FUNCTIONAL INTEGRALS FOR HUBBARD OPERATORS
AND
PROJECTION METHODS FOR STRONG INTERACTION

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Abstract

We discuss problems of functional integral formalisms in a constrained fermionic Fock space. A functional integral is set up for the Hubbard model using generalized coherent states which lie either in the constrained or in the full Fock space. The projection for the latter states is implemented through a reduction of the charge fluctuations which induce transitions between the constrained and full space. The Lagrangian is expressed in terms of two complex fields representing spin and charge excitations, and one Grassmann field signifying hole excitations. Here, the charge excitations denote transitions between states with empty and doubly occupied sites. The projection method is inspired by the observation that the local interaction in the model resembles a magnetic field in the space of charge fluctuations. Hence the projection is understood as an infinite magnetic field in a spin path integral.

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I. INTRODUCTION

Models of interacting fermions on the lattice like the Hubbard model and its derivatives, the $t - J$ and Heisenberg models, have been under intense investigation in recent years \cite{1}. These models are thought to describe much of the qualitative physics of the Mott-Hubbard metal-insulator transition, including the magnetic correlations and possibly superconductivity in its vicinity. Most importantly, there is reason to expect new types of ground states such as spin liquid states \cite{2} in the two-dimensional systems. Progress in assessing the validity and relevance to many existing ideas proposed in this context has been slow due to the lack of reliable theoretical methods. The generic problem here is the dynamics of fermions in constrained Fock space, excluding double occupancy of lattice sites. A convenient representation used in this case is in terms of slave particles \cite{3}, assigning fermion and boson creation operators to the various possible states at a given lattice site. The occupation numbers of the slave particles at any given site then have to add up to one for all times. Local constraints of this type are difficult to handle. Most treatments use a mean field description by which the constraint is only satisfied on the average \cite{4,5}. Additionally, the slave boson methods exhibit a local gauge invariance which is destroyed in the mean field description. The conserving slave boson approach presented in \cite{6}, however, preserves the local gauge invariance.

One strategy to avoid slave particles builds on a Hubbard Stratonovich decoupling of the interaction in terms of density and spin excitations. But a straightforward saddle point evaluation violates certain symmetries, e.g. the spin rotation invariance. Schulz \cite{7} considered a time dependent quantization axis for each spin which is being treated as an additional set of angular field variables. This procedure preserves the spin rotation invariance of the saddle point Lagrangian.

A different strategy is to try to work in the constrained subspace only. Conventional many body formulations build on equation of motion and diagrammatic schemes \cite{8, 9, 10}, and often
involve uncontrolled factorizations which can violate sum rules and conservation laws (except for certain limiting cases, as the limit of large spin degeneracy in [10]). The use of resolvent operator methods [11] may be well adapted to certain problems. Also Quantum Monte-Carlo techniques, which work in the constrained subspace only, were devised in [12,13].

In this paper we explore the following alternative: the construction of a path integral formalism for Hubbard operators [14,15], different from the usual fermionic representation [16]. The path integral formalism has several well-known properties:

(i) it allows a time-ordered perturbation theory to be developed
(ii) collective behavior may be incorporated from the outset
(iii) the classical limit may be easily extracted, e.g. in the case of large spin degeneracy.

In addition the path integral we develop here does not exhibit the local gauge invariance generated in slave boson approaches.

We organize the paper as follows:
First, we introduce functional integral formulations in the constrained Fock space. We note some problems in the literature concerning the measure. They may be traced back to difficulties with the resolution of the unity with normalized coherent states. Therefore we review the definition of coherent states in order to extend it to graded algebras. We derive coherent states in the full Fock space using two complex fields in order to describe the spin and charge degrees of freedom, and one Grassmann field in order to implement fermionic statistics. Working with these coherent states, we are able to resolve the unity and set up a functional integral with the Trotter formula for which the measure is known exactly. In order to test its validity we calculate the so-called atomic limit. To handle the problem of a constrained space we develop a well-defined projection method, first for spin 1/2 functional integrals [17,18] in strong magnetic fields, and later adapting it to the electron path integral for strong local interaction. We investigate the Hubbard model in the limit of strong Coulomb interaction to derive an effective Lagrangian.
As a model system we consider a fermionic lattice Hamiltonian with local interactions which is most suitable for a discussion of projection methods. The Hubbard Hamiltonian \[ H = - \sum_{\sigma=\{\uparrow, \downarrow\}} \sum_{\langle i,j \rangle} t_{ij} C_{i,\sigma}^d C_{j,\sigma} + U \sum_i C_{i,\uparrow}^d C_{i,\uparrow}^* C_{i,\downarrow}^d C_{i,\downarrow} - \mu \sum_{\sigma,i} C_{i,\sigma}^d C_{i,\sigma} \] \] allows “to turn on” the projection by sending the interaction parameter to infinity. Using canonical electron creation and annihilation operators it reads:

\[ H = - \sum_{\sigma=\{\uparrow, \downarrow\}} \sum_{\langle i,j \rangle} t_{ij} C_{i,\sigma}^d C_{j,\sigma} + U \sum_i C_{i,\uparrow}^d C_{i,\uparrow}^* C_{i,\downarrow}^d C_{i,\downarrow} - \mu \sum_{\sigma,i} C_{i,\sigma}^d C_{i,\sigma} \]

where \( \langle i,j \rangle \) is a summation over nearest neighbor sites, and we will assume that \( t_{ij} = t \) for all nearest neighbors on a hypercubic lattice.

This model has a graded structure in the following sense: local excitations of the system either belong to a bosonic or fermionic type. As bosonic excitations we classify all excitations involving an even number of electron creation and annihilation operators. Spin, particle hole and pair excitations are in this class and will be attributed to complex fields in the path integral. Fermionic excitations, with an odd number of electron operators, are creation or annihilation of electrons at empty, singly or doubly occupied sites, and will be taken care of by Grassmann fields.

To set up this formalism on the Hamiltonian level first, we introduce local operators which represent these excitations more faithfully. Knowing the algebra of these operators (the “Hubbard operators”), one is in the position to derive coherent states for the excitations. These Hubbard operators are defined as projections:

\[ X_{i}^{\mu\nu} := |i; \mu \rangle \langle i; \nu| \] (1)

where \( |i; \mu \rangle \) are orthonormal states at site \( i \), representing the empty (\( \mu = 0 \)), singly occupied (\( \mu = \uparrow, \downarrow \)) and doubly (\( \mu = 2 \)) occupied sites (we chose the convention \( |2\rangle = C_{i,\uparrow}^d C_{i,\downarrow}^d |0\rangle \)).

Then one can verify the following supercommutator relation:

\[ [X_{i}^{\mu\nu}, X_{j}^{\alpha\beta}]_{S} = \delta_{ij} \left( X_{i}^{\mu\beta} \delta_{\nu\alpha} - (-1)^{X_{i}^{\mu\alpha}} X_{j}^{\alpha\beta} X_{i}^{\alpha\nu} \delta_{\beta\mu} \right) \] (2)
where \( S = 2 \left( \Theta(\chi^{\mu\nu} + \chi^{\alpha\beta} - 3/2) - 1/2 \right) \), and the graded characters \( \chi^{\mu\nu} \) of the Hubbard operators are 0 in the case of the bosonic operators \( (X^{00}, X^{22}, X^{\sigma\sigma}, X^{\sigma-\sigma}, X^{02}, X^{20}) \) and 1 in the case of the fermionic operators \( X^{0\sigma}, X^{\sigma0}, X^{2\sigma}, X^{\sigma2} \). The algebra of the Hubbard operators has been extensively studied in [9].

Now we may write the canonical creation and annihilation operators in terms of linear combinations of Hubbard operators:

\[
C_\sigma = X^{0\sigma} + \sigma X^{-\sigma2} \\
C^\dagger_\sigma = X^{\sigma0} + \sigma X^{2-\sigma}
\]  

However, this transformation is not linear and the inverse of it reads:

\[
X^{\sigma0} = C^\dagger_\sigma (1 - n_{-\sigma}) \\
X^{\sigma2} = C_{-\sigma} n_\sigma \\
X^{\sigma\sigma} = n_\sigma (1 - n_{-\sigma}) \\
X^{00} = (1 - n_\sigma) (1 - n_{-\sigma}) \\
X^{02} = C^\uparrow C^\downarrow \\
X^{20} = C^\dagger_{\sigma} C^\dagger_{\sigma-\sigma}
\]  

The bosonic number operators automatically satisfy the local completeness relation \( \mathbb{1} = X^{00} + X^{\uparrow\uparrow} + X^{\downarrow\downarrow} + X^{22} \) which follows from the orthogonality and completeness of the local states.

Furthermore, the Hubbard Hamiltonian takes the form:

\[
H = -t \sum_{<ij>} \sum_\sigma (X_i^{0\sigma} + \sigma X_i^{2-\sigma})(X_j^{0\sigma} + \sigma X_j^{\sigma2}) - \mu \sum_i \sum_\sigma X_i^{\sigma\sigma} + (U - 2\mu) \sum_i X_i^{22}
\]  

Obviously, the kinetic energy is split into four terms, each of them representing a specific interaction process between excitations on nearest neighbor sites. The local terms in this Hamiltonian may be interpreted as chemical potentials \( \mu \) and \( 2\mu - U \) for singly and doubly occupied sites, respectively.

Now it seems very easy to project out doubly occupied states with these Hubbard operators. Since the last term in (5) attributes an exponentially small weight to doubly occupied
sites for large $U$ it appears to be obvious that the infinite $U$ limit is accomplished by discarding all terms with index 2 in equation (5). We will show that in the Lagrangian formalism, i.e. in the path integral formalism, such a projection scheme fails – except for very exotic choices of the measure of the path integration.

Construction of a path integral for the degrees of freedom represented by the Hubbard operators requires a mapping onto classical fields or Grassmann fields depending on the statistics. Wiegmann [14] formulated the path integral representation using geometric quantization. First, he introduced the projection operator $Q$ onto coherent states. The Lagrangian is:

$$L = -\text{Tr}(HQ) + \frac{1}{2} \int_0^1 du \, \text{Tr}(Q \, \partial_u Q \, \partial_t Q)$$  \hspace{1cm} (6)

where $Q(\tau, u)$ is an arbitrary differentiable extension of $Q(\tau)$—only restricted by the boundary conditions $Q(\tau, 0) = \text{const}$ and $Q(\tau, 1) = Q(\tau)$ and $\tau, u$ are imaginary time variables. The second term in (6) is the so-called Berry phase. This phase is being collected by the system while transporting it along a considered path [20]. The first part, containing the Hamiltonian of (6), is the ‘Boltzmann weight’ of this path.

In order to investigate the limit of infinitely strong local interaction ($U = \infty$) Wiegmann proposed the following form for $Q(\tau)$:

$$Q(\tau) = (1 - \psi^\dagger \psi) \sum_{\sigma \sigma'} A_{\sigma \sigma'} X^{\sigma \sigma'} + \sum_{\sigma} \psi^\dagger z_{\sigma} X^{\sigma 0} + \sum_{\sigma} X^{0 \sigma} z_{\sigma}^\dagger \psi + \psi^\dagger \psi X^{0 0}$$  \hspace{1cm} (7)

where

$$z_{\sigma} = \begin{pmatrix} \sin(\vartheta) e^{i\varphi} \\ \cos(\vartheta) \end{pmatrix} \quad \text{and} \quad A_{\sigma \sigma'} = \begin{pmatrix} \sin^2(\vartheta) & \sin(\vartheta) \cos(\vartheta) e^{i\varphi} \\ \sin(\vartheta) \cos(\vartheta) e^{-i\varphi} & \cos^2(\vartheta) \end{pmatrix}$$

and $\psi^\dagger, \psi$ are Grassmann numbers. Only empty and singly occupied states are involved in (7), making it plausible that a projection onto a constrained space has been successfully implemented. Using (6) and (7), the partition function is:
\[ Z = \text{Tr} e^{-\beta H} = \int D[\vartheta(\tau), \varphi(\tau), \psi^\dagger(\tau), \psi(\tau)] \times \exp \left[ -\int_0^\beta \left( -i\dot{\varphi} \sin^2 \vartheta + \psi^\dagger \left( \partial_\tau + i\dot{\varphi} \sin^2 \vartheta \right) \psi + \text{Tr}(QH) \right) d\tau \right] \]  

(8)

To point out the problem with the normalizability of \( Z \) we consider the following trivial limit \( \text{Tr}(QH) = 0 \). In this case the partition function should be equal to the dimension of the Fock space. Applying the relations of appendix \[ \square \], it is straightforward to integrate out the Grassmann degrees of freedom, and we find:

\[ Z = \int D[\vartheta(\tau), \varphi(\tau)] \left[ 1 + \exp \left[ \int_0^\beta d\tau i\dot{\varphi} \sin^2 \vartheta \right] \right] = \lim_{N \to \infty} (2^N + 2) \]  

(9)

using the results of appendix \[ \square \], where \( N \) is the number of time slices in the discretized partition function. This partition function cannot be normalized to the correct result, \( 1 + 2 \), with a common prefactor in the spirit of Feynman’s path integral.

To further illuminate this problem, we investigate the measure. It should be possible to resolve the unity operator with coherent states:

\[ \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \int d\psi \int d\psi^\dagger \mu(\vartheta, \varphi, \psi, \psi^\dagger) Q = X^{00} + X^{\uparrow\uparrow} + X^{\downarrow\downarrow} = 1, \]  

(10)

where \( \mu \) is a measure to be determined. It can only be a function of the spin variables, otherwise the term involving \( X^{00} \) would be eliminated. From (7) the prefactor of \( X^{00} \) in (10) is:

\[ \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \mu(\vartheta, \varphi) = 1 \]  

(11)

and accordingly of \( X^{\uparrow\uparrow}, X^{\downarrow\downarrow} \):

\[ \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \mu(\vartheta, \varphi) \sin^2(\vartheta/2) = 1 \quad \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \mu(\vartheta, \varphi) \cos^2(\vartheta/2) = 1, \]  

(12)

Adding the two last equations results in a contradiction to (11). As a consequence, the resolution of the unity operator is not possible with \( Q \) of equation (7) \[ \square \]. However, the

\[ ^{1}\text{It seems, the doubly occupied sites have not been projected out consistently.} \]
derivation of (6) requires such a resolution.

Weller [15] was aware of this problem and succeeded in setting up a resolution of the unity operator. He obtained the following relation:

\[
\int Q = \int \left[ 1 + \frac{1}{4} \psi \psi^\dagger + \psi \sin(\vartheta/2)e^{i\varphi}X^0 + \psi \cos(\vartheta/2)X^0 \right] |0\rangle \cdot |0\rangle = X^{00} + X^{\uparrow\uparrow} + X^{\downarrow\downarrow} = 1
\]  

(13)

where

\[
\int = 2 \int_{0}^{\pi} \frac{d\vartheta}{\pi} \int_{0}^{2\pi} \frac{d\varphi}{2\pi} \int d\psi \int d\psi^\dagger
\]  

(14)

But Q of [15] is not a projector, i.e. \(Q^2 \neq Q\). In other words the coherent state is not normalized. Using the relation (13), Weller derived a path integral. The resulting Berry phase has an unusual form:

\[
S_0 = \frac{1}{2} \sum_{n=1}^{N} \psi_n^\dagger \psi_n - \frac{1}{2} \sum_{n=1}^{N} \psi_{n-1}^\dagger \psi_{n-1} \times \left( \sin(\vartheta_n/2)\sin(\vartheta_{n-1}/2)e^{i(\varphi_n-\varphi_{n-1})} + \cos(\vartheta_n/2)\cos(\vartheta_{n-1}/2) \right)
\]

\[
\rightarrow \int_{0}^{\beta} d\tau \psi^\dagger (\partial_\tau - i\dot{\varphi} \sin^2(\vartheta/2)) \psi - \frac{1}{2} \sum_{n=1}^{N} \psi_n^\dagger \psi_n
\]

(15)

It is impossible to take the continuum limit because the last term is missing a prefactor \(\epsilon = \beta/N\). The Hamiltonian part, \(Tr(HQ)\), has the same form as in Wiegmann’s paper. One can prove that a resolution of the unity operator with normalized coherent states is not possible in the case of the \(U = \infty\) algebra (see appendix C 2).

To investigate the \(U = \infty\) limit, Schmeltzer [21] used a slave boson technique in the full Fock space:

\[
L = L_0 + L_\lambda + L_H
\]

(16)

with
\[ L_0 = \sum_i \left[ \psi_i^\dagger \partial_\tau \psi_i + \sum_\sigma b_{i,\sigma}^\dagger \partial_\tau b_{i,\sigma} \right] \]
\[ L_\lambda = \sum_i i\bar{\lambda}_i \left( \psi_i^\dagger \psi_i + \sum_\sigma b_{i,\sigma}^\dagger b_{i,\sigma} - 1 \right) \]
\[ L_H = \sum_i \left[ \mu \psi_i^\dagger \psi_i - \mu \right] - \sum_\sigma \sum_{<i,j>} \left( t_{ij} \psi_i^\dagger b_{i,\sigma}^\dagger b_{j,\sigma} \psi_j + \text{H.c.} \right) \] (17)

where \( b_\sigma \) are complex fields representing the spin degrees of freedom, \( \tilde{\lambda} \) is a Lagrange multiplier field, and \( \psi \) is a Grassmann field for the hole excitation.

A graded transformation was set up
\[ b_\sigma = z_\sigma \sqrt{1 - \psi_i^\dagger \psi_i} \quad \lambda = \bar{\lambda} \left( 1 - \psi_i^\dagger \psi_i \right) \] (18)

which transforms the graded constraint into a trivial complex constraint which can be solved by parameterization. Consequently, the Lagrangian is \( L = L_0 + L_\lambda + L_H \), where
\[ L_0 = \sum_i \left[ \psi_i^\dagger \partial_\tau \psi_i + \left( z_{i,\sigma}^\dagger \partial_\tau z_{i,\sigma} \right) \left( 1 - \psi_i^\dagger \psi_i \right) \right] \]
\[ L_\lambda = \sum_i i\lambda_i \left( \sum_\sigma z_{i,\sigma}^\dagger z_{i,\sigma} - 1 \right) \]
\[ L_H = \sum_i \left[ \mu \psi_i^\dagger \psi_i - \mu \right] - \sum_{<i,j>} \left( t_{ij} \psi_i^\dagger z_{i,\sigma}^\dagger z_{j,\sigma} \psi_j + \text{H.c.} \right) \] (19)

The resulting Lagrangian is identical to Wiegmann’s, and therefore suffers from the same problem of normalizability.

Schulz \[ 7 \] also worked out a path integral formalism for the full Fock space. He started with the canonical formalism and decoupled the model by a Hubbard Stratonovich transformation. Having introduced a unity at each space and time step, he chose the unity to be \( \mathbb{1} = RR^\dagger \), where \( R \) is a spin rotation matrix \( SU(2)/U(1) \). In order to make \( R \) a dynamical field, he additionally integrated over all angle variables at each space and time step using the invariant measure of the group. In this way he built in a dynamical, rotating spin reference system. After taking a saddle point approximation with second order fluctuations, he applied a \( 1/U \) expansion and integrated out the Hubbard Stratonovich field variables. Again the effective Lagrangian determined in this way is equivalent to Wiegmann’s in the
limit \( U = \infty \). Also Weng et al. \[22\] introduced a dynamical rotating spin reference system in the same manner as Schulz.

### III. COHERENT STATES

In the following sections we will derive a path integral formalism which uses only one Grassmann field variable and works with a well-defined measure. It should give a correct result for the partition function and, in addition, the measure of the path integral should possess a controlled continuum limit in the time direction.

First, we reconsider how to set up the definition of coherent states. A well known procedure is to require the coherent state to be an eigenstate of an annihilation operator. This results in an unnormalized state (see \[23\]). A straightforward generalization of this scheme to an arbitrary operator algebra is unclear. Therefore we take the definition of Perelomov \[24,25\] for generalized coherent states. The underlying idea is that the coherent states are the orbit of a Lie group represented in a Hilbert space and acting on a reference state. This scheme produces normalized coherent states. We will discuss only those coherent states which fulfill the two conditions: (I) normalization and (II) resolution of the unity operator. This will automatically result in a well-defined Berry phase in the continuum limit\[2\].

The limit of infinite local interaction is of special interest in this paper. It should be advantageous to construct normalized coherent states in the constrained space. However, we will show in appendix \[C2\] that possible coherent states with one Grassmann field in the constrained space will not fulfill (I) and (II) simultaneously.

For the coherent state to be defined uniquely, up to a phase factor, the Lie group should be divided in left cosets of the maximal isotropic subgroup, i.e. all operators, which when

\[2\] Abandoning condition (I) may result in a Berry phase which has no continuum limit, cf. Weller \[15\].
applied to the reference state generate just a phase factor, are removed.

In the case of bosons the coherent state is:

\[ e^{\alpha a^\dagger - a \alpha^\dagger} |0\rangle \]  

(20)

and in the fermionic case:

\[ e^{\psi C^\dagger - C \psi^\dagger} |0\rangle \]  

(21)

where \( \alpha \) is a complex variable, \( \psi \) a Grassmann number, \( a, a^\dagger \) bosonic creation and annihilation operators and \( C, C^\dagger \) the fermionic operators, respectively. The unity operator \( \mathbb{1} \) does not appear in the exponentials of equations (20) and (21) because it is a generator of the maximal isotropic subgroup.

The graded case is more involved. As mentioned above, bosonic and fermionic Hubbard operators are the generators of the graded Lie group. To get the new coherent state \(|G\rangle\) we write the analogous ansatz:

\[ |G\rangle = \exp \left[ \sum_{a \neq b} \chi_{ab} X^{ab} - \text{h.c.} \right] |\uparrow\rangle \]  

(22)

where we have just chosen \(|\uparrow\rangle\) to be the arbitrary reference state\(^3\). Now, we intend to use only one Grassmann field and the smallest number of complex fields possible. The minimal number of complex fields is two. This expresses the fact that we deal with a spin and a charge degree of freedom. Therefore, we choose \( \chi_{\uparrow 0} = \alpha \psi \), \( \chi_{0 \uparrow} = \alpha^\dagger \psi^\dagger \), \( \chi_{\downarrow 0} = \beta \psi \), \( \chi_{0 \downarrow} = \beta^\dagger \psi^\dagger \) and \( \alpha, \beta, \chi_{ab} \) to be complex. Then the exponential function is expanded using \( \psi^2 = 0 \), etc. :

\[ |G\rangle = \left( 1 + \sum_{ab} \chi_{ab} X_{ab} + \frac{1}{2} \sum_{a \neq b, c \neq d} \chi_{ab} \chi_{cd} X_{ab} X_{cd} + \ldots \right) |\uparrow\rangle \]

\[ = \left( a + b \psi \psi^\dagger \right) |\uparrow\rangle + \left( c + d \psi \psi^\dagger \right) |\downarrow\rangle + e \psi |2\rangle + f \psi |0\rangle \]  

(23)

\(^3\)The discussion of Klauder \[17\] concerning the correct choice of the reference state is not applicable here because both \(|\uparrow\rangle\) and \(|\downarrow\rangle\) are states with maximal weight.
where $a, b, c, d, e, f$ are complex variables which are functions of the $\chi_{ab}$. The conditions to be fulfilled by the coherent state are (I) normalization and (II) existence of a resolution of the unity operator:

**(I)**

$$\langle G | G \rangle = a^\dagger a + a^\dagger b \psi \psi^\dagger + ab^\dagger \psi \psi^\dagger + c^\dagger c + cd^\dagger \psi \psi^\dagger + c^\dagger d \psi \psi^\dagger + e^\dagger e \psi^\dagger \psi + f^\dagger f \psi^\dagger \psi = 1$$

**(II)**

$$1 = \int d\mu (a, b, c, d, e, f) d\psi^\dagger d\psi |G\rangle \langle G|$$

$$= \int d\mu (a, b, c, d, e, f) \left( ba^\dagger + ab^\dagger \right) X^{\uparrow \uparrow} + |e|^2 X^{22} + |f|^2 X^{00} + \left( cd^\dagger + dc^\dagger \right) X^{\downarrow \downarrow}$$

$$\downarrow\downarrow X^{00} + X^{\uparrow \uparrow} + X^{\downarrow \downarrow} + X^{22} = 1$$

Here, $\mu$ is an unknown measure which still has to be determined: The prefactors of the diagonal Hubbard operators are integrals and should equal 1:

$$\int d\mu (a, b, c, d, e, f) \left( ba^\dagger + ab^\dagger \right) \downarrow\uparrow 1 \quad \int d\mu (a, b, c, d, e, f) |e|^2 \downarrow\downarrow 1$$

$$\int d\mu (a, b, c, d, e, f) |f|^2 \downarrow\downarrow 1 \quad \int d\mu (a, b, c, d, e, f) \left( cd^\dagger + dc^\dagger \right) \downarrow\downarrow 1$$

(24)

In addition, the normalization condition (I) has to be fulfilled. The solution of this system of equations is not unique since there are six unknown variables and one unknown measure function $\mu$. One solution is, e.g.:

$$|G\rangle = \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) \sin (\vartheta) e^{i\varphi} |\uparrow\rangle$$

$$+ \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) \cos (\vartheta) |\downarrow\rangle$$

$$+ \psi \cos (\theta) |0\rangle$$

$$+ \psi \sin (\theta) e^{i\phi} |2\rangle$$

(25)

This state is normalized and one can resolve the unity operator and obtain a trace:

$$1 = \int |G\rangle \langle G|, \quad \text{Tr} (A) = \int \langle \chi G | A | G \rangle$$

(26)

In appendix we will show the calculation of these functions explicitly in two special cases.

The integration over the phases of $cd^\dagger$ and $(af^\dagger + be^\dagger)$ which are the prefactors of the offdiagonal Hubbard operators are supposed to give 0.
where \( f = 2 \int_0^\pi \frac{d\theta}{\pi} \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^\pi \frac{d\vartheta}{\pi} \int_0^{2\pi} \frac{d\varphi}{2\pi} \int d\psi^+ d\psi \). \( \chi \) indicates that Grassmann numbers will acquire a minus sign. In this solution we have used a so-called reduced measure (see [15,26]). There is another resolution and a trace with the invariant measure \( f = \frac{1}{2\pi^2} \int_0^{\pi/2} d\theta \sin(2\theta) \int_0^{2\pi} d\phi \int_0^{\pi/2} d\vartheta \sin(2\vartheta) \int_0^{2\pi} d\varphi \int d\psi^+ d\psi \); however the Lagrangian will be independent of this choice.

The expectation values of the Hubbard operators are listed in the following table.

| bosonic | fermionic |
|---------|-----------|
| \langle G | X^{00} | G \rangle = \psi^\dagger \psi \cos^2 (\theta) | \langle G | X^{10} | G \rangle = \psi \sin (\vartheta) e^{-i\varphi} \cos (\theta) |
| \langle G | X^{\uparrow\uparrow} | G \rangle = (1 + \psi \psi^\dagger) \sin^2 (\vartheta) | \langle G | X^{0\uparrow} | G \rangle = \psi^\dagger \sin (\vartheta) e^{i\varphi} \cos (\theta) |
| \langle G | X^{\downarrow\downarrow} | G \rangle = (1 + \psi \psi^\dagger) \cos^2 (\vartheta) | \langle G | X^{\downarrow0} | G \rangle = \psi \cos (\vartheta) \cos (\theta) |
| \langle G | X^{22} | G \rangle = \psi^\dagger \psi \sin^2 (\theta) | \langle G | X^{0\downarrow} | G \rangle = \psi^\dagger \cos (\vartheta) \cos (\theta) |
| \langle G | X^{02} | G \rangle = \psi^\dagger \psi \sin (\theta) \cos (\theta) e^{i\varphi} | \langle G | X^{1\downarrow} | G \rangle = \psi \sin (\vartheta) e^{-i\varphi} \sin (\theta) e^{i\varphi} |
| \langle G | X^{20} | G \rangle = \psi^\dagger \psi \sin (\theta) \cos (\theta) e^{-i\varphi} | \langle G | X^{1\uparrow} | G \rangle = \psi^\dagger \sin (\vartheta) e^{i\varphi} \sin (\theta) e^{-i\varphi} |
| \langle G | X^{\uparrow\downarrow} | G \rangle = (1 + \psi \psi^\dagger) \sin (\vartheta) \cos (\vartheta) e^{-i\varphi} | \langle G | X^{0\downarrow} | G \rangle = \psi \cos (\vartheta) \sin (\theta) e^{i\varphi} |
| \langle G | X^{\downarrow\uparrow} | G \rangle = (1 + \psi \psi^\dagger) \sin (\vartheta) \cos (\vartheta) e^{i\varphi} | \langle G | X^{2\downarrow} | G \rangle = \psi^\dagger \cos (\vartheta) \sin (\theta) e^{-i\varphi} |

This table allows \((\vartheta, \varphi)\) to be interpreted as angular spin variables, and \((\theta, \phi)\) as angular charge variables. The charge variables are pseudospin variables in the space of empty and doubly occupied states. They parameterize rotations in this space, as \((\vartheta, \varphi)\) do in the spin space. The Grassmann field induces transitions between spin and pseudospin space, e.g. \(\psi^\dagger\) creates a hole in the constrained space and a doubly occupied state in the complementary space.

### IV. PATH INTEGRAL REPRESENTATION

In the previous section we introduced coherent states for the Hubbard operators and fixed the measure which guarantees a resolution of the unity. Now, using the Trotter formula and this resolution of the unity operator with the coherent state [25], we are in the position to
set up a path integral for the partition function. The derivation is analogous to the spin $1/2$ case in appendix A.

\[
Z = \int \mathcal{D} \left[ \theta(\tau), \phi(\tau), \vartheta(\tau), \varphi(\tau), \psi^\dagger(\tau), \psi(\tau) \right] \exp \left[ - \int_0^\beta (L_0 + L_1 + L_t) d\tau \right]
\]  

(27)

where the Berry phase $L_0$ is:

\[
L_0 = \langle G(\tau) | \partial_\tau | G(\tau) \rangle = \sum_i \left[ i \dot{\varphi}_i \sin^2 \vartheta_i + \psi^\dagger_i \left( \partial_\tau + i \dot{\varphi}_i \sin^2 \vartheta_i - i \dot{\varphi}_i \sin^2 \vartheta_i \right) \psi_i \right]
\]  

(28)

The Hamiltonian part may be directly taken from the table. It contains the Coulomb potential $UX^{22}$ and the chemical potential $\mu (\sum_\sigma X^{\sigma\sigma} + 2X^{22})$ which corresponds to

\[
L_1 = \sum_i \left[ -\mu + \psi^\dagger_i \left( \frac{U}{2} + \left( \mu - \frac{U}{2} \right) \cos(2\vartheta_i) \right) \psi_i \right]
\]  

(29)

The form of $L_1$ allows to interpret $\mu - U/2$ as a magnetic field coupling to the pseudospin (c.f. appendix A). The discrete version of the local Lagrangian $L_0 + L_1$, will be presented in the next section.

Further it contains the kinetic term which we write in the discrete version in order to exhibit the correct time ordering of the field variables:

\[
L_t = L_{t;01} + L_{t;20} + L_{t;11} + L_{t;21}
\]  

(30)

where

\[
L_{t;01} = \sum_{<i,j>} t_{ij} \psi^\dagger_{i,n-1} \psi_{j,n} \cos \theta_{i,n-1} \cos \theta_{j,n} \times \left( \sin \vartheta_{i,n} \sin \vartheta_{j,n-1} e^{-i(\varphi_{i,n-1} - \varphi_{j,n-1})} + \cos \vartheta_{i,n} \cos \vartheta_{j,n-1} \right)
\]  

(31)

represents the exchange of a singly occupied site with its empty nearest neighbor,

\[
L_{t;20} = \sum_{<i,j>} t_{ij} \psi^\dagger_{i,n-1} \psi_{j,n-1} \cos \theta_{i,n-1} \sin \theta_{j,n-1} e^{i\phi_{j,n-1}} \times \left( \sin \vartheta_{i,n} \cos \vartheta_{j,n} e^{-i\varphi_{j,n}} - \cos \vartheta_{i,n} \sin \vartheta_{j,n} e^{i\varphi_{j,n}} \right)
\]  

(32)

signifies a transition from a state with two singly occupied nearest neighbor sites to a state with neighboring doubly occupied and empty sites,
\[ L_{t;11} = \sum_{<i,j>} t_{ij} \psi_{i,n}^\dagger \psi_{j,n}^\dagger \sin \theta_{i,n} \cos \theta_{j,n} e^{-i\phi_{i,n}} \]
\[ \times \left( \cos \partial_{i,n-1} \sin \partial_{j,n-1} e^{i\varphi_{j,n-1}} - \sin \partial_{i,n-1} \cos \partial_{j,n-1} e^{-i\varphi_{i,n-1}} \right) \] (33)

is the inverse process, and

\[ L_{t;21} = \sum_{<i,j>} t_{ij} \psi_{i,n}^\dagger \psi_{j,n-1} \sin \theta_{i,n} \sin \theta_{j,n-1} e^{-i(\phi_{i,n}-\phi_{j,n-1})} \]
\[ \times \left( \cos \partial_{i,n-1} \cos \partial_{j,n} + \sin \partial_{i,n-1} \sin \partial_{j,n} e^{i(\varphi_{i,n-1}-\varphi_{j,n})} \right) \] (34)

denotes the exchange of a singly occupied site with its doubly occupied nearest neighbor. We check that, if we set all angle-variable fields to zero, we find a Lagrangian which describes spinless fermions up to a particle hole transformation (cf. appendix B).

V. ATOMIC LIMIT

A. Continuum Version

The partition function may be calculated easily in the case of no band motion: \( t_{ij} = 0 \). Although this atomic limit is trivial physically, we consider it carefully in order to test the integration techniques and further to develop projection methods in the next two sections. In this atomic limit we integrate out the Grassmann field using appendix B.

\[ Z_{at} = \int D[\theta(\tau), \phi(\tau), \vartheta(\tau), \varphi(\tau), \psi^3(\tau), \psi^\dagger(\tau)] \exp \left[ -\int_0^\beta d\tau \left( L_0 + L_1 \right) \right] \]
\[ = \int D[\vartheta(\tau), \varphi(\tau)] \exp \left[ \mu \beta - \int_0^\beta d\tau i\dot{\varphi} \sin^2 \vartheta \right] \int D[\vartheta(\tau), \phi(\tau)] \]
\[ + \int D[\vartheta(\tau), \phi(\tau)] \exp \left[ -\int_0^\beta d\tau \left( i\dot{\varphi} \sin^2 \vartheta + \left( \mu - \frac{U}{2} \right) (\cos(2\theta) - 1) \right) \right] \int D[\vartheta(\tau), \phi(\tau)] \] (35)

The first term is a path integral for the free spin 1/2 and, therefore, yields \( 2e^{\mu\beta} \). The second term is also a spin path integral, but with the pseudo angle variables and subject to a ‘magnetic field’ \( \mu - U/2 \). Therefore we obtain

\[ Z = 2e^{\mu\beta} + \left( 1 + e^{(2\mu-U)\beta} \right) \] (36)
B. Discrete Version

As is well known, the continuum version of the action is only a short form, correct to first order in $\beta/N$, but several situations necessitate to consider the second order, e.g. magnetic field problems [27] or particle hole transformations (appendix B 1). Therefore we reformulate the previous subsection in the discrete language and introduce some notation which will be used in the following.

The vector notation of spin coherent states at time step $l$ is:

$$ |n_l\rangle = \begin{pmatrix} \sin(\vartheta_l)e^{i\varphi_l} \\ \cos(\vartheta_l) \end{pmatrix} \tag{37} $$

and for the pseudo spin coherent state:

$$ |N_l\rangle = \begin{pmatrix} \sin(\theta_l)e^{i\phi_l} \\ \cos(\theta_l) \end{pmatrix} \tag{38} $$

To first order in $\epsilon = \beta/N$ we are allowed to use:

$$ 1 - \langle n_l|n_{l-1}\rangle = i\dot{\varphi}\sin^2\vartheta\epsilon + \mathcal{O}(\epsilon) \quad \langle n_l|\sigma_z|n_{l-1}\rangle = -\cos(2\vartheta_l) + \mathcal{O}(\epsilon) \tag{39} $$

$$ 1 - \langle N_l|N_{l-1}\rangle = i\dot{\phi}\sin^2\theta\epsilon + \mathcal{O}(\epsilon) \quad \langle N_l|\sigma_z|N_{l-1}\rangle = -\cos(2\theta_l) + \mathcal{O}(\epsilon) \tag{40} $$

With these relations we rewrite the atomic limit in the following form:

$$ Z_{at} = \int \left( \prod_{l=1}^{N} \frac{1}{2\pi}d\vartheta_l d\phi_l d\varphi_l d\psi_l d\psi^\dagger_l \right) e^{\mu\beta} \prod_{l=1}^{N}\langle n_l|n_{l-1}\rangle $$

$$ \times \exp \left[ -\sum_{l=1}^{N} \left( \psi^\dagger_l \psi_l + \psi^\dagger_l \psi_{l-1} \left( -1 + \langle n_l|n_{l-1}\rangle - \langle N_l|1 \right) - \frac{U}{2} \|\epsilon + (\mu - \frac{U}{2})\sigma_z\epsilon|N_{l-1}\rangle \right) \right] \tag{41} $$

Expanding the exponential function and exploiting the fact that all higher orders vanish because of the anticommuting properties of the Grassmann fields $\psi, \psi^\dagger$ leads to:

6In functional integrals over Grassmann fields it is necessary to include the zeroth time slice explicitly due to the antiperiodic boundary conditions. However, in order to present the following calculations in a more readable form we will always skip this term.
\[ Z_{at} = \int \left( \prod_{l=1}^{N} \frac{1}{2\pi^2} d\vartheta_l d\phi_l d\psi_l d\psi_l^\dagger \right) e^{\mu\beta} \prod_{l=1}^{N} \langle n_l | n_{l-1} \rangle \]
\[ \times \prod_{l=1}^{N} \left( 1 + \psi_l \psi_l^\dagger + \psi_l^\dagger \psi_{l-1} \left( 1 - \langle n_l | n_{l-1} \rangle + \langle N_l | \mathbb{1} - \frac{U}{2} \mathbb{1} \mathbb{e} + (\mu - \frac{U}{2}) \sigma_z \mathbb{e} | N_{l-1} \rangle \right) \right) \]

In order to carry out the integrations we first collect the complete Grassmann chains as explained in appendix B.

\[ Z_{at} = \int \left( \prod_{l=1}^{N} \frac{1}{2\pi^2} d\vartheta_l d\phi_l d\psi_l d\psi_l^\dagger \right) e^{\mu\beta} \left[ \prod_{l=1}^{N} \left( \psi_l \psi_l^\dagger \langle n_l | n_{l-1} \rangle \right) \right. \]
\[ \left. + \prod_{l=1}^{N} \left( \psi_l^\dagger \psi_{l-1} \langle N_l | \mathbb{1} - \frac{U}{2} \mathbb{1} \mathbb{e} + (\mu - \frac{U}{2}) \sigma_z \mathbb{e} | N_{l-1} \rangle \right) \right] \]

Integration over the Grassmann and spin (first expression) or pseudo spin (second expression) variables yields:

\[ Z_{at} = \int \left( \prod_{l=1}^{N} \frac{1}{\pi} d\vartheta_l d\phi_l \right) \prod_{l=1}^{N} \langle n_l | n_{l-1} \rangle e^{\mu\beta} \]
\[ + \int \left( \prod_{l=1}^{N} \frac{1}{\pi} d\vartheta_l d\phi_l \right) e^{\mu\beta} \prod_{l=1}^{N} \langle N_l | \mathbb{1} - \frac{U}{2} \mathbb{1} \mathbb{e} + (\mu - \frac{U}{2}) \sigma_z \mathbb{e} | N_{l-1} \rangle \]

Using the resolution of the unity operator we immediately obtain:

\[ Z_{at} = \text{Tr}(\mathbb{1}) e^{\mu\beta} + e^{\mu\beta} \text{Tr} \left[ \exp \left( -\frac{U}{2} \mathbb{1} \beta + (\mu - \frac{U}{2}) \sigma_z \beta \right) \right] \]
\[ = 2e^{\mu\beta} + 1 + e^{(\mu - U)\beta} \]

VI. METHODS OF PROJECTION USING SPIN COHERENT STATES

In this section we introduce several methods of projection with the intention of applying one of these to the path integral (27). It was shown in section IV that the local Coulomb interaction \( U \) is similar to a magnetic field in the pseudo spin space. Therefore, we first deal with the system of a ‘spin in a magnetic field’ and investigate the limit of an infinitely strong magnetic field. This will result in a procedure with a well-defined measure which allows to take the limit of strong interaction \( U \to \infty \).
A. Method 1: Direct Integration

We write the spin path integral in its discrete version

\[
Z = \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \left( \prod_{n=1}^{N} d\varphi_n d\vartheta_n \right) \exp \left[ -i \sum_{n=1}^{N} \left( (\varphi_n - \varphi_{n-1}) \sin^2(\vartheta_n) \right) \right]
\]

(45)

and carry out the angular integrations. To this end, the \( \varphi \) integration is extended to \( L \) intervals and \( \sin^2(\vartheta_n) = \frac{1}{2} (1 - \cos(2\vartheta_n)) \) is replaced. We find:

\[
Z = \lim_{N \to \infty} \lim_{L \to \infty} \left( \frac{1}{\pi^2} \right)^N \left( \prod_{n=1}^{N} \int_{2\pi L}^{2\pi L} \frac{d\varphi_n}{2L} \int_{0}^{\pi/2} d\vartheta_n \right) \times \exp \left[ i \sum_{n=1}^{N} (\varphi_n - \varphi_{n-1}) \frac{1}{2} \cos(2\vartheta_n) \right]
\]

(46)

where periodic boundary conditions were used. Integrating out the \( N \vartheta \) variables, a \( N \)-fold convolution product of Bessel functions \( J_0 \) emerges which may be diagonalized by Fourier transformation. Furthermore we integrate out the \( \varphi_n \) and use the resulting \( \delta \) functions. It follows:

\[
Z = \lim_{N \to \infty} c \cdot \int_{-1/2}^{1/2} \frac{dk}{2\pi} \left( \frac{1}{\sqrt{1 - k^2}} \right)^N
\]

(47)

where \( c = (1/\pi)^N \). Taking the limit \( N \to \infty \), the only surviving contributions are due to both poles at \( k = \pm 1/2 \). In order to determine the contributions, we introduce a cutoff \( \epsilon_c \). Integration over \( k \) yields:

\[
Z = 2 \lim_{N \to \infty} \lim_{\epsilon_c \to 0} \frac{1}{\epsilon_c \pi (N + 2)} \left( \frac{2}{\sqrt{\epsilon_c}} \right)^N
\]

(48)

The prefactor 2 arises from the two poles. To solve the problem of the continuum limit in the spirit of Feynman requires only the quotient of path integrals with different couplings to be well-defined. The existence of this quotient is guaranteed by the precise knowledge of the normalization factor. In our case the limiting procedure is explicitly known (see (48)). Specifically, the problem of a spin in a ‘magnetic field’ is solved analogously to (45)–(48) and yields the same normalization factor as in (48)—independent of the ‘magnetic field’. Therefore the existence of quotients such as \( Z(B)/Z(B = 0) \) is ensured.
B. Method 2: Time Dependent Saddle Point Approximation

The spin path integral is the sum over all paths on a sphere. A path is a set containing points for each time and space step. In order to map the surface of the sphere onto planar coordinates uniquely the sphere is cut along the equator and each of the hemispheres is represented by a separate plane. With this stereographic projection each point will be placed on either of the two planes.

There is a natural way to extend the standard saddle point approximation to this spin path integral: at every space and time step the functional will be expanded around a point in each of the two planes. In this section we will clarify this procedure and show that it results in the exact expression for the partition function.

For the explicit evaluation of the partition function of a single spin, first, we chose north and south pole as reference points for the expansion:

\[
Z = \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \prod_{n=1}^{N} d\varphi_n d\vartheta_n \exp \left[ i \sum_{n=1}^{N} \left( \varphi_n - \varphi_{n-1} \right) \frac{1}{2} \cos(2\vartheta_n) \right] 
\]

(49)

\[
Z = \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \prod_{n=1}^{N} d\varphi_n d\tilde{\vartheta}_n \prod_{n=1}^{N} \left[ e^{-i(\varphi_n - \varphi_{n-1})\left(\tilde{\vartheta}_n - \tilde{\vartheta}_{n-1}\right)} + e^{+i(\varphi_n - \varphi_{n-1})\left(\tilde{\vartheta}_n - \tilde{\vartheta}_{n-1}\right)} \right]
\]

where we have expanded the exponentials up to second order in \( \tilde{\vartheta}_n \), where the field \( \tilde{\vartheta}_n \) is the fluctuation around north and south pole. Next we integrate out the \( \tilde{\vartheta}_n \). The integration runs from 0 to arbitrary \( \rho \). The result is an infinite convolution of Fresnel functions which can be diagonalized by a Fourier transformation. Making use of the periodic boundary conditions for \( \varphi_n \) the partition function reads:

\[
Z = \lim_{N \to \infty} c \cdot \int dk \left[ \frac{1}{\sqrt{k + \frac{1}{2}}} + \frac{1}{\sqrt{k - \frac{1}{2}}} \right]^N
\]

(50)

The only contributions to the integral are due to the poles at \( \pm \frac{1}{2} \).

One might worry that \( c \) has to be tuned separately for each kind of spin system. Hence one might infer that the quotient of two path integrals is not well-defined. Therefore we cal-
culate two spins in a magnetic field interacting via a Heisenberg coupling. Using the above saddle point approximation and introducing auxiliary fields, to write \( \cos(\varphi_n) \) as a derivative to \( \varphi_n - \varphi_{n-1} \), we show that the same limiting procedure, using \( c \) and cutoff \( \epsilon_c \), normalizes this more complicated problem.

First, we present the calculation for an Ising coupling of two spins in the presence of a magnetic field. The Lagrangian is:

\[
L = -\sum_{i=1,2} \frac{ix_{n,i}}{2\epsilon} \cos(2\varphi_{n,i}) + \frac{J}{4} \cos(2\varphi_{n,1}) \cos(2\varphi_{n,2}) + B \sum_{i=1,2} \cos(2\varphi_{n,i}) \tag{51}
\]

where \( x_{n,i} = \varphi_{n} - \varphi_{n-1} \). Now we work with the Gaussian method discussed above. Therefore, we have to add up the four combinations of north and south pole at each site. Rewriting the Ising coupling and magnetic field with auxiliary fields, the partition function reads:

\[
Z = \left( \frac{1}{\pi^2L} \right)^2 \int \prod_{i=1,2} \int \prod_{n=1}^N d\varphi_{n,i} d\varphi_{n,i} \left\{ \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \right. \\
\times \exp \left[ iJ/2\epsilon (\sigma_1 \partial_{x_{n,1}} + \sigma_2 \partial_{x_{n,2}} + \sigma_1 \sigma_2 \frac{i}{2}) \right] + 2B\epsilon i(\partial_{x_{n,1}} + \partial_{x_{n,2}}) \right. \\
\times \exp \left[ \sigma_2 i x_{n,1} \left( \frac{1}{2} - \varphi_{n,1}^2 \right) + \sigma_1 i x_{n,2} \left( \frac{1}{2} - \varphi_{n,2}^2 \right) \right] \right\} \tag{52}
\]

Next we have to do the \( \varphi \) integrations which cover the interval from 0 to \( \rho \). Fourier transformation and straightforward calculation yields:

\[
Z = \lim_{N \to \infty} c^2 \cdot \int_{-\infty}^\infty dk_1 \int_{-\infty}^\infty dk_2 (f(k_1, k_2))^N \tag{53}
\]

where

\[
f(k_1, k_2) = \frac{1}{2} \sum_{\sigma_1, \sigma_2} \left[ e^{\sigma_1 J\epsilon/4} + e^{-\sigma_1 J\epsilon/4} (\cos(iJ\epsilon/2) - 2i\sigma_1 \sin(iJ\epsilon/2)) \right] \times \\
\times \frac{e^{-2B\epsilon}}{\sqrt{1/2 + \sigma_2 k_1 \sqrt{1/2 + \sigma_1 \sigma_2 k_2}}} \tag{54}
\]

The dependence on \( \rho \) has vanished because we have applied formulas of the following kind:

\[
\int_0^\infty dx \frac{S(\sqrt{x})}{\sqrt{x}} \sin\left( \frac{b^2 x}{\rho^2} \right) = \frac{\sqrt{\pi} 2^{-5/2}}{b} \tag{55}
\]
Using the same cutoff and normalization constant as in method 1, we obtain:

$$Z = 2e^{J\beta/2} \cosh(B\beta) + 2e^{J\beta/2}$$  \hspace{1cm} (56)

which is the correct result for the model [51]. Extending these considerations to a Heisenberg coupling, we switch on the $x - y$ interaction, expand in the $x - y$ coupling to all orders, calculate the value of an arbitrary term, and sum up all terms to leading order in $\epsilon$. Using the same limiting procedure and normalization, we find the correct result for the partition function [26].

Later on, we will need a well-defined projection method to handle the $U \to \infty$ limit. Thereby we note that the north pole collects a weight $e^{\beta B}$ and the south pole $e^{-\beta B}$. The only surviving path in the limit of an infinitely strong magnetic field is the path that stays at the north pole over the full time range. However, if we set $\vartheta = 0$, we would not find the same normalization constant as before. The correct way of doing the projection is the following:

$$L = i\dot{\varphi} \sin^2(\vartheta) + B \cos(2\vartheta) \to L = i\dot{\varphi} \sin^2(\vartheta) \bigg|_{\text{north pole}} + B$$  \hspace{1cm} (57)

In this prescription the Berry phase is not eliminated, but has some small fluctuations around the pole. In the Hamiltonian part, the prescription yields the same result, as if we had set $\vartheta = 0$ without further considerations. We note that this prescription does not change the measure.

In the discrete language the corresponding prescription is:

$$\int \left( \prod_{l=1}^{N} \frac{1}{\pi^2} d\vartheta_l d\varphi_l \right) \prod_{l=1}^{N} \langle n_l | (1 + B\sigma_z \epsilon) | n_{l-1} \rangle$$

$$\to \int \left( \prod_{l=1}^{N} \frac{1}{\pi^2} d\vartheta_l d\varphi_l \right) \prod_{l=1}^{N} \langle n_l | (1 + B\sigma_z \epsilon) P_{\text{north pole}} | n_{l-1} \rangle$$  \hspace{1cm} (58)

where $P_{\text{north pole}} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. The path integral for infinite ‘magnetic field’ may be either gained by using (57) in the continuum version (analogously to (5A)) or by using (58) in the
discrete version (analogously to V B). As compared to section V, the projection onto the constrained space is now implemented into the path integral formalism ab initio.

C. Method 3: Action Angular Variables

In this section we want to present a method, interesting in a didactical sense. First, we consider the Berry phase of the spin 1/2 path integral.

\[ Z = \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \left( \prod_{n=1}^{N} d\vartheta_n d\varphi_n \right) \exp \left[ i \frac{1}{2} \sum_{n=1}^{N} (\varphi_n - \varphi_{n-1}) \cos(2\vartheta_n) \right] \] (59)

There is a geometrical interpretation to this expression: The Berry phase is the area enclosed by a single path. This reminds us of classical action angle variables in classical mechanics. Therefore, we want to implement similar variables.

To do so, we start by separating the partition function into a sum over all right and left rotating paths:

\[ Z = \frac{1}{2} \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \left( \prod_{n=1}^{N} d\vartheta_n d\varphi_n \right) \exp \left[ -i \frac{1}{2} \sum_{n=1}^{N} (\varphi_n - \varphi_{n-1}) \cos(2\vartheta_n) \right] \]

\[ + \frac{1}{2} \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \left( \prod_{n=1}^{N} d\vartheta_n d\varphi_n \right) \exp \left[ i \frac{1}{2} \sum_{n=1}^{N} (\varphi_n - \varphi_{n-1}) \cos(2\vartheta_n) \right] \]

\[ = \frac{1}{2} (Z_1 + Z_1^*) \] (60)

The classical action variable is the area enclosed by a single path. Therefore the action of the single spin is just this classical action variable, and it seems to be advantageous to transform the \( \vartheta \) field variables into action variables. Since the field \( \vartheta \) consists of \( N \) \( \vartheta_n \)-variables (and there exists only one classical action variable), we introduce new variables being defined as the areas which are swept out by the geodesic line from the north pole to the actual position on the considered path (see figure). In this way we obtain \( N \) variables:

\[ B_n = \frac{1}{2} \sum_{l=1}^{n} (\varphi_l - \varphi_{l-1}) \cos(2\vartheta_l) \] (61)

Then \( B_N \) is the Berry phase. The Jacobian is:
\[ |J|^{-1} = \begin{vmatrix} \frac{\partial B}{\partial \vartheta} & \frac{\partial B}{\partial \varphi} \\ \frac{\partial \vartheta}{\partial \vartheta} & \frac{\partial \vartheta}{\partial \varphi} \\ \frac{\partial \varphi}{\partial \vartheta} & \frac{\partial \varphi}{\partial \varphi} \\ 0 & 1 \end{vmatrix} = \begin{vmatrix} \frac{\partial B}{\partial \vartheta} & \frac{\partial B}{\partial \varphi} \\ \frac{\partial \vartheta}{\partial \vartheta} & \frac{\partial \vartheta}{\partial \varphi} \\ \frac{\partial \varphi}{\partial \vartheta} & \frac{\partial \varphi}{\partial \varphi} \\ 0 & 1 \end{vmatrix} \] (62)

where

\[ \frac{\partial B_n}{\partial \vartheta_m} = \begin{cases} (\varphi_m - \varphi_m) \sin(2\vartheta_m) & m \leq n \\ 0 & m \geq n \end{cases} \] (63)

is a triangular matrix and we find explicitly:

\[ |J|^{-1} = \prod_{l=1}^{N} |(\varphi_l - \varphi_{l-1}) \sin(2\vartheta_l)| = \sqrt{(\varphi_1 - \varphi_0)^2 + 4B_1^2} \prod_{l=2}^{N} \sqrt{(\varphi_l - \varphi_{l-1})^2 + 4(B_l - B_{l-1})^2} \] (64)

The partition function reads:

\[ Z = \lim_{N \to \infty} \left( \frac{1}{\pi^2} \right)^N \int \left( \prod_{n=1}^{N} dB_n d\varphi_n \right) |J|^{-1} e^{iB_N}, \] (65)

The action has become trivial but the integration over the Jacobian is a \( N \)-fold convolution. Fourier transformation decomposes the convolution into a product of independent integrals.

\[ \frac{1}{2} Z_1 = \int dB_N d\varphi_N dk_{1,N} dk_{2,N} e^{iB_N + iB_N k_{1,N} k_{2,N}} f^N(k_{1,N}, k_{2,N}) = \int dk_{1,N} f^N(k_{1,N}, -1) \] (65)

and

\[ \frac{1}{2} Z_1^* = \int dk_{1,N} f^N(k_{1,N}, +1) \] (66)

where

\[ f(k_1, k_2) = \int_{xy} \left[ x^2 + y^2 \right]^{-1/2} \exp \left[ i k_1 x + k_2 y \right] \]

\[ = \int rdrd\varphi \frac{e^{ikr \cos \varphi}}{r} \]

\[ \sim \frac{1}{k} = \frac{1}{\sqrt{k_1^2 + k_2^2}} \] (67)

The normalization of the resulting singularities is similar to the procedure of the section above (see 46-48). Furthermore, the analogous scheme applied to a spin in a magnetic field yields the correct result.
VII. ALTERNATIVE PROJECTION METHOD USING FERMIONIC COHERENT STATES

In the first part of this section we present an alternative projection method using the standard path integral formalism with two Grassmann fields. The basic idea is to perform projections at each time step explicitly through a suitable choice of the measure. Then, we introduce coherent states in the constrained space and show that their measure is identical to the ‘projecting’ measure of the first part.

First, we repeat the calculation for a local action, e.g. a chemical potential term:

\[
Z_{at} = \int \left( \prod_{n=1}^{N} d\psi_{\uparrow,n}^\dagger d\psi_{\uparrow,n} d\psi_{\downarrow,n}^\dagger d\psi_{\downarrow,n} \right) \exp \left[ - \sum_{n=1}^{N} \sum_{\sigma=\{\uparrow, \downarrow\}} \left( \psi_{\sigma,n}^\dagger \psi_{\sigma,n} - \psi_{\sigma,n}^\dagger \psi_{\sigma,n-1} (1 + \mu \epsilon) \right) \right]
\]

\[
= \int \left( \prod_{n=1}^{N} d\psi_{\uparrow,n}^\dagger d\psi_{\uparrow,n} d\psi_{\downarrow,n}^\dagger d\psi_{\downarrow,n} \right)
\times \left\{ \left( \prod_{n=1}^{N} \psi_{\uparrow,n} \psi_{\uparrow,n}^\dagger \right) \left[ \left( \prod_{n=1}^{N} \psi_{\downarrow,n} \psi_{\downarrow,n}^\dagger \right) + \left( \prod_{n=1}^{N} \psi_{\downarrow,n} \psi_{\downarrow,n-1} (1 + \mu \epsilon) \right) \right] + \left( \prod_{n=1}^{N} \psi_{\downarrow,n} \psi_{\downarrow,n}^\dagger \right) \left[ \left( \prod_{n=1}^{N} \psi_{\uparrow,n} \psi_{\uparrow,n}^\dagger \right) + \left( \prod_{n=1}^{N} \psi_{\uparrow,n} \psi_{\uparrow,n-1} (1 + \mu \epsilon) \right) \right] \right\} \quad (68)
\]

In the last step of (68) we expanded the exponential as in appendix B, (B6)–(B7). The last product of (68) represents the double occupation (see appendix B). Now we introduce a prefactor in the measure which destroys double occupation and, simultaneously, allows the other three states to survive with the same weight:

\[
Z_{at} = \int \left( \prod_{n=1}^{N} d\psi_{\uparrow,n}^\dagger d\psi_{\uparrow,n} d\psi_{\downarrow,n}^\dagger d\psi_{\downarrow,n} \right) \prod_{n=1}^{N} \left( -\psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} - \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} - \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} \right)
\times \exp \left[ - \sum_{\sigma} \sum_{n=1}^{N} \left( \psi_{\sigma,n}^\dagger \psi_{\sigma,n} - \psi_{\sigma,n}^\dagger \psi_{\sigma,n-1} (1 + \mu \epsilon) \right) \right] \quad (69)
\]

The quartic term annihilates all the terms of the exponential function, except the zeroth order term. In order to explore further this projecting measure we re-exponentiate as

\[
\left( -\psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} - \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} - \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} \right)
= - \int_{-\pi}^{\pi} \frac{d\lambda_n}{2\pi} \exp \left( i\lambda_n \left( 1 + \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} - \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} - \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} \right) \right) \quad (70)
\]
to find a contribution to the action:

$$S_{\lambda} = \sum_{n=1}^{N} i\lambda_n \frac{\epsilon}{\epsilon} \left( 1 + \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} - \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} - \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} \right)$$

$$\rightarrow \int_{0}^{\beta} d\tau i\lambda(\tau) \frac{1}{\epsilon} \left( 1 + \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} - \psi_{\uparrow,n}^\dagger \psi_{\uparrow,n} - \psi_{\downarrow,n}^\dagger \psi_{\downarrow,n} \right) \quad (71)$$

In the continuum limit \( \epsilon \to 0 \), \( S_{\lambda} \) diverges. This resembles an infinitely strong local interaction at each time step. After translation to operator language and performing a particle hole transformation (see appendix B) one recognizes a local interaction term with infinite strength:

$$\frac{\lambda}{\epsilon} (\mathbb{1} - B_{\uparrow}B_{\uparrow}^\dagger - B_{\downarrow}B_{\downarrow}^\dagger + B_{\uparrow}B_{\downarrow}^\dagger B_{\downarrow}B_{\uparrow}^\dagger) \rightarrow \frac{\lambda}{\epsilon} C_{\uparrow}^\dagger C_{\uparrow} C_{\downarrow}^\dagger C_{\downarrow} \quad (72)$$

This ad hoc scheme of introducing a measure, which projects into a (fermionic) subspace, may be embedded in the more general language of section III. The commutation relations of the operators \( X^{ab} \) (where \( a, b = 0, \uparrow, \downarrow \)) clearly constitute an algebra in the constrained space. So we may set up coherent states as:

$$|G_0\rangle = \exp^{\psi_{\uparrow}X^{00} + \psi_{\downarrow}X^{0\downarrow} - \text{h.c.}} |0\rangle$$

$$= \left( 1 - \frac{1}{2} \sum_{\sigma} \psi_{\sigma}^\dagger \psi_{\sigma} + \frac{3}{4} \psi_{\uparrow}^\dagger \psi_{\uparrow} \psi_{\downarrow}^\dagger \psi_{\downarrow} \right) |0\rangle$$

$$+ \left( \psi_{\uparrow} - \frac{1}{2} \psi_{\uparrow}^\dagger \psi_{\downarrow} \psi_{\uparrow} \right) |\uparrow\rangle$$

$$+ \left( \psi_{\downarrow} - \frac{1}{2} \psi_{\downarrow}^\dagger \psi_{\uparrow} \psi_{\downarrow} \right) |\downarrow\rangle \quad (73)$$

where \( \psi_{\sigma} \) are Grassmann numbers. Now the projector onto the normalized coherent states reads:

$$P = |G_0\rangle \langle G_0| = X^{00} \left( 1 - \sum_{\sigma} \psi_{\sigma}^\dagger \psi_{\sigma} - 2 \psi_{\uparrow}^\dagger \psi_{\uparrow} \psi_{\downarrow}^\dagger \psi_{\downarrow} \right)$$

$$+ X^{\uparrow\uparrow} \left( \psi_{\uparrow}^\dagger \psi_{\uparrow} + \psi_{\uparrow}^\dagger \psi_{\uparrow} \psi_{\downarrow}^\dagger \psi_{\downarrow} \right)$$

$$+ X^{\downarrow\downarrow} \left( \psi_{\downarrow}^\dagger \psi_{\downarrow} + \psi_{\uparrow}^\dagger \psi_{\uparrow} \psi_{\downarrow}^\dagger \psi_{\downarrow} \right) \quad (74)$$

For the resolution of unity we have to find a measure \( \mu(\psi_{\uparrow}^\dagger, \psi_{\uparrow}, \psi_{\downarrow}^\dagger, \psi_{\downarrow}) \) which satisfies:

$$\int d\psi_{\uparrow} d\psi_{\uparrow}^\dagger d\psi_{\downarrow} d\psi_{\downarrow}^\dagger \mu(\psi_{\uparrow}^\dagger, \psi_{\uparrow}, \psi_{\downarrow}^\dagger, \psi_{\downarrow}) P = \mathbb{1} \quad (75)$$

25
Obviously, any measure consisting of a single product of the Grassmann numbers will be inadequate to solve (73). It turns out that $\mu$ has to be of an additive form

$$\mu(\psi_\uparrow^\dagger, \psi_\uparrow, \psi_\downarrow^\dagger, \psi_\downarrow) = -\left(\psi_\uparrow^\dagger \psi_\uparrow \psi_\downarrow^\dagger \psi_\downarrow + \psi_\uparrow^\dagger \psi_\uparrow + \psi_\downarrow^\dagger \psi_\downarrow \right) \tag{76}$$

in order to ensure the resolution of the unity operator.

The Berry phase has to be calculated in the discrete version. Terms in fourth order of the Grassmann fields arise, but are eliminated by multiplication with $\mu$ of (76). The surviving contribution has the canonical form $\sum_{\sigma} \psi_\sigma^\dagger \partial_{\tau} \psi_\sigma$, as in (59). Having fixed the measure and the Berry phase, the functional integral formalism is established. One might worry that the derivation of the Hamiltonian terms of the action always involves higher orders in the field variables; e.g. the kinetic term as derived with (73) is

$$\sum_{<i,j>} t_{ij} \left( \psi_{\sigma,i,n}^\dagger - \frac{1}{2} \psi_{\sigma,i,n}^\dagger \psi_{-\sigma,i,n-1}^\dagger \psi_{-\sigma,i,n-1} - \frac{1}{2} \psi_{\sigma,i,n}^\dagger \psi_{-\sigma,i,n}^\dagger \psi_{-\sigma,i,n} \right)$$

$$\left( \psi_{\sigma,j,n}^\dagger - \frac{1}{2} \psi_{\sigma,j,n}^\dagger \psi_{-\sigma,j,n-1}^\dagger \psi_{-\sigma,j,n-1} - \frac{1}{2} \psi_{\sigma,j,n}^\dagger \psi_{-\sigma,j,n}^\dagger \psi_{-\sigma,j,n} \right) \tag{77}$$

Fortunately, the measure $\mu$ eliminates all fourth and higher order terms, similarly to the calculation of the Berry phase.

Before we try to derive an effective Lagrangian for large $U$, we should summarize the projection techniques of the last two sections: It turned out that it is possible to construct normalized coherent states which lie in the constrained space and resolve the unity. But their measure is of an additive form, i.e., a polynomial of the Grassmann variables for up and down spin. The minimal number of complex Grassmann fields for such a resolution in the constrained space is two, so that the proposed coherent state does not render the path integrals more tractable as compared to the canonical formalism with two Grassmann fields in the full space: The local interaction is suppressed but at the expense of a most inconvenient measure. Therefore, coherent states should be set up in the full space in which we may reduce the number of Grassmann fields to one. Additional complex fields have to be introduced for spin and pseudospin. Since the local interaction denotes a ‘magnetic field’ in the pseudospin space, we investigated an elaborate saddle point technique for spins in
magnetic fields. It serves to constrain the excitations to the considered subspace by sending
the magnetic field to infinity in a controlled way: The pseudospin fields may be fixed to their
‘subspace direction’ everywhere except in the Berry phase where small fluctuations about
this direction have to be kept, even for infinite \( U \).

**VIII. CUMULANT EXPANSION FOR LARGE LOCAL INTERACTION**

Now we will show how to gain the effective action to lowest order in \( t/U \) using the
coherent states (25) and the projection method of section [VI]. The effective action will be
similar, but not identical, to the action derived by Schulz through a Hubbard Stratonovich
decoupling scheme.

The Lagrangian for the Hubbard model was introduced in section [IV]:

\[
L = \sum_i \left( -\mu + i\dot{\phi}_i \sin^2 \vartheta_i + \psi_i^\dagger \left( \partial_\tau + \mu + i\dot{\phi}_i \sin^2 \theta_i - i\dot{\phi}_i \sin^2 \vartheta_i + \left( \mu - \frac{U}{2} \right) \cos(2\theta_i) \right) \psi_i \right) + L_t
\]  

(78)

Applying the projection prescription (57), the Lagrangian reads for \( U = \infty \):

\[
\mathcal{L} = \sum_i \left( -\mu + i\dot{\phi}_i \sin^2 \vartheta_i + \psi_i^\dagger \left( \partial_\tau + \mu + i\dot{\phi}_i \sin^2 \theta_i \bigg|_{\text{north pole}} - i\dot{\phi}_i \sin^2 \vartheta_i \right) \psi_i \right) + \mathcal{L}_t
\]  

(79)

where \( \mathcal{L}_t \) restricts hopping to the exchange of a hole with either a \( \uparrow \)-spin or a \( \downarrow \)-spin on the
nearest neighbor site:

\[
\mathcal{L}_t = \sum_{<i,j>} t_{ij} \psi_i^\dagger \psi_j^\dagger \left[ \left( \sin \vartheta_i \sin \vartheta_j e^{-i(\phi_i - \phi_j)} + \cos \vartheta_i \cos \vartheta_j \right) \right]
\]  

(80)

The path integral with \( \mathcal{L} \) from (79) may be cast into a more conventional form without
a prescription. Through a redefinition of the measure

\[
\mathcal{D} \left[ \theta(\tau), \phi(\tau), \vartheta(\tau), \varphi(\tau), \psi^\dagger(\tau), \psi(\tau) \right]
\rightarrow \mathcal{D} \left[ \theta(\tau), \phi(\tau), \vartheta(\tau), \varphi(\tau), \psi^\dagger(\tau), \psi(\tau) \right] \exp \left[ -\sum_i \int_0^\beta d\tau \left( \psi_i^\dagger \psi_i \ i \dot{\phi}_i \sin^2 \theta_i \bigg|_{\text{north pole}} \right) \right]
\]  

(81)
the projected Lagrangian acquires the form:

\[
L_{U=\infty} = \sum_i \left( -\mu + i \dot{\phi}_i \sin^2 \theta_i + \psi_i^\dagger \left( \partial_\tau + \mu - i \dot{\phi}_i \sin^2 \theta_i \right) \psi_i \right) \\
+ \sum_{<i,j>} t_{ij} \psi_i \psi_j^\dagger \left[ \sin \theta_i \sin \theta_j e^{-i(\phi_i - \phi_j)} + \cos \theta_i \cos \theta_j \right] \tag{82}
\]

This form of the path integral would be more useful if we were able to integrate over the purely kinematical fields \( \theta \) and \( \phi \) first.

In the next stage, we will explicitly calculate local propagators in order to gain an effective Lagrangian which is generated by a hopping expansion. The dynamical processes of this effective Lagrangian lie in the constrained space only. We will find the propagator by integrating first over the Grassmann fields and then the (pseudo) spin fields. As an introductory exercise we calculate \( Z \) for the atomic limit with \( \bar{T}_0 = T - T_t \) (analogously to section [VE]):

\[
Z = \int D \left[ \vartheta(\tau), \varphi(\tau), \theta(\tau), \phi(\tau), \psi(\tau), \psi^\dagger(\tau) \right] \exp \left[ - \int_0^\beta \bar{T}_0 \ d\tau \right] \\
= \int \left( \prod_{l=1}^N \frac{1}{\pi} d\vartheta_l d\varphi_l \right) \prod_{l=1}^N \langle n_l|n_{l-1}\rangle e^{\mu^2} + \\
+ \int \left( \prod_{l=1}^N \frac{1}{\pi} d\theta_l d\phi_l \right) e^{\mu^2} \prod_{l=1}^N \langle N_l| (\mathbb{1} + \mu \sigma_z \epsilon) P_{north \ pole} | N_{l-1} \rangle \\
= 2e^{\mu^2} + 1 \tag{83}
\]

where \( P_{north \ pole} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \) and we have used the fact that only the two complete Grassmann chains survive.

Similarly, we may evaluate the local propagators necessary for a cumulant resummation. In order to check the consistency of the calculation we compare the propagator obtained with \( L \) to the projected propagator assigned to \( \bar{T} \).

First we expand the functional in terms of the hopping parameter \( t \). Odd orders in the hopping expansion vanish because they contain an odd number of Grassmann numbers.
at each of the sites involved in the hopping process. In second order we average with the original action $S_{at} = \int_0^\beta d\tau (L - L_1)$. For example the propagator $Z \cdot \langle T X_{i=0}^{\tau_m-1} X_{i=0}^{\tau_n} \rangle$ is:

$$
\int \mathcal{D} \left[ \vartheta(\tau), \varphi(\tau), \theta(\tau), \phi(\tau), \psi(\tau), \psi^\dagger(\tau) \right] \\
\times \psi_{m-1} \psi_n^\dagger \cos(\theta_{m-1}) \cos(\theta_n) \cos(\phi_m) \cos(\phi_{n-1}) \exp \left[ -S_{at} \right]
$$

(84)

where $n \leq m$ is assumed. With the identity

$$
\cos(\theta_n) \cos(\theta_{m-1}) = \langle N_{m-1} | \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} | N_n \rangle
$$

(85)

we get

$$
e^{\mu \beta} \int \mathcal{D} \left[ \vartheta(\tau), \varphi(\tau), \theta(\tau), \phi(\tau), \psi^\dagger(\tau), \psi(\tau) \right] \\
\times \left( \prod_{l=m}^{n-1} \psi_l^\dagger \psi_l \right) \left( \prod_{l=m+1}^{n-1} \langle n_l | n_{l-1} \rangle \right) \langle n_m | \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} | n_{n-1} \rangle \\
\times \left( \prod_{l=n+1}^{m-1} \left( \psi_l^\dagger \psi_{l-1} \langle N_l | \mathbb{I} - \left( \frac{U}{2} \mathbb{I} - (\mu - \frac{U}{2}) \sigma_z \right) \epsilon | N_{l-1} \rangle \right) \langle N_n | \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} | N_{m-1} \rangle \right)
$$

$$
= e^{\mu \beta} \int \mathcal{D} \left[ \psi^\dagger(\tau), \psi(\tau) \right] \\
\times \psi_{m-1} \psi_n^\dagger \text{Tr} \left[ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \prod_{l=m}^{n-1} \psi_l^\dagger \psi_l \prod_{l=n+1}^{m-1} \psi_l^\dagger \psi_{l-1} \right]
$$

$$
\times \text{Tr} \left[ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \exp \left[ -\frac{U}{2} \mathbb{I} + (\mu - \frac{U}{2}) \sigma_z \epsilon (m - n - 1) \right] \right]
$$

$$
= e^{\mu \beta} e^{-\mu (m-n-1) \epsilon}
$$

(86)

where the following convention is introduced: if there is a sum (product), whose upper index is smaller than its lower index, the sum (product) denotes a sum (product) from the lower index to $\beta$ and from 0 to the upper index. With this convention we can also prove the result to be true in the case of $n \geq m$.

By exploiting the identity
\[
\sin(\theta_{m-1}) \sin(\theta_n) e^{i(\phi_{m-1} - \phi_n)} = \langle N_n | \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} | N_{m-1} \rangle \tag{87}
\]

we are able to calculate remaining term from the second order cumulant expansion. It which
will generate virtual double occupations in the effective action below.

\[
\int \mathcal{D} [\vartheta(\tau), \varphi(\tau), \theta(\tau), \phi(\tau), \psi(\tau), \psi(\tau)] \psi_{m-1} \psi_n^\dagger \\
\times \sin(\theta_{m-1}) \sin(\theta_n) e^{i(\phi_{m-1} - \phi_n)} \cos(\vartheta_m) \cos(\vartheta_{n-1}) e^{-S_{at}}
\]

\[
= e^{\mu \beta} \int \mathcal{D} [\psi(\tau)] \psi_{m-1} \psi_n^\dagger \text{Tr} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}^{n-1} \prod_{l=m}^{n-1} \psi_l \psi_l^\dagger \prod_{l=m+1}^{n-1} \psi_l \psi_l - 1 \\
\times \text{Tr} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \exp \left[ \left( -\frac{U}{2} \mathbb{I} + \left( \mu - \frac{U}{2} \sigma_z \right) \epsilon (m - n - 1) \right) \right]
\]

\[
= e^{\mu \beta} e^{(\mu - U)(m - n - 1) \epsilon} \tag{88}
\]

We have to pay attention to the correct sequence of the limits, i.e. to take first \( U \to \infty \) and
then \( \epsilon \to 0 \) (for \( \mu \ll U \)). In the case of large \( U \), it is an excellent approximation to substitute
for the last result a Kronecker delta with weight given by the integral of the exponential
over all positive times \( \tau = (m - n - 1) \epsilon \) [\( \mathbb{I} \)]:

\[
\approx \frac{1}{U} e^{\mu \beta} \delta_{m-1, n} \tag{89}
\]

Now we calculate the analogous averages using the projected action, \( \overline{S}_{at} = f_0^\beta d \tau (L - \overline{L}_t) \).

The calculation corresponds to the preceding:

\[
\int \mathcal{D} [\vartheta(\tau), \varphi(\tau), \psi(\tau), \psi(\tau)] \psi_{m-1} \psi_n^\dagger \cos(\vartheta_m) \cos(\vartheta_{n-1}) e^{-\overline{S}_{at}}
\]

\[
= \int \mathcal{D} [\vartheta(\tau), \varphi(\tau), \psi(\tau), \psi(\tau)] \psi_{m-1} \psi_n^\dagger e^{\mu \beta} \langle n_m | \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} | n_{n-1} \rangle
\]

\[
= e^{\mu \beta} e^{-\mu (m - n - 1) \epsilon} \tag{90}
\]
which is obviously equivalent to (84)–(86). Therefore we are led to introduce the following translation rules regarding the transition from the unconstrained to the constrained (infinite \( U \)) problem.

\[
\langle \psi_n^\dagger \psi_{m-1} \cos(\theta_n) \cos(\theta_{m-1}) \rangle_{S_{\text{at}}} \rightarrow \langle \psi_n^\dagger \psi_{m-1} \rangle_{S_{\text{at}}}
\]

\( (91) \)

\[
\langle \psi_n^\dagger \psi_{m-1} \sin(\theta_n) \sin(\theta_{m-1}) \rangle_{S_{\text{at}}} \rightarrow \frac{1}{U} \delta_{n,m-1} \langle \ldots \rangle_{S_{\text{at}}}
\]

\( (92) \)

The ellipses stand for the various spin variables. (91) and (92) exemplify how to gain all the required propagators. The hopping expansion has to be done to fourth order. After using these translation rules we re-exponentiated to obtain the following effective Lagrangian:

\[
L_{\text{eff}} = \sum_i L_0 - t \sum_{<i,j>} \psi_{i,n-1}^\dagger \psi_{j,n}^\dagger \alpha(n_i, n_j) + \frac{t^2}{U} \sum_{<i,j>} \left( \psi_{i,n-1}^\dagger \psi_{i,n}^\dagger + \psi_{j,n-1}^\dagger \psi_{j,n}^\dagger \right) (1 - n_i n_j) + \frac{t^2}{U} \sum_{<i,j,k>} \psi_{i,n-1}^\dagger \psi_{k,n}^\dagger \alpha(n_i, n_j) \alpha(n_j, n_k)
\]

\( (93) \)

Here \( L_0 = \mathcal{L} - \mathcal{L}_t \) and

\[
\alpha(n_i, n_j) = \sqrt{\frac{1}{2} (1 + n_i n_j)} \exp [i \mathcal{A}(n_i, n_j, \hat{z}) / 2]
\]

\( (94) \)

\( \mathcal{A}(n_i, n_j, \hat{z}) \) is the area of the spherical triangle defined by the three unit vectors, and \( \hat{z} \) points to the north pole of the unit sphere. \(<i,j,k>\) denotes the following convention: \( j \) has to be a nearest neighbor of \( i \), and \( k \) a nearest neighbor of \( j \), excluding \( k = i \). To compare this effective Lagrangian with Schulz [7], we have to perform a particle-hole transformation. On the operator level the well known anticommutator relation

\[
C^\dagger C = \mathbb{1} - CC^\dagger
\]

holds. In the path integral formalism we work with the corresponding ‘anticommutator relation’:

\[
\]
\[
\int \left( \prod_{n=1}^{N} d\psi d\psi \dagger \right) \psi_n \psi_{n-1} \exp \left[ -\sum_{l=1}^{N} \psi_l^\dagger (\psi_l - \psi_{l-1}(1 + \mu \epsilon)) \right] = \int \left( \prod_{n=1}^{N} d\psi d\psi \dagger \right) (1 - \psi_n \psi_n^\dagger) \exp \left[ -\sum_{l=1}^{N} \psi_l^\dagger (\psi_l - \psi_{l-1}(1 + \mu \epsilon)) \right]
\]

(96) is proved by using relations of appendix B 1. Obviously, the information about the anticommutator is contained in the time index (see also [27]). The transformation results in:

\[
\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_t + \mathcal{L}_J + \mathcal{L}_{\text{pair}}
\]

where

\[
\mathcal{L}_0 = \frac{1}{\epsilon} \sum_i \left( -\mu \epsilon + 1 - \langle \mathbf{n}_{i,n} | \mathbf{n}_{i,n-1} \rangle + \psi^\dagger_{i,n} \psi_{i,n} + \psi^\dagger_{i,n} \psi_{i,n-1} \left( \mu \epsilon - 1 + \langle \mathbf{n}_{i,n} | \mathbf{n}_{i,n-1} \rangle - \langle \mathbf{N}_{i,n} | \mathbf{N}_{i,n-1} \rangle \right) \right)
\]

contains the Berry phase which differs from [7] by pseudo spin fluctuations about the north pole,

\[
\mathcal{L}_t = -t \sum_{<i,j>} \psi^\dagger_{i,n} \psi_{j,n-1} \alpha \left( \mathbf{n}_i, \mathbf{n}_j \right)
\]

is the hopping term,

\[
\mathcal{L}_J = \frac{t^2}{U} \sum_{<i,j>} \left( 2 - \psi^\dagger_{i,n} \psi_{i,n} - \psi^\dagger_{j,n-1} \psi_{j,n} \right) \left( 1 - \mathbf{n}_i \mathbf{n}_j \right)
\]

denotes the Heisenberg term, and

\[
\mathcal{L}_{\text{pair}} = \frac{t^2}{U} \sum_{<i,j,k>} \psi^\dagger_{i,n} \psi_{k,n} \alpha \left( \mathbf{n}_i, \mathbf{n}_j \right) \alpha \left( \mathbf{n}_j, \mathbf{n}_k \right)
\]

is the pair hopping term which represents hopping to the next nearest neighbor site and thereby transports a pair of spins. We refer the reader to the literature for a discussion of these terms, e.g. [1,7].

Schulz derived an additional term:

\[
\frac{1}{4U} \sum_j (1 - \psi^\dagger_j \psi_j) \mathbf{n}_j^2
\]

Such a term is not generated in our formalism because no operation will produce a quadratic time derivative.
IX. CONCLUSIONS

In this paper we addressed the question of how to set up a path integral formalism in a constrained Fock space. We only tackled methods which do not involve additional ‘graded constraints’ as in the slave boson method. The projection was implemented through either, (i) a suitable modification of the measure of the path integral, or, (ii) through adequately generalized coherent states.

The first approach allows the use of Grassmann fields which correspond to the canonical creation and annihilation operators of electrons. A ‘projecting measure’ was introduced which explicitly projects at every time step.

Alternatively, one might want to consider generalized coherent states which lie in the constrained space, exclusively. Such normalized states were constructed explicitly but they resolve the unity operator only if the number of complex Grassmann fields is equal to the number of spin states. But even then, the path integration is awkward because the Grassmann valued measure is of an additive form which turns out to be exactly the ‘projecting’ measure of the first approach. This implies that normalized coherent states should be set up in the full Fock space first. We presented such states, involving only one (complex) Grassmann field and the smallest number of complex fields possible, i.e. one for the spin and one for the charge degree of freedom. The ‘charge field’, which here signifies transitions between states with empty and doubly occupied sites, was shown to be a pseudo spin coupled to a ‘magnetic field’, linear in the local interaction parameter. Accordingly, this approach had to establish a procedure how to send the pseudo magnetic field to infinity in order to implement the constraint of no double occupancy. This procedure fixes the pseudo spin field at the north pole in the Hamiltonian terms of the action but keeps fluctuations around the north pole in the Berry phase. It seems to be a generic feature of such constrained systems that forces us to keep the Berry phase fluctuations in the unconstrained space, in order to work with ‘normalizable’ path integrals. Finally, this method was elaborated and tested on the Hubbard model to derive an effective Lagrangian for strong local interaction.
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APPENDIX A: SPIN PATH INTEGRAL

A spin coherent state is given by [24]:

\[ |n\rangle = \begin{pmatrix} \sin(\vartheta)e^{i\varphi} \\ \cos(\vartheta) \end{pmatrix} \quad (A1) \]

Furthermore we can find a resolution of unity and a trace with this overcomplete set of coherent states:

\[ \mathbb{1} = \int d\mu(n) |n\rangle\langle n| \]

\[ = \frac{1}{\pi^2} \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \begin{pmatrix} \sin^2(\vartheta) & \sin(\vartheta) \cos(\vartheta)e^{i\varphi} \\ \sin(\vartheta) \cos(\vartheta)e^{-i\varphi} & \cos^2(\vartheta) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

\[ \text{Tr}(A) = \frac{1}{\pi^2} \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \langle n|A|n\rangle \quad (A2) \]

Now a path integral is derived using the Trotter formula and introducing an imaginary time index:

\[ Z = \text{Tr} e^{-\beta H} \]

\[ = \lim_{N \to \infty} \text{Tr} \left( e^{-\epsilon H}\mathbb{1}_1 e^{-\epsilon H}\mathbb{1}_2 e^{-\epsilon H} \ldots \mathbb{1}_{N-2} e^{-\epsilon H}\mathbb{1}_{N-1} e^{-\epsilon H} \right) \]

\[ = \lim_{N \to \infty} \int \prod_{l=1}^N d\mu(n_l) \prod_{l=1}^N \langle n_l|\mathbb{1} - \epsilon H|n_{l-1}\rangle \]

\[ = \lim_{N \to \infty} \int \prod_{l=1}^N d\mu(n_l) \exp \left[ -\sum_{l=1}^N \left( \epsilon \langle n_l|\partial_\tau|n_l\rangle + \epsilon \langle n_l|H|n_l\rangle + O(\epsilon^2) \right) \right] \quad (A3) \]
In the last step the continuum limit was taken. Thereby the discrete time index \( n \) became a continuum variable \( n(\tau) \) with \( \tau = l\epsilon \) and the measure is \( d\mu(n) = \frac{d\theta d\varphi}{\pi^2} \). The continuum path integral is written as:

\[
Z = \int D[\theta(\tau), \varphi(\tau)] \exp \left[ -\int_0^\beta \left( i\dot{\varphi} \sin^2(\vartheta) + \langle n | H | n \rangle \right) d\tau \right]
\] (A4)

We finish this appendix with a note of warning: Usually a path integral with complex fields is evaluated through a saddle point approximation. In the spin case it will break down. Consider the spin in a magnetic field proportional to \( B \). The Lagrangian is:

\[
L = i\dot{\varphi} \sin^2(\vartheta) + B \cos(2\vartheta)
\] (A5)

The general solution of the classical equations of motion restricts the spin dynamics to north and south pole if the periodic boundary conditions are taken care of. The classical action is \( S_{cl} = \pm B\beta \), for north and south pole, respectively. Although the saddle point solution yields the correct result, fluctuations around the classical path are divergent, already in lowest order. This originates from an expansion of the action about its maximum at the south pole. A path on the sphere, on which the spins live, can be described only by two complex numbers at each space and time step. In section \( \text{VI} \) methods were devised in order to generalize the conventional saddle point approximation for spin path integrals.

APPENDIX B: FERMIONIC PATH INTEGRAL

In this appendix we want to derive a path integral for a system with spinless fermions using normalized coherent states. We take the following definition for coherent states:

\[
|G\rangle = e^{\psi C^\dagger - C^\dagger \psi} |0\rangle
\] (B1)

Because of the anticommuting properties of the Grassmann numbers the exponential function is trivially determined to be:

\[
|G\rangle = \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) |0\rangle + \psi |1\rangle
\] (B2)
This state is normalized

\[ \langle G | G \rangle = \left( \langle 0 | \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) \right) + \langle 1 | \psi^\dagger \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) | 0 \rangle + \psi | 1 \rangle \right) = 1 \]  

and we can easily find a resolution of the unity operator

\[
\int d\psi^\dagger d\psi |G\rangle \langle G| = \int d\psi^\dagger d\psi \left\{ \left( 1 + \psi \psi^\dagger \right) |0\rangle \langle 0| + \psi \psi^\dagger |1\rangle \langle 1| - \psi^\dagger |0\rangle \langle 1| \right\}
\]

\[
= |0\rangle \langle 0| + |1\rangle \langle 1| = \mathbb{1}
\]

and the trace is:

\[
\text{Tr } A = \int d\psi^\dagger d\psi \left( \langle 0 | \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) - \langle 1 | \psi^\dagger \right) A \left( \left( 1 + \frac{1}{2} \psi \psi^\dagger \right) |0\rangle + \psi | 1 \rangle \right)
\]

In the same manner as in appendix A we derive a path integral using the Trotter formula:

\[
Z = \int \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \exp \left[ - \sum_{n=1}^{N} \epsilon \left( \psi_n^\dagger (\psi_n - \psi_{n-1}) + \langle G_n | H | G_{n-1}\rangle \right) \right]
\]

If we only consider a chemical potential \( \mu C^\dagger C \), we have to replace \( \langle G_n | H | G_{n-1}\rangle \rightarrow -\mu \psi_n^\dagger \psi_{n-1} \). The evaluation of the path integral is equivalent to the calculation of a determinant. Alternatively, we can expand the exponential function. Then we have to collect a large number of terms which seem to be difficult to handle. But, only the complete chains of Grassmann numbers will survive the Grassmann integrations. Thereby ‘complete chain’ denotes a product of Grassmann numbers over all time steps \( \prod_{n=1}^{N} \psi_n \psi_n^\dagger \). This implies that the partition function may be written in the following way:

\[
Z = \int \left( \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \right) \left( \prod_{n=1}^{N} \psi_n \psi_n^\dagger - \prod_{n=1}^{N} \psi_n^\dagger \psi_{n-1} \left( 1 + \mu \epsilon \right) \right)
\]

\[
= 1 + \prod_{n=1}^{N} \left( 1 + \mu \epsilon \right) = 1 + e^{\mu \beta}
\]

The assumption of the continuum limit to exist requires \( \mu(\tau) \) to be a smooth function.

With this assumption we are able to calculate the partition function of a time dependent (chemical) potential:

\[\text{Heed the footnote of section V B}\]
\[ Z = 1 + \prod_{n=1}^{N} (1 + \mu_n \epsilon) = 1 + e^{\int_0^\beta \mu(\tau) d\tau} \quad (B8) \]

In order to set up more involved path integrals we would like to investigate the question of the minimal number of complex fields. Specifically, one might have the idea to introduce an additional complex field in \((B1)\).

\[ |G\rangle = e^{\alpha \psi C^\dagger - \alpha^\dagger C \psi^\dagger} |0\rangle = \left( 1 + \frac{1}{2} \alpha \alpha^\dagger \psi \psi^\dagger \right) |0\rangle + \alpha \psi |1\rangle \quad (B9) \]

The state is also normalized and we can resolve the unity:

\[ \mathbb{1} = \int d\psi^\dagger d\psi \int d\alpha d\alpha^\dagger \mu(\alpha) |G\rangle \langle G| \quad (B10) \]

Here, the measure has to obey the relation:

\[ \int d\alpha d\alpha^\dagger \mu(\alpha) \alpha^\dagger \alpha = 1 \quad (B11) \]

The following Berry phase arises in the path integral:

\[ \mathcal{L}_o = \alpha^\dagger \psi^\dagger \partial_\tau (\alpha \psi) = \alpha^\dagger \alpha \psi^\dagger \partial_\tau \psi + \alpha^\dagger (\partial_\tau \alpha) \psi^\dagger \psi \quad (B12) \]

With our consideration of ‘complete chains of Grassmann numbers’ we can write the partition function:

\[ Z = \int \left( \prod_{n=1}^{N} d\alpha_n^\dagger d\alpha_n d\psi_n^\dagger d\psi_n \right) \left( \prod_{n=1}^{N} \alpha_n^\dagger \alpha_n \psi_n^\dagger \psi_n - \prod_{n=1}^{N} \alpha_n^\dagger \alpha_n \psi_n^\dagger \psi_{n-1} (1 + \mu \epsilon) \right) \]

We note that each of the two chains possesses a complete product of the complex fields \(\alpha_n\). Therefore we can integrate out the \(\alpha_n\) and we get the known result

\[ Z = \text{const} \int \left( \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \right) \left( \prod_{n=1}^{N} \psi_n^\dagger \psi_n^\dagger - \prod_{n=1}^{N} \psi_n^\dagger \psi_{n-1} (1 + \mu \epsilon) \right) \quad (B13) \]

which can be re-exponentiated:

\[ Z = \int \mathcal{D} \left[ \psi^\dagger(\tau), \psi(\tau) \right] \exp \left[ - \int_0^\beta d\tau \left( \psi^\dagger \partial_\tau \psi - \mu \psi^\dagger \psi \right) \right] \quad (B14) \]

In this way we have shown the additional field to be superfluous.
1. Particle Hole Transformation

The particle hole transformation is a special case of an unitary transformation for electronic states. On the operator level it reads:

\[ C \rightarrow B^\dagger, \quad C^\dagger \rightarrow B \]  \hspace{1cm} (B15)

Under this transformation the trivial Hamilton operator \( H = -\mu C^\dagger C \) transforms to \( H' = -\mu B B^\dagger = -\mu \mathbb{1} + \mu B^\dagger B \). So, why not introduce the analogous unitary transformation in the path integral formalism

\[ \psi_n \rightarrow \psi_n^\dagger, \quad \psi_n^\dagger \rightarrow \psi_n \]  \hspace{1cm} (B16)

In the path integral \( \mu \psi_n^\dagger \psi \) transforms into \( -\mu \psi_n^\dagger \psi \). However, we expect the particle hole transformed result to be \( \mu - \mu \psi_n^\dagger \psi \). Obviously, we have to do further considerations to find a Lagrangian analogous to a particle hole transformed Hamiltonian.

The path integral consists of two complete Grassmann chains. One of them is the particle chain \( \prod \psi_l^\dagger \psi_{l-1} \) and the other is the hole chain \( \prod \psi_l \psi_l^\dagger \). The particle hole transformation should exchange the two chains. Therefore the particle hole transformation is not unitary, but ‘almost unitary’:

\[ \psi_n^\dagger \rightarrow \psi_n (1 - \mu \epsilon), \quad \psi_{n-1} \rightarrow \psi_{n}^\dagger \]  \hspace{1cm} (B17)

and the Jacobian is\[^8\]:

\[ |J| = \prod_{n=1}^{N} (1 + \mu \epsilon) = e^{\beta \mu} \]  \hspace{1cm} (B18)

The Berry phase transforms to (first order in \( \epsilon \)):

\[^8\]The Jacobian for the Grassmann numbers is defined inversely in comparison to the complex numbers.
\[
\lim_{N \to \infty} \sum_{n=1}^{N} \psi_n^\dagger (\psi_n - \psi_{n-1})
\]

\[
\rightarrow \lim_{N \to \infty} \sum_{n=1}^{N} \psi_n (1 - \mu \epsilon) (\psi_n^\dagger - \psi_n^\dagger - 1) = \lim_{N \to \infty} \sum_{n=1}^{N} \psi_n^\dagger (\psi_n - \psi_{n-1}) + \mathcal{O}(\epsilon^2)
\]  \hspace{1cm} (B19)

and the partition function accordingly:

\[
Z = \int \left( \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \right) \exp \left[ - \sum_{n=1}^{N} \epsilon (\psi_n^\dagger (\psi_n - \psi_{n-1}) - \mu \psi_n^\dagger \psi_{n-1}) \right]
\]

\[
\rightarrow \mid J \mid \int \left( \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \right) \exp \left[ - \sum_{n=1}^{N} \epsilon (\psi_n^\dagger (\psi_n - \psi_{n-1}) - \mu \psi_n^\dagger \psi_{n-1} + \mathcal{O}(\epsilon)) \right]
\]  \hspace{1cm} (B20)

If we take the continuum limit, i.e. keep the first order in \( \epsilon \) only, we find:

\[
Z = e^{\mu \beta} \int \left( \prod_{n=1}^{N} d\psi_n^\dagger d\psi_n \right) \exp \left[ - \sum_{n=1}^{N} \epsilon (\psi_n^\dagger (\psi_n - \psi_{n-1}) + \mu \psi_n^\dagger \psi_n) \right]
\]  \hspace{1cm} (B21)

So, transformation (B17) produced the expected \( e^{\mu \beta} \)-prefactor.

**APPENDIX C: RESOLUTION OF UNITY FOR INFINITE INTERACTION?**

In this appendix we will investigate the possibility to resolve the unity operator with normalized coherent states which exist in the constrained Fock space. We remind the reader that the resolution of the unity operators with such coherent states would result in a well-defined Berry phase in the continuum limit. For this purpose we will explicitly construct coherent states with either one or two complex Grassmann fields which are clearly normalized.

However, it will be proved by contradiction that neither of them will resolve the unity operator (further discussions in [26]) – assuming a sufficiently ‘simple’ measure which is not a sum of several Grassmann valued terms.

1. **Coherent state with two complex Grassmann numbers**

We write the normalized coherent state in exponential form as in Perelomov [24] (cf. (22)). The bosonic operators will acquire a complex prefactor, and the fermionic a Grassmann prefactor. In the following formula \( \alpha \) is a complex field, but \( \beta \) is proportional to a
Grassmann number $\psi_{\uparrow}$ and $\gamma$ proportional to a Grassmann number $\psi_{\downarrow}$. The reference state is chosen to be $|0\rangle$.

$$|g\rangle = \exp \left[ \alpha X_{\uparrow\uparrow} + \beta X_{\uparrow\downarrow} + \gamma X_{\downarrow\downarrow} - \alpha^* X_{\downarrow\uparrow} + \beta^* X_{\downarrow\downarrow} + \gamma^* X_{\uparrow\downarrow} \right] |0\rangle$$

$$= |0\rangle + \beta|\uparrow\rangle + \gamma|\downarrow\rangle$$

$$+ \frac{1}{2!} \left\{ (\alpha\gamma|\uparrow\rangle - \alpha^*\beta|\downarrow\rangle - (\beta^*\beta + \gamma^*\gamma)|0\rangle \right\}$$

$$+ \frac{1}{3!} \left\{ (-\alpha\alpha^*\beta - \beta^*\gamma^*\gamma) |\uparrow\rangle + (\alpha^*\alpha\gamma - \gamma^*\beta^*\beta)|\downarrow\rangle + (\gamma^*\alpha^*\beta - \beta^*\alpha\gamma)|0\rangle \right\}$$

$$+ \ldots$$  \hspace{1cm} (C1)

The construction scheme is found by expanding to eighth order. The coherent state then is:

$$\left\{ \frac{\beta \sin(|\alpha|) + \gamma \frac{1 - \cos(|\alpha|)}{|\alpha|}}{\alpha^*} + \beta^* \gamma^* \frac{\sin(|\alpha|) - |\alpha|}{|\alpha|^3} \right\} |\uparrow\rangle$$

$$+ \left\{ \frac{\gamma \sin(|\alpha|) - \beta \frac{1 - \cos(|\alpha|)}{|\alpha|}}{\alpha} + \gamma^* \beta \frac{\sin(|\alpha|) - |\alpha|}{|\alpha|^3} \right\} |\downarrow\rangle$$

$$+ \left\{ 1 - \gamma^* \beta \frac{\sin(|\alpha|) - |\alpha|}{|\alpha|^2} + \beta^* \gamma \frac{\sin(|\alpha|) - |\alpha|}{|\alpha|^2} \right\}$$

$$- (\beta^* \beta + \gamma^* \gamma) \frac{1 - \cos(|\alpha|)}{|\alpha|^2} - 2\beta^* \beta \gamma^* \gamma \frac{1 - \cos(|\alpha|) - |\alpha|^2/2}{|\alpha|} \right\} |0\rangle$$  \hspace{1cm} (C2)

which is proved by induction. This state is normalized. Next the resolution of the unity operator is tackled. Therefore we have to take the projector onto the coherent state and integrate with some unknown measure. This measure is either a constant, a single product of Grassmann numbers, or a sum of such terms. The single product is ruled out, since it destroys prefactors of the diagonal Hubbard operators in the projection operator. The sum of products yields the measure of section VII as the only possible choice. Finally, the case that the measure is a constant is investigated below.

The arg($\alpha$) phase integration over $\alpha$ is supposed to yield 0 in order to destroy the terms with off-diagonal Hubbard operators. The remaining terms, with diagonal Hubbard operators, contain integrals as prefactors which should equal 1:

$$X_{\uparrow\uparrow} : \int 2\beta^* \gamma^* \gamma \frac{\sin(|\alpha|)}{|\alpha|} \frac{|\alpha| - \sin(|\alpha|)}{|\alpha|^3} \frac{1}{|\alpha|^2} = 1$$  \hspace{1cm} (C3)
\[ X^{\uparrow \uparrow} : \int 2\beta^*\gamma^* \frac{\sin(|\alpha|) |\alpha| - \sin(|\alpha|)}{|\alpha|^3} = 1 \]  \hspace{1cm} (C4)

\[ X^{00} : \int \beta^*\gamma^* \left[ \frac{4\cos(|\alpha|) - 1 + |\alpha|^2/2}{|\alpha|^4} - 2 \frac{|\alpha| - \sin(|\alpha|))^2}{|\alpha|^4} + 2 \frac{(\cos(|\alpha|) - 1)^2}{|\alpha|^4} \right] = 1 \]  \hspace{1cm} (C5)

The square brackets can be written as:

\[[...]|\alpha|] = \frac{4 \sin(|\alpha|)(|\alpha| - \sin(|\alpha|))}{|\alpha|^4} \]  \hspace{1cm} (C6)

Now, adding the first two equations \((C3),(C4)\) results in a contradiction to equation \((C5)\).

To complete the proof one can choose another reference state, for example \(|\uparrow\rangle\) or \(|\downarrow\rangle\).

Carrying through the same steps as before one obtains a similar contradiction.

2. Coherent state with one complex Grassmann number

Analogously, we try to find a resolution of unity with one Grassmann number. For this purpose we take the calculation from the previous section and substitute \(\psi_1 = \psi_2\). Then the coherent state is calculated to be:

\[
\begin{align*}
\{ \frac{\beta^*\sin(|\alpha|)}{|\alpha|} + \gamma^* \frac{1 - \cos(|\alpha|)}{|\alpha|^2} \} |\uparrow\rangle \\
+ \{ \frac{\gamma^*\sin(|\alpha|)}{|\alpha|} - \beta^* \frac{1 - \cos(|\alpha|)}{|\alpha|^2} \} |\downarrow\rangle \\
+ \left\{ 1 - \gamma^*\beta^*\frac{\sin(|\alpha|) - |\alpha|}{|\alpha| |\alpha|^*} + \beta^*\gamma^* \frac{\sin(|\alpha|) - |\alpha|}{|\alpha| |\alpha|^*} - (\beta^*\beta + \gamma^*\gamma) \frac{1 - \cos(|\alpha|)}{|\alpha|^2} \right\} |0\rangle
\end{align*}
\]  \hspace{1cm} (C7)

Again, this state is normalized. To resolve the unity we have to integrate with an unknown measure. Using the same procedure as before we get:

\[ X^{\uparrow \uparrow} : \int \beta^*\gamma^* \frac{\sin^2(|\alpha|)}{|\alpha|^2} + \gamma^* \frac{(1 - \cos(|\alpha|))^2}{|\alpha|^2} = 1 \]  \hspace{1cm} (C8)

\[ X^{\downarrow \downarrow} : \int \gamma^*\beta^* \frac{\sin^2(|\alpha|)}{|\alpha|^2} + \beta^* \frac{(1 - \cos(|\alpha|))^2}{|\alpha|^2} = 1 \]  \hspace{1cm} (C9)

\[ X^{00} : \int 2(\beta^*\gamma^* \frac{\cos(|\alpha|) - 1)^2}{|\alpha|^2} = 1 \]  \hspace{1cm} (C10)

Adding the first two lines results in a contradiction to the last.
APPENDIX D: SLAVE PARTICLE CONSTRAINTS

To contrast the projection methods discussed in this paper with slave boson techniques, we sketch the treatment of slave boson constraints within a path integral formulation. The trace in the partition function is constrained to some subspace characterized by $q = 0$,

$$Z = \text{Tr} \left[ e^{-\beta H} | q = 0 \rangle \langle q = 0 | \right] \quad (D1)$$

where $q$ labels the eigenvalues of operator $Q$. We may write

$$Z = \text{Tr} \left[ e^{-\beta H} \delta(Q) \right] = \int \frac{d\lambda'}{2\pi} \text{Tr} \left[ e^{-\beta H} e^{i\lambda' Q} \right] \quad (D2)$$

The delta function makes sense if we evaluate the trace in the basis of eigenstates of $Q$. We now assume that $Q$ commutes with $H$ to get

$$Z = \int_{-\pi}^{\pi} \frac{d\lambda'}{2\pi} \text{Tr} \left[ e^{-\beta H + i\lambda' Q} \right] \quad (D3)$$

The integral runs from $-\pi$ to $\pi$ because the eigenvalues of the number operator $Q$ are supposed to be integers. Now, the coherent state functional integral may be set up in the usual way ($\lambda = \lambda' / \beta$),

$$Z = \lim_{n \to \infty} \int_{-\pi T}^{\pi T} \frac{d\lambda}{2\pi} \text{Tr} \left[ \mathbb{1} : e^{-\Delta \tau H(\lambda)} : \mathbb{1} : e^{-\Delta \tau H(\lambda)} : \mathbb{1} : e^{-\Delta \tau H(\lambda)} : \ldots \mathbb{1} \right] \quad (D4)$$

where $H(\lambda) = H - i\lambda Q$. We may expand the exponentials in this Trotter formula only because $\beta \lambda$ is limited to the interval $[-\pi, \pi]$. It remains to express the unities by a closure relation for coherent states.

We should draw the readers attention to the following two facts concerning the constraint term:

\[ e.g. \text{ a path integral for } H = \sum_{i,j} \sum_{\sigma} t_{ij} C_{i\sigma} C_{j\sigma} \text{ with constraint } \lambda' Q = \lambda' (\sum_i n_{i\uparrow} n_{i\downarrow} - 0) \text{ is invalid because } Q \text{ does not commute with } H. \]
(i) The constraint is not implemented at each time step separately – nor at the initial
time step. It was implemented at the operator level and is now ‘smeared’ over all time steps.
This contrasts with the projection methods introduced in the main body of the paper.

(ii) $\lambda$ is a parameter (one for each site), and not a (time-dependent) field. It is not
correct to make $\lambda$ time dependent ($\lambda \rightarrow \lambda_n$). However, since $Q$ is a number operator, say
$i\lambda Q = i\lambda \left( \sum_{\alpha} a_{\alpha}^\dagger a_{\alpha} - 1 \right) \rightarrow i\lambda \sum_{\alpha} \Phi_{\alpha n}^* \Phi_{\alpha n-1} - i\lambda$, we may perform a gauge transformation
of the fields $\Phi_{\alpha n} \rightarrow e^{i\chi_n} \Phi_{\alpha n}$ to generate additional terms in the Berry phase:

$$
\Phi_{\alpha n}^* \left( \Phi_{\alpha n} - \Phi_{\alpha n-1} \right) \rightarrow \Phi_{\alpha n}^* e^{-i\chi_n} \left( \Phi_{\alpha n} e^{i\chi_n} - \Phi_{\alpha n-1} e^{i\chi_{n-1}} \right)
$$

$$
= \Phi_{\alpha n}^* \left( \Phi_{\alpha n} - \Phi_{\alpha n-1} \right) + \Phi_{\alpha n}^* \Phi_{\alpha n-1} \left( 1 - e^{i(\chi_{n-1} - \chi_n)} \right)
$$

(D5)

The additional term may be written as $i\Phi_{\alpha n}^* \Phi_{\alpha} \partial_\tau \chi$, if $\partial_\tau \chi$ stays finite (i.e. if $\chi_n - \chi_{n-1} = O(\Delta \tau)$). This gauge field has to obey the boundary condition $\chi(0) - \chi(\beta) = 2\pi m$ to keep
$\exp(iS)$ invariant, and $\lambda \rightarrow \lambda + i\dot{\chi}(\tau) =: \lambda(\tau)$ (see the discussion in [1]). Now we sum all
paths of $\lambda(\tau)$ in order to obtain a functional integration of the Lagrange multiplier field
$\lambda(\tau)$. Interpretation of this procedure is as follows: The static component of the field $\lambda(\tau)$
enforces the constraint whereas the Fourier components may be gauged away.
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