi}(t)$ and $\psi(t)$. The derivative of the arbitrary superpotential $P(\phi(t))$ is taken with respect to ϕ, i.e. $P' = \frac{\partial P}{\partial \phi}$ and $P'' = \frac{\partial^2 P}{\partial \phi^2}$. For infinite temporal extent and fields vanishing at infinity, the action is invariant under the $\mathcal{N} = 2$ supersymmetry transformations $\delta_{1,2}$,

$$\begin{aligned} &\delta_1 \phi = \bar{\epsilon} \psi, && \delta_2 \phi = \overline{\psi} \epsilon, \\ &\delta_1 \psi = 0, && \delta_2 \psi = \left(\dot{\phi} - P' \right) \epsilon, \\ &\delta_1 \overline{\psi} = -\bar{\epsilon} \left(\dot{\phi} + P' \right), && \delta_2 \overline{\psi} = 0, \end{aligned} \tag{3}$$

where $\bar{\epsilon}$ and ϵ are Grassmann parameters and $\dot{\phi} = \frac{d\phi}{dt}$. For finite extent, however, the variation of the action under the supersymmetry transformations $\delta_{1,2}$ yields the nonvanishing terms

$$\delta_1 S = \int_0^\beta dt \left(-\bar{\epsilon} \left(\psi P'' \dot{\phi} + \dot{\psi} P' \right) \right) = \bar{\epsilon} \psi P' \Big|_0^\beta, \tag{4}$$

$$\delta_2 S = \int_0^\beta dt \left(\dot{\overline{\psi}} \dot{\phi} + \overline{\psi} \ddot{\phi} \right) \epsilon = \overline{\psi} \dot{\phi} \epsilon \Big|_0^\beta \tag{5}$$

which can only be brought to zero by imposing periodic boundary conditions for the fermionic degrees of freedom, i.e.,

$$\psi(\beta) = \psi(0), \qquad \overline{\psi}(\beta) = \overline{\psi}(0). \tag{6}$$

Thus, choosing thermal, i.e., antiperiodic boundary conditions for the fermionic degrees of freedom breaks supersymmetry explicitly.

For specific choices of the superpotential $P(\phi)$ the supersymmetric system may enjoy additional symmetries. With the superpotential

$$P_u(\phi) = \frac{1}{2} \mu \phi^2 + \frac{1}{4} g \phi^4 \tag{7}$$

the resulting action is for example invariant under a parity transformation $\phi \to -\phi$, since

$$\left(P_u'(-\phi) \right)^2 = \left(P_u'(\phi) \right)^2, \qquad P_u''(-\phi) = P_u''(\phi), \tag{8}$$

and thus has an additional $\mathbb{Z}_2$-symmetry. This is the potential we will use in the following as an illustrating example for a quantum mechanical system with unbroken supersymmetry, hence the subscript u. Using the superpotential

$$P_b(\phi) = -\frac{\mu^2}{4\lambda} \phi + \frac{1}{3} \lambda \phi^3 \tag{9}$$

which we will use as an illustrating example for a system with broken supersymmetry, one finds that the action is invariant under a combined *CP* symmetry,

$$\phi(t) \to -\phi(t), \tag{10}$$

$$\psi(t) \to \overline{\psi}(t), \tag{11}$$

$$\overline{\psi}(t) \to \psi(t). \tag{12}$$

In the Schroedinger formalism, the partner potentials $\frac{1}{2}P_b'^2 \pm P_b''$ of a system with broken supersymmetry are connected through a mirror symmetry, and it turns out that the combined *CP* symmetry is just a manifestation of this mirror symmetry in the field theory language.

We now formulate the theory on a discrete lattice Λ by replacing the continuous (Euclidean) time variable $t \in [0, L]$ by a finite set of L_t lattice sites $x_n = an$, $n = 0, \ldots, L_t - 1$ separated by the lattice spacing $a = \frac{L}{L_t}$,

$$\Lambda = \{x \in a\mathbb{Z} \mid 0 \leq x \leq a(L_t - 1)\}. \tag{13}$$

Then, in order to formulate the path integral of supersymmetric quantum mechanics as a one-dimensional lattice field theory, we define the path integral measure on the lattice as

$$\int \mathcal{D}\phi\mathcal{D}\overline{\psi}\mathcal{D}\psi \equiv \prod_{x=0}^{L_t-1} \int_{-\infty}^{\infty} d\phi_x \int d\overline{\psi}_x \int d\psi_x, \tag{14}$$

such that the lattice partition function is given by

$$Z = \int \mathcal{D}\phi\mathcal{D}\overline{\psi}\mathcal{D}\psi \; \mathrm{e}^{-S_\Lambda(\phi,\overline{\psi},\psi)}, \tag{15}$$

where S_Λ is a suitable discretisation of the action. It requires the replacement of the temporal integration in the action by a discrete sum over all lattice sites,

$$\int_0^L dt \longrightarrow a \sum_{x=0}^{L_t-1}, \tag{16}$$

and the replacement of the continuous derivatives by suitable lattice derivatives. In the following two Subsections 2.1 and 2.2 we discuss in detail two suitable lattice actions.

In principle, it is now straightforward to evaluate the partition function (15), for example numerically using Monte Carlo algorithms. However, for a system with broken supersymmetry one encounters a severe fermion sign problem when standard Metropolis update algorithms are employed. We will address this issue in more detail in Subsection 2.3.

Finally, we note that the continuum limit of the lattice theory is taken by fixing the dimensionful parameters μ, g, λ and L while taking the lattice spacing $a \to 0$. In practice, the dimensionless ratios $f_u = g/\mu^2$, $f_b = \lambda/\mu^{3/2}$ fix the couplings and μL the extent of the system in units of μ, while $a\mu$ and a/L are subsequently sent to zero. Then, by attaching a physical scale to L for example, the physical values for all other dimensionful quantities follow immediately. Employing antiperiodic boundary conditions for the fermion, the extent L corresponds to the inverse temperature, hence the system at finite μL represents a system at finite temperature and the limit $\mu L \to \infty$ implies a system at zero temperature.

2.1. Standard discretisation

The most obvious choice for discretising the continuous derivatives in the action is to use the discrete symmetric derivative

$$\widetilde{\nabla} = \frac{1}{2}(\nabla^+ + \nabla^-) \tag{17}$$

where

$$\nabla^- f_x = \frac{1}{a}(f_x - f_{x-a}), \tag{18}$$

$$\nabla^+ f_x = \frac{1}{a}(f_{x+a} - f_x) \tag{19}$$

are the backward and forward derivatives, respectively. However, it is well known that the symmetric derivative leads to the infamous fermion doubling which, for the sake of maintaining supersymmetry, should be avoided. This can be achieved by introducing an additional Wilson term which removes all fermion doublers from the system,

$$\nabla^W(r) = \widetilde{\nabla} - \frac{ra}{2}\Delta,$$

where $\Delta = \nabla^+\nabla^-$ is the Laplace operator and the Wilson parameter takes values $r \in [-1, 1]\backslash\{0\}$. It turns out that for one-dimensional derivatives the standard choice $r = \pm 1$ yields $\nabla^W(\pm 1) = \nabla^{\mp}$, hence for $r = 1$ the discretised action reads

$$S_\Lambda = a\sum_x \left\{\frac{1}{2}(\nabla^-\phi_x)^2 + \frac{1}{2}P'(\phi_x)^2 + \overline{\psi}_x(\nabla^- + P''(\phi_x))\psi_x\right\} \tag{20}$$

and setting the lattice spacing $a = 1$ we obtain

$$S_\Lambda = \sum_x \left\{\frac{1}{2}(P'(\phi_x)^2 + 2\phi_x^2) - \phi_x\phi_{x-1} + (1 + P''(\phi_x))\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1}\right\}. \tag{21}$$

This is the standard discretisation for the action of supersymmetric quantum mechanics on the lattice. Correspondingly, the supersymmetry transformations (3) discretised on the lattice Λ read

$$\begin{aligned} &\delta_1\phi = \bar{\epsilon}\psi, && \delta_2\phi = \overline{\psi}\epsilon, \\ &\delta_1\psi = 0, && \delta_2\psi = \left(\nabla^-\phi - P'\right)\epsilon, \\ &\delta_1\overline{\psi} = -\bar{\epsilon}\left(\nabla^-\phi + P'\right), && \delta_2\overline{\psi} = 0, \end{aligned} \tag{22}$$

and the variation of the action under δ_1 yields

$$\delta_1 S_\Lambda = -\bar{\epsilon}\sum_x \left\{\psi_x P''(\phi_x)(\nabla^-\phi_x) + P'(\phi_x)(\nabla^-\psi_x)\right\}, \tag{23}$$

and similarly for δ_2. Note, that (23) is the lattice version of the surface term in the continuum, Eq. (4). Since the Leibniz rule does not apply on the lattice, it is not possible to integrate this term by parts and S_Λ is therefore not invariant under the supersymmetry transformations δ_1 and δ_2. This is the explicit supersymmetry breaking by the lattice discretisation which we already pointed out in the introduction. In addition, the Wilson term also breaks the time reversal symmetry, or equivalently the charge conjugation for the fermion in our quantum mechanical system. This can

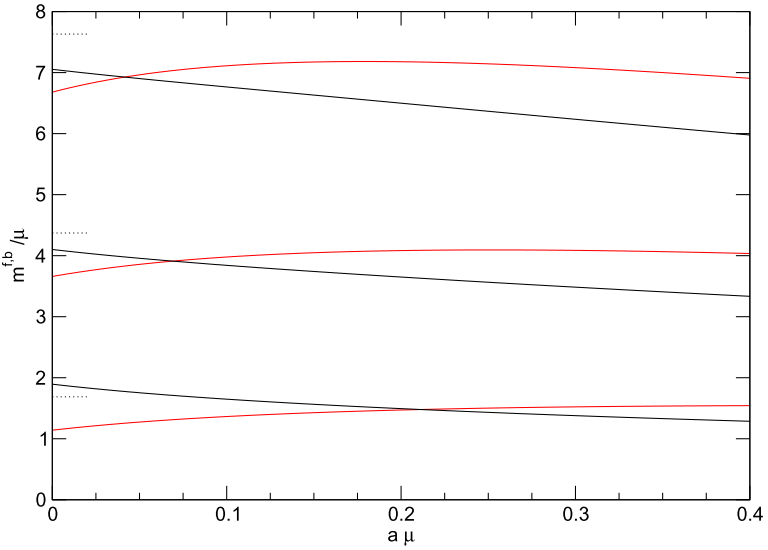

Fig. 1. Continuum extrapolation $a\mu \to 0$ of the bosonic (red lines) and fermionic (black lines) mass gaps expressed in units of μ for unbroken supersymmetry at the coupling $f_u = 1$ using the standard discretisation. The expected continuum values are indicated by dotted lines. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

be seen from the fact that the oriented hopping term $\overline{\psi}_x \psi_{x-1}$ is directed only in forward direction $x - 1 \to x$, while the backward hopping is completely suppressed.[1] As a matter of fact, the discretised system only describes a fermion propagating forward in time, but not the corresponding antifermion propagating backward in time. As we will see later, this has an important consequence for the fermion bond formulation. In the continuum the symmetry is restored and this comes about by the relative contributions of the fermion and antifermion approaching each other in this limit.

At this point, it is necessary to stress that the action in Eq. (20) does not correctly reproduce the continuum limit of the theory [15,19,22]. In Fig. 1, we illustrate this failure by extrapolating the lowest mass gaps of the fermion and the boson for the system with superpotential P_u (unbroken supersymmetry) to the continuum $a\mu \to 0$. The exact calculation is based on the extraction of the mass gaps via transfer matrix techniques which will be discussed in detail in the second paper of this series [37], see also [38]. Note, that the extrapolation of the masses does not yield the known continuum values indicated by the horizontal dotted lines. In fact the bosonic and fermionic mass gaps are not even degenerate in the continuum and supersymmetry is not restored for this discretisation. It turns out that the mismatch is due to perturbative corrections and a careful analysis of those in the lattice theory is therefore mandatory [15]. However, since this quantum mechanics model is superrenormalisable, there are only a finite number of terms which do not converge to the correct continuum limit, and it is therefore sufficient to add a finite number of counterterms to the lattice action. Note that as opposed to a quantum field theory in higher dimensions, the counterterms do not diverge in quantum mechanics, but remain finite as $a \to 0$.

[1] For an arbitrary choice of the Wilson parameter $0 < |r| < 1$ both directions would be present.

As explicitly shown in [15], in order to restore supersymmetry in the continuum, it is necessary and sufficient to add the term $P''/2$ to the lattice action, i.e.,

$$S_\Lambda \longrightarrow S_\Lambda^c = S_\Lambda + \frac{1}{2}\sum_x P''(\phi_x)\,. \tag{24}$$

The term can be understood as a radiative correction and we will see in Section 2.3 how the term arises in the explicit calculation of the determinant of the Wilson Dirac matrix. Finally, it is important to note that the resulting lattice theory is not supersymmetric at finite lattice spacing, but in the continuum limit it will nevertheless flow to the correct supersymmetric theory without any further fine tuning.

2.2. *Q-exact discretisation*

A discretisation of supersymmetric quantum mechanics which avoids the fine tuning of counterterms is based on the idea that it might be sufficient to preserve only a subset of the full supersymmetry at finite lattice spacing in order to reach the correct continuum limit. This approach, known under the name of twisted supersymmetry, was first applied to supersymmetric quantum mechanics in [19] and can be established in the context of topological field theory [39], or from a lattice superfield formalism [14]. For $\mathcal{N} = 2$ supersymmetric quantum mechanics it relies on the observation that the lattice variation $\delta_1 S_\Lambda$ of the standard discretised action in (23) can be written – up to a minus sign – as the variation of the lattice operator

$$O = \sum_x P'(\phi_x)(\nabla^- \phi_x) \tag{25}$$

under the same supersymmetry transformation δ_1, such that we have

$$\delta_1 S_\Lambda = -\delta_1 O. \tag{26}$$

It is then clear that the invariance of the action under the supersymmetry transformation δ_1 can be restored by simply adding the term O to the action. The bosonic part of the so constructed action can be written as

$$S^Q_{\Lambda,\text{bosonic}} = \sum_x \left\{\frac{1}{2}(\nabla^-\phi_x)^2 + \frac{1}{2}P'(\phi_x)^2 + P'(\phi_x)(\nabla^-\phi_x)\right\}, \tag{27}$$

and the total action in more compact form as

$$S^Q_\Lambda = \sum_x \left\{\frac{1}{2}\left((\nabla^-\phi_x) + P'(\phi_x)\right)^2 + \overline{\psi}_x(\nabla^- + P''(\phi_x))\psi_x\right\}. \tag{28}$$

This is the Q-exact lattice action which preserves the supersymmetry δ_1 exactly (but not δ_2) for finite lattice spacing. The Q-exactness can be best seen in the off-shell formulation of the total action. Using an auxiliary field and defining the fermionic variation by $\delta_1 = \bar{\epsilon}\,Q$, where Q is the generator of the supersymmetry transformation [39], one can write the total action off-shell as the Q-variation of a particular function F, i.e. $S_\Lambda = QF$. This makes the Q-exact invariance of the action explicit via the nilpotency property $Q^2 = 0$ [9]. Maintaining this single supersymmetry on the lattice is sufficient to protect the theory from radiative contributions which would otherwise spoil the continuum limit. Note, that this action corresponds to the Ito prescription in [22]. In complete analogy, one can also construct a Q-exact action invariant under δ_2 but not δ_1, or in fact a Q-exact action invariant under any linear combination of δ_1 and δ_2, but not invariant under

the corresponding orthogonal linear combination. This property is related to the fact that the improved lattice field theory is topological and hence the improvement term O can be added to the action with any prefactor different from zero to obtain a Q-exact action [39]. Each variant leads to a different discretisation of the bosonic part of the action. For the loop formulation we will concentrate on the form given in Eqs. (27) and (28), but of course the reformulation can be achieved for any Q-exact action. Before getting more specific, we will now discuss the fermion sign problem emerging in simulations of systems with broken supersymmetry.

2.3. Fermion sign problem from broken supersymmetry

In this section we discuss the fermion sign problem which affects standard Monte Carlo simulations of supersymmetric systems with broken supersymmetry. The problem is generic and affects all supersymmetric systems with (spontaneously) broken supersymmetry since it is related to the vanishing of the Witten index accompanying any spontaneous supersymmetry breaking. In the particularly simple supersymmetric quantum mechanics case we consider here in this paper, the problem can be illustrated very explicitly.

In order to evaluate the partition function in Eq. (15), in a first step one usually integrates out the fermionic degrees of freedom in the path integral which then yields the determinant of the fermion Dirac operator $D(\phi)$, i.e.,

$$Z = \int \mathcal{D}\phi \ \det(D(\phi)) \ \mathrm{e}^{-S^B_\Lambda(\phi)}, \tag{29}$$

with $S^B_\Lambda(\phi)$ being the purely bosonic part of the lattice action. In the following we will concentrate on the Wilson Dirac operator $D(\phi) = \nabla^- + P''(\phi)$, but the considerations apply equally to any fermion discretisation. It turns out that depending on the specific choice of the superpotential $P(\phi)$ the determinant is not positive definite. In that case the effective Boltzmann weight $\det(D(\phi))\exp\{-S^B_\Lambda(\phi)\}$ cannot be interpreted as a probability distribution and the standard Monte Carlo approach breaks down. In fact, since the partition function with periodic boundary conditions is proportional to the Witten index, which vanishes in systems with (spontaneously) broken supersymmetry, the partition function itself must be zero. From Eq. (29) it then becomes clear that this can only be achieved by the determinant being indefinite and in fact zero on average. The cancellations between positive and negative contributions of the determinant to the partition function are hence maximal and constitute a severe fermion sign problem. Since the fermion determinant $\det(D(\phi))$ can be calculated analytically both in the continuum [22,40,41] and on the lattice, one can illustrate this explicitly and we will do so in the next two subsections. Moreover, the considerations will also be useful for the interpretation of the reformulation in terms of fermion loops.

2.3.1. The fermion determinant in the continuum

For the evaluation of the fermion determinant in the continuum, some regularisation is necessary. A suitable choice is given by dividing the determinant by the fermion determinant of the free theory, $\det(\partial_t + \mu)$. Moreover, the computation of the fermion determinant depends essentially on the choice of the boundary conditions for the fermionic degrees of freedom.

For antiperiodic boundary conditions $\psi(L) = -\psi(0)$, the regularised determinant yields

$$\det\left(D(\phi)\right) \doteq \det\left(\frac{\partial_t + P''(\phi)}{\partial_t + \mu}\right) = \frac{\cosh\left(\frac{1}{2}\int_0^L dt \ P''(\phi)\right)}{\cosh\left(\frac{1}{2}\mu L\right)} \tag{30}$$

and we observe that this is always positive. Furthermore, writing the cosh function in terms of exponentials, we find that

$$\det\left(D(\phi)\right) \propto \exp\left(+\frac{1}{2}\int_0^L dt\ P''(\phi)\right) + \exp\left(-\frac{1}{2}\int_0^L dt\ P''(\phi)\right) \tag{31}$$

and hence the partition function (29) decomposes into two parts which just correspond to the bosonic and the fermionic sector, respectively. To be specific, one has

$$\int \mathcal{D}\phi\ \det\left(D(\phi)\right)\ \mathrm{e}^{-S^B(\phi)} = \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_-(\phi)} + \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_+(\phi)} \equiv Z_0 + Z_1\,, \tag{32}$$

where the actions

$$S^B_\pm(\phi) = \int_0^L dt \left\{\frac{1}{2}\left(\frac{d\phi(t)}{dt}\right)^2 + \frac{1}{2}P'(\phi(t))^2 \pm \frac{1}{2}P''(\phi(t))\right\} \tag{33}$$

remind us of the partner potentials in the usual Hamilton formulation of supersymmetric quantum mechanics, and Z_0 and Z_1 are the partition functions in the bosonic and fermionic sector, respectively. Since we have calculated the determinant for antiperiodic boundary conditions, we have

$$Z_0 + Z_1 = Z_a \tag{34}$$

and we note that Z_a is positive since both Z_0 and Z_1 are positive.

For periodic boundary conditions $\psi(L) = \psi(0)$, the analogous calculation of the regularised fermion determinant yields

$$\det\left(D(\phi)\right) = \frac{\sinh\left(\frac{1}{2}\int_0^L dt\ P''(\phi)\right)}{\sinh\left(\frac{1}{2}\mu L\right)} \tag{35}$$

and writing out the sinh function as a sum of exponentials, we find

$$\int \mathcal{D}\phi\ \det\left(D(\phi)\right)\ \mathrm{e}^{-S^B(\phi)} = \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_-(\phi)} - \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_+(\phi)} = Z_0 - Z_1 \equiv Z_p\,. \tag{36}$$

More importantly, we note that for this choice of boundary conditions the partition function is indefinite and the fermion determinant is hence not necessarily positive.

We now recalling the definition of the Witten index W from quantum mechanics [42],

$$W = \mathrm{Tr}\left[(-1)^F e^{-\beta H}\right] = \mathrm{Tr}_B\left[e^{-\beta H}\right] - \mathrm{Tr}_F\left[e^{-\beta H}\right] \tag{37}$$

where H is the Hamilton operator and F the fermion number, while $\mathrm{Tr}_{B,F}$ denotes the trace over the bosonic and fermionic states, respectively. Identifying β with L we realise that the Witten index is in fact proportional to the expectation value of the fermion determinant, i.e., the partition function with fully periodic boundary conditions,

$$W \propto Z_p\,. \tag{38}$$

The relation is given as a proportionality because the path integral measure is only defined up to a constant multiplicative factor as compared to the traces in Eq. (37).

In order to see the implications of these results, we consider the two superpotentials P_u and P_b defined in the introduction of Section 2. Recall that the superpotential P_u in Eq. (7) is invariant under the parity transformation $\phi \to -\phi$. Furthermore, for $\mu > 0$ and $g \geq 0$, $P_u''(\phi) > 0$, and Eqs. (35) and (36) then imply that $Z_p \neq 0$ and hence the Witten index is nonzero, $W \neq 0$. Thus, we conclude that for this superpotential supersymmetry is indeed unbroken, in agreement with the generic expectation from supersymmetric quantum mechanics. Next, we consider the superpotential P_b in Eq. (9) which we recall is odd under the parity transformation $\phi \to -\phi$, and so is its second derivative, $P_b''(-\phi) \to -P_b''(\phi)$. On the other hand, the bosonic action $S^B(\phi)$ for this superpotential,

$$S^B(\phi) = \int dt \left\{ \frac{1}{2} \left(\frac{d\phi}{dt} \right)^2 - \frac{1}{2} \left(\frac{\mu^2}{2} \phi^2 - \lambda^2 \phi^4 \right) \right\}, \tag{39}$$

is invariant under the parity transformation, $S^B(-\phi) \to S^B(\phi)$. Therefore, Eqs. (35) and (36) imply that with periodic b.c. for each configuration contributing to the partition function, there is the parity transformed one with exactly the same weight but opposite sign coming from the fermion determinant. Consequently, the partition function Z_p vanishes and the Witten index is $W = 0$. Indeed, for the superpotential P_b one expects on general grounds that supersymmetry is broken.

Obviously, the argument can be reversed leading to the conclusion discussed at the beginning of this section: since the Witten index is zero for a supersymmetric system with broken supersymmetry, the partition function with periodic boundary conditions Z_p, and hence the expectation value of $\det(D)$, vanishes, and this then leads to the fermion sign problem for numerical simulations.

2.3.2. The fermion determinant on the lattice

Next, we calculate the fermion determinant on the lattice. The lattice provides a regularisation, such that we can calculate the determinant directly without division by the determinant of the free theory. Using the lattice discretisation introduced in Section 2.1, the determinant of the fermion matrix can easily be seen to be

$$\det\left(\nabla^- + P''(\phi_x)\right) = \prod_x (1 + P''(\phi_x)) \mp 1, \tag{40}$$

where the -1 $(+1)$ in the last term is associated with periodic (antiperiodic) boundary conditions. Note that this result is consistent with the expression derived for supersymmetric Yang–Mills quantum mechanics in [30]. As in the continuum the fermion determinant decomposes into a bosonic part, the product over all lattice sites x, and a fermionic part, the term ∓ 1. We will see later in Section 3 from the fermion loop formulation that this interpretation is indeed correct.

At this point it is interesting to discuss the continuum limit of the lattice determinant. In principle, one would expect to recover the expressions in Eq. (30) and Eq. (35) when dividing the lattice determinant by the determinant of the free lattice theory and then taking the lattice spacing to zero, $a \to 0$. However, one finds

$$\lim_{a\to 0} \det\left(\frac{\nabla^- + P''(\phi_x)}{\nabla^- + \mu \cdot \mathbb{1}} \right) = \frac{\exp\left(\frac{1}{2} \int_0^L dt \; P''(\phi) \right)}{\exp\left(\frac{1}{2} \mu L \right)} \det\left(\frac{\partial_t + P''(\phi)}{\partial_t + \mu} \right), \tag{41}$$

i.e., taking the naive continuum limit apparently yields an additional factor in front of the continuum determinant. This factor can be understood as the remnants of the radiative corrections

from the Wilson discretisation which survive the naive continuum limit [15]. The term is in fact responsible for the wrong continuum limit of the fermion and boson masses discussed in Section 2.1 and illustrated in Fig. 1.

Let us now proceed by discussing the determinant of the Wilson Dirac matrix for both superpotentials P_u and P_b explicitly. Using the superpotential for unbroken supersymmetry P_u, the determinant yields

$$\det(\nabla^- + P_u''(\phi_x)) = \prod_x (1 + \mu + 3g\phi_x^2) \mp 1 \tag{42}$$

which for $\mu > 0$ and $g \geq 0$ is strictly positive, independent of the boundary conditions. Using the superpotential for broken supersymmetry P_b, the determinant yields

$$\det(\nabla^- + P_b''(\phi_x)) = \prod_x (1 + 2\lambda\phi_x) \mp 1 \tag{43}$$

which is indefinite even for $\lambda > 0$. While this is necessary in order to accommodate a vanishing Witten index, it imposes a serious problem on any Monte Carlo simulation, for which positive weights, and hence positive determinants, are strictly required. Moreover, the sign problem is severe in the sense that towards the continuum limit (i.e., when the lattice volume goes to infinity), the fluctuations of the first summand in Eq. (43) around 1 tend to zero, such that $W \to 0$ is exactly realised in that limit. Hence, the source of the fermion sign problem lies in the exact cancellation between the first and the second summand in Eq. (43), i.e., of the bosonic and fermionic contributions to the partition function, and this observation also holds more generally in higher dimensions [31–33]. In the loop formulation, to be discussed in the next section, the separation of the partition function into the various fermionic and bosonic sectors is made explicit and allows the construction of a simulation algorithm that samples these sectors separately, and more importantly also samples the relative weights between them. In this way, the loop formulation eventually provides a solution to the fermion sign problem.

3. Loop formulation of supersymmetric quantum mechanics

We will now discuss in detail the reformulation of supersymmetric quantum mechanics in terms of bosonic and fermionic bonds, eventually leading to the so-called loop formulation. The bond formulation is based on the hopping expansion for the bosonic and fermionic degrees of freedom. For the latter, the hopping expansion becomes particularly simple due to the nilpotent character of the fermionic variables and in addition reveals the decomposition of the configuration space into the bosonic and fermionic subspaces.

3.1. Loop formulation of the fermionic degrees of freedom

We start by splitting the action into a bosonic and fermionic part

$$S_\Lambda = S_\Lambda^B(\phi) + S_\Lambda^F(\phi, \overline{\psi}, \psi) \tag{44}$$

with

$$S_\Lambda^B(\phi) = \sum_x \left\{ \frac{1}{2}(\nabla^-\phi_x)^2 + \frac{1}{2}P'(\phi_x)^2 \right\}, \tag{45}$$

$$S_\Lambda^F(\phi, \overline{\psi}, \psi) = \sum_x \left\{ \overline{\psi}_x(\nabla^- + P''(\phi_x))\psi_x \right\}, \tag{46}$$

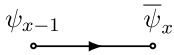

Fig. 2. Graphical representation of the directed fermionic bond b^F.

so that the partition function can be written as

$$Z = \int \mathcal{D}\phi \, \mathrm{e}^{-S^B_\Lambda(\phi)} \int \mathcal{D}\overline{\psi}\mathcal{D}\psi \, \mathrm{e}^{-S^F_\Lambda(\phi,\overline{\psi},\psi)} . \tag{47}$$

Rewriting the fermionic action as in Eq. (21) and introducing $M(\phi) = 1 + P''(\phi)$ for the monomer term we have

$$S^F_\Lambda(\phi, \overline{\psi}, \psi) = \sum_x \left\{ M(\phi_x)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1} \right\}, \tag{48}$$

and expanding separately the two terms in the Boltzmann factor yields

$$\mathrm{e}^{-S^F_\Lambda} = \prod_x (1 - M(\phi_x))\overline{\psi}_x\psi_x \prod_x \left(1 + \overline{\psi}_x\psi_{x-1}\right) . \tag{49}$$

Due to the nilpotency of the Grassmann variables, all terms of second or higher order in $\overline{\psi}_x\psi_x$ or $\overline{\psi}_x\psi_{x-1}$ vanish in the expansion. Introducing fermionic monomer occupation numbers $m(x) \in \{0, 1\}$ as well as the fermionic bond occupation numbers $n^f(x) \in \{0, 1\}$, we can further rewrite the expansion as

$$\mathrm{e}^{-S^F_\Lambda} = \prod_x \left(\sum_{m(x)=0}^{1} \left(-M(\phi_x)\overline{\psi}_x\psi_x\right)^{m(x)} \right) \prod_x \left(\sum_{n^f(x)=0}^{1} \left(\overline{\psi}_x\psi_{x-1}\right)^{n^f(x)} \right) . \tag{50}$$

The fact that the fermionic occupation numbers can only take the values 0 or 1 can be seen as a realisation of the Pauli exclusion principle and follows naturally from the nilpotency property of the fermion fields. Obviously, it is natural to assign the bond occupation number $n^f(x)$ to the link connecting the sites $x - 1$ and x, while the monomer occupation number $m(x)$ lives on the lattice site. The directed fermionic bond can be represented as illustrated in Fig. 2 by an arrow associated to the hopping term $\overline{\psi}_x\psi_{x-1}$ which is either occupied or not.

In a next step we can now integrate out the fermionic variables. The Grassmann integration rule

$$\int d\overline{\psi}d\psi \; \overline{\psi}\psi = -1 \tag{51}$$

tells us that each site x must be occupied by exactly one variable ψ_x and one variable $\overline{\psi}_x$ in order to obtain a nonzero contribution to the path integral. The Grassmann integration at a given site x is either saturated by the monomer term $\propto \overline{\psi}_x\psi_x$, yielding the contribution $M(\phi_x)$ after the integration, or by exactly one ingoing and one outgoing fermionic bond $\propto \overline{\psi}_{x+1}\psi_x \cdot \overline{\psi}_x\psi_{x-1}$, yielding the contribution 1 for each bond after the Grassmann integration. The fact that these two possibilities are exclusive at each site leads to a local constraint on the monomer and bond occupation numbers $m(x)$ and $n^f(x)$ given by

$$m(x) + \frac{1}{2}\left(n^f(x) + n^f(x-1)\right) = 1, \qquad \forall x . \tag{52}$$

As a consequence, the integration over the Grassmann degrees of freedom ψ and $\overline{\psi}$ is replaced by a sum over all possible configurations of monomer and bond occupation numbers satisfying the local constraint (52). The constraint implies that there are only two possible fermionic

bond configurations with nonzero weight. On the one hand, Eq. (52) is satisfied if $m(x) = 1$ and $n^f(x) = 0\ \forall x$. In this case, there are no fermionic bonds, i.e. the fermion number is $F = 0$, and such a configuration hence contributes to the bosonic sector. Each site is then saturated with the monomer term and by applying the Grassmann integration rules we identify the total fermionic contribution to the weight of a configuration to be the product of monomer weights $M(\phi_x)$ at each site x, i.e., $\prod_x (1 + P''(\phi_x))$. On the other hand, Eq. (52) can also be satisfied by $n^f(x) = 1$ and $m(x) = 0\ \forall x$. For such a configuration the fermion number is $F = 1$, since all sites x are connected by fermionic bonds forming a fermionic loop which winds around the lattice. The fermionic bonds contribute with weight 1, hence the total fermionic contribution to the weight of such a configuration is just a factor (-1) where the minus sign follows from integrating out the cyclic loop of hopping terms and is the usual, characteristic fermion sign associated with closed fermion loops. In addition, the fermion loop receives an additional minus sign if antiperiodic boundary conditions for the fermion field are employed. We will discuss this in more detail in Section 3.3.

Summarising the two contributions to the path integral from the integration of the fermionic variables, we have

$$\prod_x \Big(1 + P''(\phi_x)\Big) \mp 1 \tag{53}$$

for periodic and antiperiodic b.c., respectively, and we recognise this as the determinant of the lattice Dirac operator, cf. Eq. (40). The first term from the configuration without any fermionic bonds is identified as the bosonic contribution to the path integral, while the second term from the fermion loop configuration is identified as the fermionic contribution. The partition function can hence be written as

$$Z_{p,a} = Z_0 \mp Z_1 \tag{54}$$

with

$$Z_0 = \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_\Lambda(\phi)} \prod_x \Big(1 + P''(\phi_x)\Big), \tag{55}$$

$$Z_1 = \int \mathcal{D}\phi\ \mathrm{e}^{-S^B_\Lambda(\phi)} \tag{56}$$

where the subscript 0 and 1 denotes the fermion winding number of the underlying fermionic bond configuration, or equivalently the fermion number F. We have thus confirmed the interpretation of the bosonic and fermionic parts contributing to the fermion determinant alluded to in Section 2.3.2.

3.2. *Loop formulation of the bosonic degrees of freedom*

In complete analogy to the previous section we can also replace the continuous bosonic variables ϕ by integer bosonic bond occupation numbers. To keep the discussion simple we first consider the standard discretisation. The bosonic action S^B_Λ in Eq. (21) can be written in the form

$$S^B_\Lambda = \sum_x \{-w \cdot \phi_x \phi_{x-1} + V(\phi_x)\} \tag{57}$$

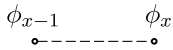

Fig. 3. Graphical representation of the bosonic bond $b^B_{1\to 1}$.

where we have separated the (nonoriented) hopping term $w \cdot \phi_x \phi_{x-1}$ with the hopping weight $w = 1$ from the local potential term $V(\phi_x) = \frac{1}{2}(P'(\phi_x)^2 + 2\phi_x^2)$. Expanding now the exponential of the hopping term in the Boltzmann factor we obtain

$$\mathrm{e}^{-S^B_\Lambda} = \prod_x \left(\sum_{n^b(x)=0}^{\infty} \frac{(w \cdot \phi_{x-1}\phi_x)^{n^b(x)}}{n^b(x)!} \right) \prod_x \mathrm{e}^{-V(\phi_x)}. \tag{58}$$

The summation indices $n^b(x)$ can be interpreted as bosonic bond occupation numbers, but in contrast to the fermionic case there is no Pauli exclusion principle which truncates the expansion, and hence the summation runs from 0 to infinity.

To make further progress we now need to combine this with the result from the expansion in the fermionic variables, and so we obtain for the full partition function

$$Z = \int \mathcal{D}\phi \prod_x \left(\sum_{n^b(x)=0}^{\infty} \frac{(w \cdot \phi_{x-1}\phi_x)^{n^b(x)}}{n^b(x)!} \right) \prod_x \mathrm{e}^{-V(\phi_x)} \prod_x \left(\sum_{m(x)=0}^{1} M(\phi_x)^{m(x)} \right). \tag{59}$$

In order to integrate over the variable ϕ_x locally at each site we select a particular entry in each of the sums. This is equivalent to choosing a particular bond configuration $\{n^b(x)\}$ and fermionic monomer configuration $\{m(x)\}$. The rearrangement of the bosonic fields, essentially collecting locally all powers of ϕ_x, yields local integrals of the form

$$Q(N(x), m(x)) = \int_{-\infty}^{\infty} d\phi_x \; \phi_x^{N(x)} \mathrm{e}^{-V(\phi_x)} M(\phi_x)^{m(x)} \tag{60}$$

where the site occupation number

$$N(x) = n^b(x) + n^b(x-1) \tag{61}$$

counts the total number of bosonic bonds attached to the site x. This can be visualised by a graphical representation of the bond as a (dashed) line connecting the sites $x-1$ and x as in Fig. 3. The site occupation number is then just the number of bonds connected to a site from the left and the right.

As a consequence of the reordering, the weight of the chosen bond and monomer configuration factorises as

$$W\left(\{n^b(x)\}, \{m(x)\}\right) = \prod_x \frac{w^{n^b(x)}}{n^b(x)!} Q(N(x), m(x)). \tag{62}$$

Depending on the specific form of the superpotential $P(\phi)$ the site weight Q might vanish for certain values of N and m. This essentially induces a local constraint on the number of bosonic bonds attached to a site, e.g. $N \bmod 2 = 0$ for potentials even in ϕ, similar to the constraint on the fermionic bond occupation numbers. The constraint simply reflects the symmetry property of the underlying bosonic field and has important consequences e.g. for the observables as discussed in Section 4.

Let us now consider how the bosonic hopping expansion is modified when the action with a counterterm, Eq. (24), or the Q-exact action in Eq. (27) is employed. While the counterterm simply changes $V(\phi) \to V(\phi) + P''(\phi)/2$ and hence the site weight Q, the Q-exact discretisation has a more severe impact on the hopping expansion. To be more specific, the Q-exact actions demand for additional kinds of bosonic bonds as can be seen by explicitly calculating the term O in Eq. (25). Using for example the superpotential P_u we have

$$O = \sum_x P'_u(\phi_x)(\nabla^- \phi_x) = \sum_x \left\{ \mu\phi_x^2 + g\phi_x^4 - \mu\phi_x\phi_{x-1} - g\phi_x^3\phi_{x-1} \right\}. \tag{63}$$

While the first two terms $\mu\phi_x^2$ and $g\phi_x^4$ just modify the potential $V(\phi)$ describing the local bosonic self-interaction, the third term $-\mu\phi_x\phi_{x-1}$ matches the standard hopping term and modifies the hopping weight $w = 1 \to w = 1 + \mu$. The fourth term $-g\phi_x^3\phi_{x-1}$, however, introduces a new kind of bosonic hopping and hence a new bosonic bond with weight g. Since the hopping carries one power of the bosonic variable ϕ at the left ending and three powers ϕ^3 at the right ending the new bosonic bond is directed. In order to distinguish the two different types of bosonic bonds, we label them by indicating the number of bosonic variables they carry at each ending, i.e. $b^B \to b^B_{1\to 1}$ and $b^B_{1\to 3}$ for the new bond. Of course the new bosonic bond also contributes to the site occupation number,

$$N(x) = n^b_{1\to 1}(x) + n^b_{1\to 1}(x-1) + n^b_{1\to 3}(x) + 3 \cdot n^b_{1\to 3}(x-1)\,, \tag{64}$$

and the total weight of a bond configuration becomes

$$W = \prod_x \frac{(1+\mu)^{n^b_{1\to 1}(x)}}{n^b_{1\to 1}(x)!} \frac{g^{n^b_{1\to 3}(x)}}{n^b_{1\to 3}(x)!} Q\left(N(x), m(x)\right). \tag{65}$$

For the superpotential P_b, the explicit expression for the surface term reads

$$O = \sum_x P'_b(\phi_x)(\nabla^- \phi_x) = \sum_x \left\{ \lambda\phi_x^3 - \lambda\phi_x^2\phi_{x-1} \right\}. \tag{66}$$

The first term $\lambda\phi_x^3$ modifies the local potential $V(\phi)$ and therefore just changes the site weight Q. In contrast to the previous case there is no additional term $\propto \phi_x\phi_{x-1}$, hence the corresponding hopping weight $w = 1$ is unchanged. The hopping term $-\lambda\phi_x^2\phi_{x-1}$ generates a new type of bosonic bond $b^B_{1\to 2}$ with weight λ. This directed bond carries one power of the bosonic variable ϕ at the left ending and two powers ϕ^2 at the right ending, so the site occupation number is therefore modified as

$$N(x) = n^b_{1\to 1}(x) + n^b_{1\to 1}(x-1) + n^b_{1\to 2}(x) + 2 \cdot n^b_{1\to 2}(x-1)\,. \tag{67}$$

Eventually, the total weight of a bond configuration is then found to be

$$W = \prod_x \frac{w^{n^b_{1\to 1}(x)}}{n^b_{1\to 1}(x)!} \frac{\lambda^{n^b_{1\to 2}(x)}}{n^b_{1\to 2}(x)!} Q\left(N(x), m(x)\right) \tag{68}$$

with $w = 1$. In analogy to the illustration for the $b^B_{1\to 1}$ bond in Fig. 3, we give a graphical representation of the new bonds $b^B_{1\to 3}$ and $b^B_{1\to 2}$ in Fig. 4 illustrating their contributions to the site weights at each ends. As a side remark we note that it is in fact not too surprising to find directed bosonic hopping terms for the Q-exact actions: since these preserve part of the supersymmetry the oriented fermion hopping needs to be matched in some way by corresponding oriented boson hopping terms.

Fig. 4. Graphical representation of the bosonic bonds $b^B_{1\to 3}$ and $b^B_{1\to 2}$ appearing in the bond formulation for the Q-exact action with the superpotentials P_u and P_b, respectively.

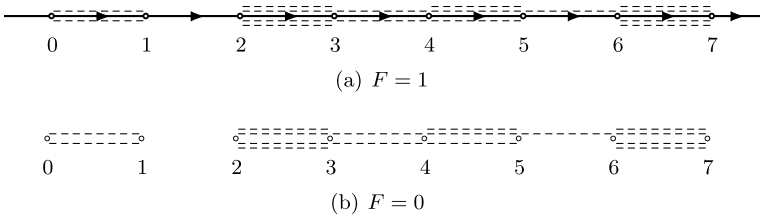

Fig. 5. Illustration of a possible bosonic bond configuration in the fermionic sector $F = 1$ and the same configuration in the bosonic sector $F = 0$ on a $L_t = 8$ lattice.

It is straightforward to generalise the above construction to even more complicated discretisations. For example, we mentioned before that the addition of the surface term in Eq. (25) to the original action with any weight different from zero yields a whole class of Q-exact actions [39]. Another example is the discretisation of the action using the Stratanovich prescription [21,22,43]. In general, in addition to the bonds of type $(1 \to 1)$ and $(1 \to 2)$ or $(1 \to 3)$, these actions will also generate bonds of type $(2 \to 1)$ or $(3 \to 1)$ for the superpotentials P_b and P_u. Superpotentials of higher order produce bonds of correspondingly higher order. All these bonds can be treated in exactly the same way as discussed above. Each new hopping of type $(i \to j)$ induces a new bond $b^B_{i\to j}$ carrying weight $w_{i\to j} \equiv w$ and a corresponding bond occupation number $n^b_{i\to j} \equiv n$, contributing a factor $w^n/n!$ to the local weight and eventually also modifies the site occupation number N.

3.3. Partition functions in the loop formulation

After having integrated out the fermionic and bosonic fields $\overline{\psi}$, ψ and ϕ, respectively, we are left with discrete fermionic and bosonic bond occupation numbers as the degrees of freedom. The path integral has eventually been replaced by a sum over all allowed bond configurations, possibly restricted by local constraints, and hence represents a discrete statistical system. By itself this is already a huge reduction in complexity. Any bond configuration contributing to the partition function consists of the superposition of a generic bosonic bond configuration with one of the two allowed fermionic bond configurations, namely the one representing a closed fermion loop winding around the lattice or the one without any fermionic bonds. Therefore, each bond configuration is either associated with the fermionic sector with fermion number $F = 1$, or with the bosonic sector with $F = 0$. In Fig. 5 we illustrate two such possible configurations in the fermionic and bosonic sectors on a $L_t = 8$ lattice. Collecting our results from the previous two sections we can now write down the contribution of a generic bond configuration $\mathcal{C} = \{n^b_i(x), m(x)\}$ to the partition function. It depends on the fermion number and reads

$$W_F(\mathcal{C}) = \prod_x \left(\prod_i \frac{w_i^{n_i^b(x)}}{n_i^b(x)!} \right) \prod_x Q_F(N(x)) \tag{69}$$

where the index i runs over all the types of bosonic bonds appearing for the specific discretisation under consideration, i.e. $i \in \{1 \to 1, 1 \to 2, 1 \to 3\}$. In Appendix A we summarise the various bond types and corresponding weights for the discretisations and superpotentials discussed in the previous two sections. The site weights are given by

$$Q_F(N(x)) = \int_{-\infty}^{\infty} d\phi\, \phi^{N(x)} \mathrm{e}^{-V(\phi)} M(\phi)^{1-F}\,, \tag{70}$$

where the site occupation number $N(x)$ counts all the bosonic bonds connected to the site x,

$$N(x) = \sum_{j,k} \left(j \cdot n^b_{j\to k}(x) + k \cdot n^b_{j\to k}(x-1) \right). \tag{71}$$

The potential $V(\phi)$ depends on the first derivative of the superpotential, $P'(\phi)$, while the monomer term $M(\phi)$ depends on second derivative $P''(\phi)$ and is present if the fermion is not ($F = 0$) and vice versa ($F = 1$). For superpotentials of polynomial form they can be written as

$$V(\phi) = \sum_n k_n \phi^n\,, \quad M(\phi) = \sum_n m_n \phi^n\,. \tag{72}$$

The values of the various coefficients for the superpotentials discussed in this paper are compiled in the tables in Appendix A, where we summarise the details of the various discretisations. Finally, the full partition functions in the two sectors can be written as the sum over all configurations $\mathcal{C}$ in the corresponding configuration space $\mathcal{Z}_F$,

$$Z_F = \sum_{\mathcal{C}\subset\mathcal{Z}_F} W_F(\mathcal{C})\,. \tag{73}$$

The separation of the bond configuration space into the bosonic and fermionic sectors comes about naturally in the loop formulation, since the bond configurations fall into separate equivalence classes $\mathcal{Z}_F$ specified by the fermion number F. In principle one can consider each sector separately and the partition functions simply describe canonical quantum mechanical systems with fixed fermion number $F = 0$ or 1. In terms of a winding fermion this corresponds to boundary conditions which fix the topology of the winding fermion string, i.e., topological boundary conditions. In order to specify the usual fermion boundary conditions,

$$\overline{\psi}_{x+L_t} = (-1)^{\varepsilon}\overline{\psi}_x\,, \qquad \psi_{x+L_t} = (-1)^{\varepsilon}\psi_x \tag{74}$$

with $\varepsilon = 0$ and 1 for periodic and antiperiodic boundary conditions, respectively, the two partition functions need to be combined. From our discussion in Section 3.1 we know that the configurations in the fermion sector, apart from having different weights, pick up a relative sign (-1) coming from the closed fermion loop. An additional sign stems from the fermion loop crossing the boundary if antiperiodic boundary conditions are employed. The relative sign between the contributions of the two sectors can therefore be summarised as $(-1)^{\varepsilon\cdot F}$, and the partition functions for the systems with periodic or antiperiodic fermionic boundary conditions can be written as

$$Z_{p,a} = Z_0 \mp Z_1\,. \tag{75}$$

Depending on the relative size of Z_0 and Z_1 the combination for Z_p vanishes or can even be negative. This has important consequences for the Witten index W which is proportional

to Z_p. The index vanishes whenever $Z_0 = Z_1$, i.e., when the contributions from the bosonic and fermionic sectors cancel each other exactly. In this case, the free energies of the bosonic and fermionic vacuum must be equal and hence there exists a gapless, fermionic excitation which oscillates between the two vacua, namely the Goldstino mode. As discussed before, the Witten index is regulated at finite lattice spacing, essentially through the fact that Z_0 and Z_1 have different lattice artefacts and therefore do not cancel exactly. More precisely, the finite lattice spacing breaks the degeneracy between the vacuum states by inducing a small free energy difference between the bosonic and fermionic vacua. Consequently, the Goldstino mode receives a small mass, which only disappears in the continuum limit, and is hence also regulated. From that point of view standard Monte Carlo simulations seem to be safe in the sense that there is no need to simulate at vanishing fermion mass. Nevertheless, sufficiently close to the massless limit in a supersymmetry broken system, standard simulation algorithms will almost certainly suffer from critical slowing down and from fluctuating signs of the determinant due to the sign problem discussed before.

The separation of the partition function into a bosonic and fermionic part offers several ways to approach and in fact solve the sign problem when the supersymmetry is broken. Firstly, one can in principle perform simulations in each sector separately, but of course one then misses the physics of the Goldstino mode. Secondly, one can devise an algorithm which efficiently estimates the relative weights of the sectors and hence directly probes the signal on top of the potentially huge cancellations between Z_0 and Z_1. Fortunately, such an algorithm is available [29,44]. Since this so-called open fermion string algorithm directly samples the Goldstino mode, there is no critical slowing down and the physics of the Goldstino is properly captured. The application of the algorithm to the quantum mechanical system is the topic of our third paper in the series [45].

Finally, we note that the equivalence classes $\mathcal{Z}_F$ of the bond configurations specified by the fermion number F can also be characterised by the winding of the fermion around the lattice. In our quantum mechanical system the two characterisations are equivalent, but in more complicated systems the classification in terms of the topology of the fermion winding is more appropriate. It turns out that the discussion of the topological sectors with fixed fermion winding number is in fact crucial for the successful operational application of the fermion loop formulation in more complicated quantum mechanical systems [30], or in higher dimensions [29,46]. As a matter of fact, the separation of the bond configurations into topological classes provides the basis for the solution of the fermion sign problem in the $\mathcal{N} = 1$ Wess–Zumino model [31–34] in complete analogy to how it is illustrated here in the quantum mechanical system.

4. Observables in the loop formulation

We now discuss how bosonic and fermionic observables are expressed in the loop formulation and how the calculation of vacuum expectation values is affected by the decomposition of the partition function into its bosonic and fermionic parts. In general, the expectation value of an observable $\langle \mathcal{O} \rangle$ is given by

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \mathcal{D}\overline{\psi} \mathcal{D}\psi \; \mathcal{O}(\phi, \overline{\psi}, \psi) \; \mathrm{e}^{-S(\phi, \overline{\psi}, \psi)} \tag{76}$$

and the explicit expression for periodic and antiperiodic boundary conditions is

$$\langle \mathcal{O} \rangle_{p,a} = \frac{\langle\!\langle \mathcal{O} \rangle\!\rangle_0 \mp \langle\!\langle \mathcal{O} \rangle\!\rangle_1}{Z_0 \mp Z_1} \,. \tag{77}$$

Here, we have denoted the non-normalised expectation value of the observable in the sector F by $\langle\langle\mathcal{O}\rangle\rangle_F \equiv \langle\mathcal{O}\rangle_F \cdot Z_F$. According to our discussion at the end of the previous section, it is important that in order to calculate the expectation values it is not sufficient to determine $\langle\mathcal{O}\rangle$ in each sector separately, but it is mandatory to calculate the ratio Z_0/Z_1, or similar ratios which contain the same information such as $Z_F/(Z_0+Z_1)$.

Recalling that for broken supersymmetry the Witten index is $W=0$, and hence $Z_p = Z_0 - Z_1 = 0$, it is obvious from Eq. (77) that the vacuum expectation values for periodic boundary conditions $\langle\mathcal{O}\rangle_p$ require a division by zero. Of course this is simply a manifestation of the fermion sign problem discussed earlier in Section 2.3. One might then wonder whether vacuum expectation values of observables are well defined at all when the supersymmetry is broken. It turns out, however, that the finite lattice spacing in fact provides a regularisation for this problem. For the standard discretisation, supersymmetry is explicitly broken, such that $Z_p \neq 0$ for $a \neq 0$. It is therefore possible to calculate expectation values for periodic b.c. at finite lattice spacing, when they are well defined, and then take the continuum limit. Whether or not Eq. (77) with periodic b.c. remains finite or diverges in that limit depends on the observable under consideration. For sensible observables, both the numerator and the denominator go to zero such that their ratio remains finite It is then possible to give continuum values for periodic b.c. even when the supersymmetry is broken in the continuum and $Z_0 - Z_1 \to 0$. Sensible observables are those which couple to the Goldstino mode in the same way as $Z_0 - Z_1$ does, i.e., observables for which the expectation values in both the bosonic and fermionic sector converge to the same value towards the continuum limit. For Q-exact discretisations, the situation is more complicated since in systems with broken supersymmetry $Z_0 - Z_1 = 0$ even at finite lattice spacing. In that case, the physics of the Goldstino mode is realised exactly at $a \neq 0$. It is then more useful to calculate observables separately in the fermionic and bosonic sectors and to verify that they agree.

Important examples for observables are the moments of the bosonic field and two-point functions. The latter are typically used to measure the mass gaps in the particle spectrum by extracting the energy difference between the excited states and the vacuum state, but they also play important roles in the determination of Ward identities. In the following subsections, we will derive the representation of these observables in the loop formulation. This will turn out to be very useful also for the exact calculation of two-point functions and other observables using transfer matrices in the second paper of this series [37], where we discuss a plethora of results, and for the discussion of the simulation algorithm in the third paper of this series [45].

4.1. Moments of ϕ

The expectation value of the n-th moment of the field variable ϕ is defined as

$$\langle\phi^n\rangle = \langle\phi_x^n\rangle = \frac{1}{Z}\int \mathcal{D}\phi\mathcal{D}\overline{\psi}\mathcal{D}\psi\ \phi_x^n\ \mathrm{e}^{-S}. \tag{78}$$

When repeating the reformulation in terms of bosonic and fermionic bonds for this case, it is easy to see that the bond configurations contributing to the partition functions Z_F also contribute to $\langle\phi^n\rangle$. The only difference lies in the weight of each configuration which is modified due to the additional fields ϕ_x^n present at site x. The additional fields only change the local weight $Q_F(N(x))$ through a change of the local bosonic site occupation number at site x,

$$N(x) \to N(x) + n\,. \tag{79}$$

Hence, the non-normalised expectation value reads

$$\langle\langle \phi^n \rangle\rangle_F = \sum_{\mathcal{C}\subset\mathcal{Z}_F} \frac{Q_F(N(x)+n)}{Q_F(N(x))} W_F(\mathcal{C}) \tag{80}$$

$$= \langle\langle \frac{Q_F(N(x)+n)}{Q_F(N(x))} \rangle\rangle_F \tag{81}$$

and $\langle \phi^n \rangle$ then follows directly from Eq. (77).

We noted earlier that the symmetry properties of the underlying fields are reflected in local constraints on the bond occupation numbers which in turn express themselves in the values of the site weights Q_F. As a consequence, the symmetry properties are then also promoted to the observables through the weights in Eq. (80). Considering for example potentials $V(\phi)$ even in ϕ, such as the one following from P_u, one finds the constraint $N \bmod 2 = 0$ which is realised by all site weights with an odd occupation number being identically zero, i.e. $Q_F(N \bmod 2 = 1) = 0$. Consequently, the contributions to odd moments vanish for all bond configurations, $\langle \phi^n \rangle = 0$, n odd, because $Q_F(N(x)+n) = 0$.

4.2. The bosonic n-point correlation function

The bosonic two-point function is defined as

$$C^b(x_1 - x_2) \equiv \langle \phi_{x_1} \phi_{x_2} \rangle = \frac{g^b(x_1 - x_2)}{Z}, \tag{82}$$

where

$$g^b(x_1 - x_2) = \int \mathcal{D}\phi \mathcal{D}\overline{\psi} \mathcal{D}\psi \; \phi_{x_1} \phi_{x_2} \, \mathrm{e}^{-S} \equiv \langle\langle \phi_{x_1} \phi_{x_2} \rangle\rangle. \tag{83}$$

In the following we will abbreviate the configuration space of the bosonic two-point function g^b with $\mathcal{G}^b$. It is again straightforward to rederive the loop formulation in terms of fermionic and bosonic bond occupation numbers also for this case. In general one finds that the bond configurations contributing to $\mathcal{G}^b$ and $\mathcal{Z}$ are the same, but their weights differ due to the insertion of the additional bosonic field variables ϕ at site x_1 and x_2 in the configurations contributing to g^b. The additional sources only change the local bosonic site occupation numbers at site x_1 and x_2,

$$N(x) \to N(x) + \delta_{x,x_1} + \delta_{x,x_2} \,. \tag{84}$$

For $x_1 = x_2$ the situation reduces to the one for the second moment discussed in the previous section. The fermion number F is not affected by these sources. Thus, analogously to the configuration space $\mathcal{Z}$, the configuration space $\mathcal{G}^b$ decomposes into the bosonic part with $F = 0$ and the fermionic part with $F = 1$. We denote the separated configuration spaces by adding the subscript F, i.e. $\mathcal{G}^b \equiv \mathcal{G}^b_F$. In Fig. 6 we show two possible configurations with $F = 0$ and $F = 1$ contributing to the bosonic two-point function in the corresponding sectors. The weight of a configuration where bosonic sources are inserted at the sites $x_1 \neq x_2$ is then given by

$$W_{\mathcal{G}^b_F} = \prod_x \left(\prod_i \frac{w_i^{n_i^b(x)}}{n_i^b(x)!} \right) \left[\prod_{x \neq x_1, x_2} Q_F(N(x)) \right] Q_F(N(x_1)+1) \cdot Q_F(N(x_2)+1) \tag{85}$$

and the non-normalised expectation value reads

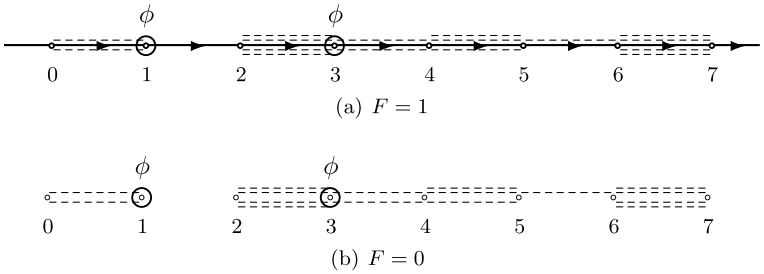

Fig. 6. Graphical representation of possible configurations similar to the closed path configurations in Fig. 5, contributing to the bosonic two-point function (a) in the fermionic sector $F = 1$ and (b) the same configuration in the bosonic sector $F = 0$ on a $L_t = 8$ lattice. The additional bosonic variables are marked with a ○.

$$\langle\langle \phi_{x_1} \phi_{x_2} \rangle\rangle_F = \sum_{\mathcal{C} \subset \mathcal{G}_F^b} \frac{Q_F(N(x_1)+1)}{Q_F(N(x_1))} \cdot \frac{Q_F(N(x_2)+1)}{Q_F(N(x_2))} \cdot W_F(\mathcal{C}) \tag{86}$$

$$= \langle\langle \frac{Q_F(N(x_1)+1)}{Q_F(N(x_1))} \cdot \frac{Q_F(N(x_2)+1)}{Q_F(N(x_2))} \rangle\rangle_F \,. \tag{87}$$

It is straightforward to generalise the construction to arbitrary bosonic n-point functions. One simply adds n bosonic sources $\phi_{x_k}^{p_k}$, $k = 1, \ldots, n$, to a given configuration. The additional sources then contribute to the bosonic site occupation numbers with additional terms $p_k \cdot \delta_{x,x_k}$ modifying the site weights at positions x_k in analogy to Eq. (84). Eventually one gets

$$\langle\langle \phi_{x_1}^{p_1} \ldots \phi_{x_n}^{p_n} \rangle\rangle_F = \langle\langle \prod_{k=1}^{n} \frac{Q_F(N(x_k)+p_k)}{Q_F(N(x_k))} \rangle\rangle_F \,. \tag{88}$$

As discussed before, for some actions there are constraints imposed on the bond configurations reflecting the symmetry properties of the bosonic field. In such a case, the bond configurations in the configuration spaces $\mathcal{Z}_F$ and $\mathcal{G}_F^b$ need no longer be the same. Considering again the example of a potential $V(\phi)$ even in ϕ such that the parity transformation $\phi \to -\phi$ is a symmetry of the action, the constraint $N \bmod 2 = 0$ requires an odd number of bosonic bonds connected to a site containing an odd power of ϕ as a source term, but the corresponding underlying bond configuration contributes with weight zero to $\mathcal{Z}_F$. Hence the sets of configurations with nonvanishing weights contributing to Z_F and g_F^b have no overlap. In addition, from the symmetry it follows that operators with different quantum numbers, in this case the parity, do not mix, i.e. their correlation is exactly zero, e.g. $\langle \phi_{x_1}^2 \phi_{x_2} \rangle = 0$. It is easy to see that this property is strictly enforced in the loop formulation, since there exist no bond configurations which can accommodate the sources and fulfil the constraints $N(x) \bmod 2 = 0$ at the same time.

4.3. The fermionic correlation function

The fermionic two-point correlation function is defined as

$$C^f(x_1 - x_2) \equiv \langle \psi_{x_1} \overline{\psi}_{x_2} \rangle = \frac{g^f(x_1 - x_2)}{Z}, \tag{89}$$

where

$$g^f(x_1 - x_2) = \int \mathcal{D}\phi \mathcal{D}\overline{\psi} \mathcal{D}\psi \;\; \psi_{x_1} \overline{\psi}_{x_2} \, \mathrm{e}^{-S} \equiv \langle\langle \psi_{x_1} \overline{\psi}_{x_2} \rangle\rangle \,. \tag{90}$$

Similarly to the bosonic correlation function, configurations contributing to the fermionic correlation function have additional fermionic variables $\overline{\psi}$ and ψ inserted in the path integral at positions x_1 and x_2. We will refer to these variables as the source and the sink, respectively. To derive the weight of a configuration in the configuration space $\mathcal{G}^f$ of the fermionic two-point functions, we repeat the expansion of the fermionic Boltzmann factor in Eq. (50) while including the additional fermionic variables. The expansion yields

$$\begin{aligned}&\psi_{x_1}\overline{\psi}_{x_2}\mathrm{e}^{-S_\Lambda^F}\\&\quad=\psi_{x_1}\overline{\psi}_{x_2}\prod_x\left(\sum_{m(x)=0}^{1}\left(-M(\phi_x)\overline{\psi}_x\psi_x\right)^{m(x)}\right)\prod_x\left(\sum_{n^f(x)=0}^{1}\left(\overline{\psi}_x\psi_{x-1}\right)^{n^f(x)}\right)\end{aligned}\tag{91}$$

and the subsequent Grassmann integration, still requiring exactly one pair of variables $\overline{\psi}$ and ψ at each site x, yields an adjustment of the fermionic occupation numbers $m(x)$ and $n^f(x)$ in order to obtain a nonvanishing contribution to the two-point function.

We first consider the case where $x_1 = x_2 \equiv y$. It is easy to see that the only possibility to saturate each site is given by the choice

$$n^f(x) = 0 \qquad \forall x, \tag{92}$$

$$m(x) = \begin{cases} 0 \text{ if } x = y, \\ 1 \text{ otherwise.} \end{cases} \tag{93}$$

For such a configuration, the site y is saturated through the source and the sink, yielding a factor 1 as the fermionic contribution to the bosonic integration. All other sites are saturated via the monomer terms which have to be accounted for by including the corresponding factors $M(\phi)$ into the bosonic integration for each of these sites, so one eventually obtains

$$\langle\langle\psi_y\overline{\psi}_y\rangle\rangle_0 = \sum_{\mathcal{C}\subset\mathcal{G}^f}\prod_x\left(\prod_i\frac{w_i^{n_i^b(x)}}{n_i^b(x)!}\right)\left[\prod_{x\neq y}Q_0(N(x))\right]\cdot Q_1(N(y)) \tag{94}$$

$$= \sum_{\mathcal{C}\subset\mathcal{G}^f}\frac{Q_1(N(y))}{Q_0(N(y))}W_0(\mathcal{C}) \tag{95}$$

$$= \langle\langle\frac{Q_1(N(y))}{Q_0(N(y))}\rangle\rangle_0\,. \tag{96}$$

If the additional fermionic variables are not at the same site, $x_1 \neq x_2$, source and sink can only be paired with the ending of a fermionic bond. Keeping in mind that the fermionic bonds are directed, it is straightforward to see that one needs $(x_1 - x_2) \bmod L_t$ of these bonds to connect the source with the sink, thus forming an open fermionic string. This is illustrated in Fig. 7 where we show two typical bond configurations using the symbols $\bigcirc$ and $\times$ to denote the sink ψ_{x_1} and the source $\overline{\psi}_{x_2}$, respectively. It is clear that each site along the open fermion string is automatically saturated by the variables of one ingoing and one outgoing fermionic bond. Those sites and the ones which are saturated with either the source or the sink and a fermionic bond attached to it yield a factor 1 as the fermion contribution to the bosonic integration, while all other sites contribute with the monomer weight $M(\phi)$.

Because the fermionic bonds are directed, the order of the source and the sink matters and we need to distinguish between the cases $x_2 > x_1$ and $x_1 > x_2$. For $x_2 > x_1$, the open string connects

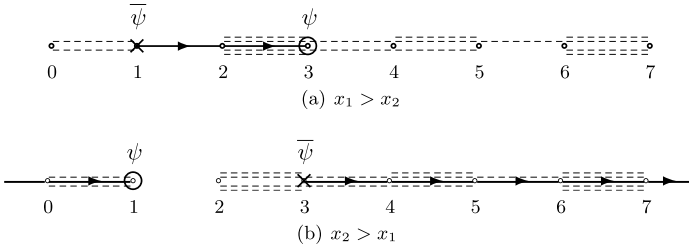

Fig. 7. Graphical representation of possible configurations similar to the constrained path configurations in Fig. 5, contributing to the fermionic two-point function (a) for $x_1 > x_2$ and (b) the same configuration for $x_2 > x_1$ on a $L_t = 8$ lattice. The additional variables are marked with a $\circ$ for ψ_{x_1} and a $\times$ for $\overline{\psi}_{x_2}$.

source and sink without crossing the boundary and each configuration is characterised by the numbers

$$n^f(x) = \begin{cases} 1 \text{ if } x_2 \leq x < x_1, \\ 0 \text{ otherwise,} \end{cases} \tag{97}$$

$$m(x) = \begin{cases} 0 \text{ if } x_2 \leq x \leq x_1, \\ 1 \text{ otherwise,} \end{cases} \tag{98}$$

while for $x_1 < x_2$, the fermionic string crosses the boundary and the numbers to characterise the configuration are given by

$$n^f(x) = \begin{cases} 0 \text{ if } x_1 \leq x < x_2, \\ 1 \text{ otherwise,} \end{cases} \tag{99}$$

$$m(x) = \begin{cases} 1 \text{ if } x_1 < x < x_2, \\ 0 \text{ otherwise.} \end{cases} \tag{100}$$

Whether or not the open fermionic string crosses the boundary of the lattice is relevant for the overall sign of the configuration. Namely, the crossing yields one extra factor of (-1) for antiperiodic boundary conditions, and this has to be taken into account in the overall book keeping for the 2-point function.

We are now able to give an explicit expression for the weight of an open fermion string configuration in $\mathcal{G}^f$ contributing to $C^f(x_1 - x_2)$. Each site x_i contributing a factor 1 to the bosonic integration amounts to a site weight $Q_1(N(x_i))$, while a site x_j contributing the monomer weight $M(\phi_{x_j})$ to the bosonic integration yields a site weight $Q_0(N(x_j))$. To simplify the notation we define the set $\mathcal{F}$ of lattice sites belonging to the open fermion string as

$$\mathcal{F}(x_1, x_2) = \begin{cases} \{x \in \Lambda \mid x_2 \leq x \leq x_1\} & \text{if } x_2 \leq x_1, \\ \{x \in \Lambda \mid x \leq x_1 \cup x \geq x_2\} & \text{if } x_1 < x_2. \end{cases} \tag{101}$$

The weight of a configuration contributing to $\mathcal{G}^f$ can then be written as

$$W_{\mathcal{G}^f} = \prod_x \left(\prod_i \frac{w_i^{n_i^b(x)}}{n_i^b(x)!} \right) \left[\prod_{x \in \mathcal{F}} Q_1(N(x)) \right] \left[\prod_{x \notin \mathcal{F}} Q_0(N(x)) \right], \tag{102}$$

and the non-normalised expectation value of the fermionic two-point function is

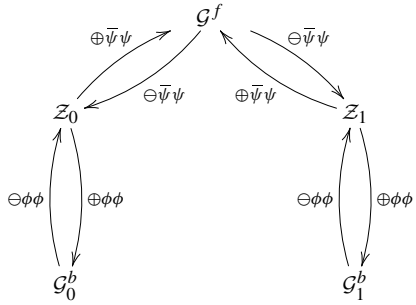

Fig. 8. Schematic representation of the configuration spaces. The configuration space $\mathcal{G}^f \equiv \mathcal{G}_0^f = \mathcal{G}_1^{\overline{f}}$ mediates between the bosonic and the fermionic sector. By the symbols $\oplus$ and $\ominus$, we denote the addition and removal of the source and sink field variables, respectively.

$$\langle\!\langle \psi_{x_1} \overline{\psi}_{x_2} \rangle\!\rangle_0 = \sum_{\mathcal{C}\subset\mathcal{G}^f} W_{\mathcal{G}^f}(\mathcal{C}) \tag{103}$$

$$= \sum_{\mathcal{C}\subset\mathcal{G}^f} \left[\prod_{x\in\mathcal{F}} \frac{Q_1(N(x))}{Q_0(N(x))} \right] \cdot W_0(\mathcal{C}) \tag{104}$$

$$= \langle\!\langle \prod_{x\in\mathcal{F}} \frac{Q_1(N(x))}{Q_0(N(x))} \rangle\!\rangle_0 \,. \tag{105}$$

This result implies that the configuration space $\mathcal{G}^f$ does not decompose into the bosonic and fermionic sector $F = 0$ and $F = 1$. Rather, all configurations in the configuration space of fermionic two point functions are associated with the bosonic sector. In a way, the configuration space $\mathcal{G}^f$ mediates between the bosonic and the fermionic sectors $\mathcal{Z}_0$ and $\mathcal{Z}_1$. The transition from one configuration space to another is induced by adding or removing the additional field variables $\overline{\psi}\psi$. The relation between the various bond configuration spaces is schematically illustrated in Fig. 8. The picture suggests to interpret the fermionic correlation function $C^f(x-y)$ as an open fermion string on the background of bosonic bond configurations in sector $\mathcal{Z}_0$, or as an open antifermion string on the background of bond configurations in sector $\mathcal{Z}_1$, i.e., as a antifermionic correlation function $-C^{\overline{f}}(y-x)$. It is this property which forms the basis for an efficient simulation algorithm which will be discussed in detail in the third paper of this series [45].

Finally, the reformulation of the fermionic correlation functions in terms of bond variables can be generalised to include more complicated fermionic source and sink operators such as $\psi_x \phi_x^k$ or $\overline{\psi}_x \phi_x^k$. The construction is rather straightforward and yields

$$\langle\!\langle \psi_{x_1} \phi_{x_1}^k \cdot \overline{\psi}_{x_2} \phi_{x_2}^l \rangle\!\rangle_0 = \sum_{\mathcal{C}\subset\mathcal{G}^f} \left[\prod_{x\in\mathcal{F}} \frac{Q_1(N(x) + k\cdot\delta_{x,x_1} + l\cdot\delta_{x,x_2})}{Q_0(N(x))} \right] \cdot W_0(\mathcal{C}) \tag{106}$$

$$= \langle\!\langle \prod_{x\in\mathcal{F}} \frac{Q_1(N(x) + k\cdot\delta_{x,x_1} + l\cdot\delta_{x,x_2})}{Q_0(N(x))} \rangle\!\rangle_0 \,, \tag{107}$$

i.e., only the site occupation numbers at site x_1 and x_2 are modified accordingly. Similarly to the discussion concerning the bosonic n-point correlation function, operators with different quantum numbers, for example the parity for actions symmetric under $\phi \to -\phi$, do not mix if the

symmetry is intact, e.g. $\langle \psi_{x_1} \phi_{x_1}^2 \cdot \overline{\psi}_{x_2} \phi_{x_2} \rangle = 0$. It is again easy to see that this property is strictly enforced through the constraints $N(x) \bmod 2 = 0$ for parity symmetric actions.

5. Conclusions

Simulations of supersymmetric models on the lattice with (spontaneously) broken supersymmetry suffer from a fermion sign problem related to the vanishing of the Witten index. This problem is a generic one and must occur whenever a massless Goldstino mode is present in the system. In this paper we discussed a novel approach which solves this problem for $\mathcal{N} = 2$ supersymmetric quantum mechanics by formulating its Euclidean path integral on the lattice in terms of fermion loops. The formulation is based on the exact hopping expansion of the fermionic action and allows the explicit decomposition of the partition function into a bosonic and a fermionic sector associated with the corresponding vacua. Since the two vacua contribute with opposite signs, the separation isolates the cause of the sign problem and opens the way for its solution. In fact, the explicit separation of the sectors in the fermion loop formulation allows the construction of a simulation algorithm which samples these sectors separately, and more importantly also samples the relative weights between them. We demonstrate in the third paper of this series [45] that in this way, the loop formulation indeed provides a solution to the fermion sign problem. The solution is not restricted to the quantum mechanics case, but it is in fact also applicable in higher dimensions. In particular, it also applies to the supersymmetric $\mathcal{N} = 1$ Wess–Zumino model [34], where the formulation has proven to successfully solve the fermion sign problem.

In addition to the sign problem, in this paper we have discussed various discretisation schemes for regularising $\mathcal{N} = 2$ supersymmetric quantum mechanics on the lattice using Wilson fermions. Because the lattice formulations break supersymmetry explicitly, special care has to be taken to guarantee the restoration of the supersymmetries in the continuum limit. A very straightforward discretisation for example requires the addition of a single counterterm which compensates certain perturbative loop corrections. We demonstrate explicitly by means of the boson and fermion mass spectra how the absence of such a term spoils the correct continuum limit. Another discretisation is based on the insertion of the Wilson term directly in the superpotential. This construction leads to the Q-exact discretisation which maintains one of the two supersymmetries exactly at finite lattice spacing. This eventually guarantees the automatic restoration of the full supersymmetries in the continuum.

For both discretisation schemes, in addition to the fermion loop reformulation, we have reformulated the quantum mechanics system on the lattice in terms of bosonic bonds. As in the fermionic case, the formulation is based on the exact hopping expansion of the bosonic actions. The bosonic bond formulation is not a necessary ingredient in the solution of the fermion sign problem, but completes the description of the quantum mechanical system in terms of solely discrete variables. In fact, while the fermion loop formulation is not affected by the choice of discretisation, the bond formulation is and in general requires arbitrary types of bonds beyond the simple one. We have discussed in detail how the simple bosonic bond formulation needs to be adapted in order to accommodate more complicated discretisations, such as the Q-exact one, as well as arbitrary superpotentials.

Furthermore, we also derived explicit expressions for various observables in the bond formulation, such as moments of the bosonic field, bosonic n-point correlation functions, and fermionic 2-point functions with arbitrary fermionic operators. For the latter we emphasised its interpretation as an open fermion string. In addition, we argued that the fermion correlator in the bosonic vacuum can equally well be interpreted as the antifermion correlator in the fermionic vacuum.

More importantly, however, is the fact that the configurations including the open fermion string represent the configuration space mediating between the bosonic and fermionic configuration spaces. This eventually forms the basis for the efficient simulation algorithm discussed in paper three of this series [45].

Finally, as an outlook, we point out that using the bond formulation it is straightforward to construct transfer matrices separately for the bosonic and fermionic sector. They allow in turn to solve the lattice system exactly. This construction and the subsequent solution will be the subject of the second paper in this series [37].

Appendix A. Summary of the discretisations

In this appendix, we write out explicitly the actions for which we discussed in detail the derivation of the loop formulation. The generic lattice actions are given by Eqs. (20), (24) and (27),

$$S_L = \sum_x \left\{ \frac{1}{2}(\nabla^- \phi_x)^2 + \frac{1}{2} P'(\phi_x)^2 + \overline{\psi}_x (\nabla^- + P''(\phi_x))\psi_x \right\}, \tag{108}$$

$$S_L^c = S_L + \frac{1}{2} \sum_x P''(\phi_x), \tag{109}$$

$$S_L^Q = S_L + \sum_x P'(\phi_x)(\nabla^- \phi_x). \tag{110}$$

For the polynomial superpotentials discussed in this paper the resulting bosonic self-interaction $V(\phi)$ and the fermionic monomer term $M(\phi)$ can be described by

$$V(\phi) = \sum_{n=1}^{6} k_n \phi^n, \qquad M(\phi) = \sum_{n=0}^{2} m_n \phi^n. \tag{111}$$

The weights of the directed bosonic bonds are given by $w_{1\to n}$, where n indicates the number of bosonic sources carried at the right ending of the specific bond. In the following we explicitly write out the actions and tabulate the coefficients k_n and m_n as well as the bond weights $w_{1\to n}$ for the two superpotentials

$$P_u(\phi) = \frac{1}{2}\mu\phi^2 + \frac{1}{4} g\phi^4, \tag{112}$$

$$P_b(\phi) = -\frac{\mu^2}{4\lambda}\phi + \frac{1}{3}\lambda\phi^3, \tag{113}$$

which yield systems with unbroken and broken supersymmetry, respectively.

A.1. The actions for the superpotential P_u

Writing out explicitly the actions for the superpotential P_u, we have

$$S_L = \sum_x \left\{ \frac{1}{2}\left(2+\mu^2\right)\phi_x^2 + \mu g \phi_x^4 + \frac{1}{2} g^2 \phi_x^6 - \phi_x \phi_{x-1} + \left(1+\mu+3g\phi_x^2\right)\overline{\psi}_x \psi_x - \overline{\psi}_x \psi_{x-1} \right\}, \tag{114}$$

Table 1
Unbroken supersymmetric quantum mechanics: coefficients and hopping weights for the superpotential $P_u(\phi) = \frac{1}{2}\mu\phi^2 + \frac{1}{4}g\phi^4$.

	S_L	S_L^c	S_L^Q
k_1	0	0	0
k_2	$1 + \frac{1}{2}\mu^2$	$1 + \frac{1}{2}\mu^2 + \frac{3}{2}g$	$1 + \mu + \frac{1}{2}\mu^2$
k_3	0	0	0
k_4	μg	μg	$g(1+\mu)$
k_5	0	0	0
k_6	$\frac{1}{2}g^2$	$\frac{1}{2}g^2$	$\frac{1}{2}g^2$
$w_{1\to 1}$	1	1	$1+\mu$
$w_{1\to 3}$	0	0	g
m_0	$1+\mu$	$1+\mu$	$1+\mu$
m_1	0	0	0
m_2	$3g$	$3g$	$3g$

$$S_L^c = \sum_x \Big\{ \frac{1}{2}\left(2 + \mu^2 + 3g\right)\phi_x^2 + \mu g\phi_x^4 + \frac{1}{2}g^2\phi_x^6 - \phi_x\phi_{x-1} + \left(1 + \mu + 3g\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1}\Big\}, \tag{115}$$

$$S_L^Q = \sum_x \Big\{ \frac{1}{2}\left(2 + 2\mu + \mu^2\right)\phi_x^2 + g(\mu+1)\phi_x^4 + \frac{1}{2}g^2\phi_x^6 - g\phi_x^3\phi_{x-1} - (1+\mu)\,\phi_x\phi_{x-1} + \left(1 + \mu + 3g\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1}\Big\}, \tag{116}$$

and the coefficients and hopping weights can directly be read off. They are compiled in Table 1.

A.2. The actions for the superpotential P_b

So far we have concentrated on the superpotential with broken supersymmetry of the form

$$P_b(\phi) = -\frac{\mu^2}{4\lambda}\phi + \frac{1}{3}\lambda\phi^3, \tag{117}$$

yielding a potential for the bosonic field which is symmetric under the parity transformation $\phi \to -\phi$. Writing out explicitly the actions for this superpotential we obtain

$$S_L = \sum_x \Big\{ \frac{1}{2}\left(2 - \frac{\mu^2}{2}\right)\phi_x^2 + \frac{1}{2}\lambda^2\phi_x^4 - \phi_x\phi_{x-1} + \left(1 + 2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1}\Big\}, \tag{118}$$

$$S_L^c = \sum_x \Big\{ \lambda\phi_x + \frac{1}{2}\left(2 - \frac{\mu^2}{2}\right)\phi_x^2 + \frac{1}{2}\lambda^2\phi_x^4 - \phi_x\phi_{x-1} + \left(1 + 2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1}\Big\}, \tag{119}$$

Table 2
Broken supersymmetric quantum mechanics: coefficients and hopping weights for the superpotential $P_b(\phi) = -\frac{\mu^2}{4\lambda}\phi + \frac{1}{3}\lambda\phi^3$.

	S_L	S_L^c	S_L^Q
k_1	0	λ	0
k_2	$\frac{1}{4}(4-\mu^2)$	$\frac{1}{4}(4-\mu^2)$	$\frac{1}{4}(4-\mu^2)$
k_3	0	0	λ
k_4	$\frac{1}{2}\lambda^2$	$\frac{1}{2}\lambda^2$	$\frac{1}{2}\lambda^2$
k_5	0	0	0
k_6	0	0	0
$w_{1\to1}$	1	1	1
$w_{1\to2}$	0	0	λ
m_0	1	1	1
m_1	2λ	2λ	2λ
m_2	0	0	0

Table 3
Broken supersymmetric quantum mechanics: coefficients and hopping weights for the superpotential $P_b(\phi) = \frac{1}{2}\mu\phi^2 + \frac{1}{3}\lambda\phi^3$.

	S_L	S_L^c	S_L^Q
k_1	0	λ	0
k_2	$\frac{1}{2}(2+\mu^2)$	$\frac{1}{2}(2+\mu^2)$	$\frac{1}{2}(2+2\mu+\mu^2)$
k_3	$\mu\lambda$	$\mu\lambda$	$(1+\mu)\lambda$
k_4	$\frac{1}{2}\lambda^2$	$\frac{1}{2}\lambda^2$	$\frac{1}{2}\lambda^2$
k_5	0	0	0
k_6	0	0	0
$w_{1\to1}$	1	1	$1+\mu$
$w_{1\to2}$	0	0	λ
m_0	$1+\mu$	$1+\mu$	$1+\mu$
m_1	2λ	2λ	2λ
m_2	0	0	0

$$S_L^Q = \sum_x \Big\{ \frac{1}{2}\left(2 - \frac{\mu^2}{2}\right)\phi_x^2 + \lambda\phi_x^3 + \frac{1}{2}\lambda^2\phi_x^4 - \lambda\phi_x^2\phi_{x-1} - \phi_x\phi_{x-1} + \left(1 + 2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1} \Big\}, \tag{120}$$

and the corresponding coefficients and hopping weights are given in Table 2.

In order to apply perturbation theory it is more useful to consider the shifted superpotential

$$P_b(\phi) = \frac{1}{2}\mu\phi^2 + \frac{1}{3}\lambda\phi^3 \tag{121}$$

which is obtained from Eq. (117) by applying the shift $\phi \to \phi + \mu/2\lambda$ and neglecting any constant terms. The potential for the bosonic field then has a minimum at $\phi = 0$, but the parity symmetry is no longer manifest. Writing out explicitly the actions for this form of the superpotential P_b, we have

$$S_L = \sum_x \left\{ \frac{1}{2}\left(2+\mu^2\right)\phi_x^2 + \mu\lambda\phi_x^3 + \frac{1}{2}\lambda^2\phi_x^4 - \phi_x\phi_{x-1} + \left(1+\mu+2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1} \right\}, \tag{122}$$

$$S_L^c = \sum_x \left\{ \lambda\phi_x + \frac{1}{2}\left(2+\mu^2\right)\phi_x^2 + \mu\lambda\phi_x^3 + \frac{1}{2}\lambda^2\phi_x^4 - \phi_x\phi_{x-1} + \left(1+\mu+2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1} \right\}, \tag{123}$$

$$S_L^Q = \sum_x \left\{ \frac{1}{2}\left(2+2\mu+\mu^2\right)\phi_x^2 + \lambda(\mu+1)\phi_x^3 + \frac{1}{2}\lambda^2\phi_x^4 - \lambda\phi_x^2\phi_{x-1} - (1+\mu)\,\phi_x\phi_{x-1} + \left(1+\mu+2\lambda\phi_x^2\right)\overline{\psi}_x\psi_x - \overline{\psi}_x\psi_{x-1} \right\}, \tag{124}$$

and the corresponding coefficients and hopping weights are given in Table 3.

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