Quantum lattice gas model of spin-2 Bose-Einstein condensates and closed-form analytical continuation of nonlinear interactions in spin-2 superfluids

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Presented is an unitary operator splitting method for handling the spin-density interaction in spinor Bose-Einstein condensates. The zero temperature behavior of a spinor BEC is given by mean field theory, where the Hamiltonian includes a nonlinear hyperfine spin interaction. This hyperfine interaction has a diagonal probability-density term (leading to the usual Gross-Pitaevskii type equation of motion) but also has a nondiagonal spin-density term. Since the $F = 2$ spinor BEC (spin-2 BEC) has a non-Abelian superfluid phase (nonperturbative cyclic phase in the strong spin-density coupling regime), an infinite-order expansion of the quantum evolution operator is needed for quantum simulation applications. An infinite-order expansion, obtained by analytical continuation and expressed in analytically closed form, for the spin-2 BEC is presented.

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INTRODUCTION

Through magneto-optical trapping combined with laser and evaporative cooling, ultracold quantum gases can be cooled within the timespan of a couple seconds to the submicrokelvin temperature range for phase change to a Bose-Einstein condensate (BEC), theoretically predicted 90 years ago \[2\]. Two decades ago, BECs were experimentally realized using dilute atomic vapors \[2, 3\]. Since their initial realization using magneto-optical trapping, new trapping techniques have emerged, for example using an atom chip in an encapsulated vacuum cell \[4\] and optical lattices \[7–11\]. Improvements in lasers and atom-chip vacuum cells has allowed for an experimental test system to fit into a small platform \[12\] not much bigger than the size of computer workstations when they were originally introduced.

Spinor BECs can be reliably reproduced at every few seconds, with repeated observations made through high numerical aperture contrast imaging. Such experimental systems are useful for studying superfluidity and topological solitons in spinor BECs. A spinor BEC has a $(2F + 1)$-multiplet quantum matter field that represents its spin degrees of freedom in the Zeeman manifold. An example spin-2 BEC is an ultracold quantum gas of alkali Rubidium-87 atoms with total angular momentum $F = L + S + I = 2\hbar$, when the orbital angular momentum is $L = 0$, since the intrinsic electron spin is $S = \hbar/2$ and the nuclear spin of $^{87}$Rb is $I = 3\hbar/2$. The Zeeman manifold of hyperfine level is $2F + 1 = 5$ dimensional. A spin-2 BEC has ferromagnetic, polar, and cyclic phases. The cyclic phase of a spin-2 BEC is analogous to $d$-wave Bardeen-Cooper-Schrieffer (BCS) superfluid \[13\], and it is this phase that admits non-Abelian quantum vortex solitons. So when confined in a magneto-optical trap, an atom-chip trap, or an optical lattice, a spin-2 BEC can be used to study non-Abelian superfluid dynamics. Experimental realizations of a spin-2 BEC provides a way to study a non-Abelian gauge theory in a table-top platform. Furthermore, designing the next generation of small-platform BEC test systems for applications such as quantum computing \[14\], analog quantum simulation \[10, 12, 16\], studying topological solitons in spinor BECs \[17\], and BEC interferometry \[20, 26\] all require accurate time-dependent quantum simulation of spinor BECs to advance the state of the art.

The purpose of this communication is to present a quantum computing method to accurately model a spin-2 BEC. The method is based on an infinite-order expansion of the hyperfine spin-density interaction. It is useful for modeling the time-dependent dynamics and interaction of solitons in the non-Abelian superfluid phase of a spin-2 BEC. Infinite-order expansions of the spin density and singlet-pair density (nondiagonal) parts of the hyperfine interaction unitary operator, denoted $U_f$, are presented in analytically closed form for the spin $f = 2$ BEC in the strongly-coupled nonperturbative regime. An exact expansion of $U_{f=1}^{\text{full}}$ is provided as a warm-up exercise before treating the spin-2 case.

The method is a quantum lattice gas model that uses an operator splitting technique that avoids the Baker-Campbell-Hausdorff (BCH) catastrophe that normally occurs because the kinetic energy operator in the free part of the Hamiltonian does not commute with the potential energy (nonlinear point-contact) operator in the interaction part of the Hamiltonian for a spinor BEC. So the operator splitting method in the quantum lattice gas algorithm does not require the Lie-Trotter product formula \[23\] to separate the kinetic energy and interaction potential energy operators during the time evolution. Instead, each component of the spin-$f$ bosonic field is repre-
sent by a pair of spin-1/2 fermionic fields. The method is useful for computational physics applications of spin-2 BECs on parallel computers. The numerical results obtained using this quantum lattice gas algorithm will be reported in an accompanying manuscript on interacting non-Abelian quantum vortices.

**SPINOR BECS**

The effective Hamiltonian of a spinor BEC constructed from a bosonic alkali atom of mass $m$ follows from mean-field theory \[28\]. Here a quantum computing algorithm is presented for the many-body system. The main approximation is reducing the boson-boson interaction to point-contact form. Each hyperfine spin state can be treated as a separate bosonic species. For integer atomic spin $f$, there are $2f + 1$ hyperfine states labeled with quantum numbers $m = f, f - 1, \ldots, 0, \ldots, -f$. Thus, a hyperfine multiplet spinor bosonic field operator, say $\hat{\varphi}$, has $2f + 1$ operator components

$$\hat{\varphi} = (\hat{\varphi}_f \hat{\varphi}_{f-1} \cdots \hat{\varphi}_{1-f} \hat{\varphi}_{-f})^T.$$

Neglecting an external trapping potential and a background uniform magnetic field, the diagonal part of the Hamiltonian is

$$H_{\text{diag}}[\hat{\varphi}] = \int d^3r \sum_m \hat{\varphi}_m^\dag \left[ -\frac{\hbar^2}{2m} \nabla^2 - \mu_m + \frac{g_0}{2} (\hat{\varphi}_m^\dag \hat{\varphi}_m) \right] \hat{\varphi}_m,$$

for $m = -f, \ldots, f$, and (up to $f = 2$) the nondiagonal part is

$$H_{\text{non-diag}}[\hat{\varphi}] = \frac{g_1}{2\hbar^2} \int d^3r \hat{\varphi}_0^\dag \hat{\varphi}_0 + \frac{g_2}{2} \int d^3r \hat{\varphi}_0^\dag \hat{\varphi}_0 \hat{A}_{00}(r),$$

where the spin density vector is

$$\hat{\varphi}(r) = \hat{\varphi}_f(r) \hat{\varphi}_{f-1}(r) \cdots \hat{\varphi}_{1-f}(r) \hat{\varphi}_{-f}(r),$$

where the spin vector is $\hat{f} = (f_x, f_y, f_z)$, and where the singlet-pair density is $\hat{N}_{00}(r) = \hat{A}_{00}(r) \hat{A}_{00}(r)$. The annihilation operator for the singlet-pair is

$$\hat{A}_{00}(r) = \hat{\varphi}^\dag_0(r) \hat{N}_{00}(r) \hat{\varphi}_0(r),$$

where the components of $N_{00}$ are

$$N_{00}^{mm'} = (-1)^{f-m} \sqrt{2f+1} \delta_{m,-m'}.$$  

The equal-time commutators are

$$[\hat{\varphi}_m(x_a), \hat{\varphi}_n^\dag(x_b)] = \delta^{(3)}(x_a - x_b) \delta_{mn}$$

$$[\hat{\varphi}_m(x_a), \hat{\varphi}_n(x_b)] = 0$$

$$[\hat{\varphi}_m^\dag(x_a), \hat{\varphi}_n^\dag(x_b)] = 0,$$

where $m$ and $n$ denote the Zeeman levels. The full Hamiltonian is $H[\hat{\varphi}] = H_{\text{diag}}[\hat{\varphi}] + H_{\text{non-diag}}[\hat{\varphi}]$, and the equation of motion for the $m$th component is

$$i\hbar \partial_t \hat{\varphi}_m = \frac{\delta H_{\text{diag}}[\hat{\varphi}]}{\delta \hat{\varphi}_m^\dag} + \frac{\delta H_{\text{non-diag}}[\hat{\varphi}]}{\delta \hat{\varphi}_m^\dag}.$$  

Quantum simulations using \(2f + 1\) coupled Gross-Pitaevskii equations \[24\] need a tractable way to handle the nondiagonal part of the hyperfine spin-density interaction in \[25\], which is

$$\frac{\delta H_{\text{non-diag}}[\hat{\varphi}]}{\delta \hat{\varphi}_m^\dag} = \frac{g_1}{\hbar^2} \hat{\varphi}_0 \hat{F}^\dag \hat{\varphi}_0 + \frac{g_2}{2} \left( \frac{\delta \hat{A}_{00}^\dag}{\delta \hat{\varphi}_m^\dag} \right) \hat{A}_{00}.$$  

Since $\frac{g_1}{\hbar^2} \hat{\varphi}_0 \hat{F}^\dag \hat{\varphi}_0 = \frac{g_2}{\hbar^2} \hat{\varphi}_0 \hat{F}^\dag \hat{\varphi}_0$ and $\frac{g_2}{2} \left( \frac{\delta \hat{A}_{00}^\dag}{\delta \hat{\varphi}_m^\dag} \right) \hat{A}_{00} = \frac{g_2}{2} (N_{00} \hat{\varphi}_0^\dag \hat{\varphi}_0),$ the equation of motion \[26\] of the spinor BEC is

$$i\hbar \partial_t \hat{\varphi} = \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu + g_0 \hat{\varphi}^\dag \hat{\varphi} \right) \hat{\varphi} + \frac{g_1}{\hbar^2} \hat{\varphi}_0 \hat{F}^\dag \hat{\varphi}_0 \hat{\varphi} + \frac{g_2}{2} (N_{00} \hat{\varphi}_0^\dag \hat{\varphi}_0 \hat{\varphi}) \hat{\varphi},$$

where $\mu$ is a diagonal matrix with components $\mu_m$. For a point-contact interaction, the coupling strengths for a spin-1 BEC are $g_0 = \frac{4\pi \hbar^2 a_{s} + a_{s}}{m}$, $g_1 = \frac{4\pi \hbar^2 a_{s} + a_{s}}{m}$, and $g_2 = 0$. For a spin-2 BEC they are $g_0 = \frac{4\pi \hbar^2 a_{s} + a_{s}}{m}$, $g_1 = \frac{4\pi \hbar^2 a_{s} + a_{s}}{m}$, and $g_2 = \frac{4\pi \hbar^2 a_{s} + a_{s}}{m}$, where $a_{s}$ is the $s$-wave scattering length for the binary interaction between two bosons of total spin $F = 0, 2, 4$ \[28\].

**QUANTUM LATTICE GAS ALGORITHM**

One may write the equation of motion \[10\] of a spinor BEC in unitary evolution operator form

$$\hat{\varphi}(r, t + \tau) = e^{-i \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu + g_0 \hat{\varphi}^\dag \hat{\varphi} + \frac{g_1}{\hbar^2} \hat{\varphi}_0 \hat{F} \hat{\varphi} + \frac{g_2}{2} (N_{00} \hat{\varphi}_0^\dag \hat{\varphi}_0 \hat{\varphi}) \right)} \hat{\varphi}(r, t),$$

where the spin-$f$ multiplet field operator is

$$\hat{\varphi} = (\hat{\varphi}_f \hat{\varphi}_{f-1} \cdots \hat{\varphi}_{1-f} \hat{\varphi}_{-f})^T.$$

The method presented here is based on performing a quantum computational decomposition of the equation of motion \[11\] that employs a fermionic 2-spinor field operator $\hat{\psi} = (\hat{\psi}^L, \hat{\psi}^R)^T$

$$\hat{\psi}^L = \left( \hat{\psi}_f^L \hat{\psi}_{f-1}^L \cdots \hat{\psi}_{1-f}^L \hat{\psi}_{-f}^L \right)^T$$

$$\hat{\psi}^R = \left( \hat{\psi}_f^R \hat{\psi}_{f-1}^R \cdots \hat{\psi}_{1-f}^R \hat{\psi}_{-f}^R \right)^T$$

(13a) (13b)

to represent each component of the spin-$f$ multiplet \[12\] as

$$\hat{\varphi}_m = (\hat{\psi}_m^L + \hat{\psi}_m^R) \sqrt{2},$$

(14)
for $m \in [-f, f]$. To construct a multiple qubit and quantum gate compatible representation, the unitary operator in (11) is split into kinetic energy and interaction energy parts. Since the spin-$f$ field $\phi$ is generalized to a fermionic field operator $\hat{\phi}$, the equation of motion that governs the $\hat{\phi}$ field operator is time-symmetrical. The equation of motion (11) is modeled by an ultraviolet unitary model

$$\hat{\psi}(\mathbf{r}, t + \tau) = e^{-i\left(\frac{g_1}{\hbar^2} \hat{\mathbf{F}} \cdot \mathbf{f} \right)} e^{-i\left(\frac{g_2}{2} \hat{\mathbf{N}}^0 \hat{\mathbf{N}}^0 \right)} e^{-i\left(\frac{g_3}{2} \hat{\mathbf{N}}^0 \hat{\mathbf{N}}^0 \right)} \hat{\psi}(\mathbf{r}, t),$$

where $\mathbf{1}_{2f+1}$ is the identity matrix of size $(2f+1) \times (2f+1)$, and where the Pauli spin matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (16)$$

The quantum dynamics is represented in a product space of gauge groups $SO(3) \otimes SU(2)$. The spin-$f$ representation of $SO(3)$ is $2f + 1$ dimensional for the spin texture. The spin-1/2 representation of $SU(2) \cong SO(3,1)$ is 2 dimensional because it is a nonrelativistic representation.\(^1\) In this product space representation, these generators are anticommuting as they respectively reside in separate subspaces

$$\left[ \frac{g_1}{\hbar^2} (\hat{\mathbf{F}} \cdot \mathbf{f}) \otimes 1 + \frac{g_2}{2} \hat{\mathbf{N}}^0 \otimes 1, \mathbf{1}_{2f+1} \otimes \sigma_x \nabla^2 \right] = 0. \quad (17)$$

This serves as the basis for the operator splitting method used in the quantum lattice gas model.

The fermionic field $\psi(x)$ is represented on a qubit array that encodes spacetime as a lattice, the fermionic field operators $\hat{\psi}$ and $\hat{\psi}^\dagger$ are represented by qubit creation and annihilation operators, and the quantum algorithm is constructed in such a way as to reduce the particle dynamics to a sequence of unitary quantum gate operations. The desired quantum lattice gas algorithm to represent (11) has second-order numerical convergence (i.e. doubling the grid resolution reduces the numerical error by one fourth for the spin-1 BEC and by over one third for the spin-2 BEC). In short, the ansatz is to split the quantum dynamics (11) into a product of unitary operators (15), and then deconstruct the unitary operators in this equation in a way that is suitable for quantum computing. The quantum algorithm for the many-body quantum system takes the split form

$$\hat{\psi}(\mathbf{r}, t + \tau) = U_{f}^{\dagger}[\hat{\psi}]U_{f}[\hat{\psi}]U_{o}[\hat{\psi}(\mathbf{r}, t), \quad (18)$$

where the free particle motion is generated by the kinetic energy $U_0 = e^{-i\left(-i\sigma_z \otimes 1_{f+1} \frac{\mathbf{p}^2}{2m^2} \right)}$, where the diagonal part of the nonlinear interaction is generated by the probability density $U_f^{\dagger}[\hat{\psi}] \equiv e^{-i\left(-1_{f+1} \otimes \sigma_x \left(\frac{\gamma}{\hbar^2} \hat{\psi}^\dagger \hat{\psi} - \mu \right) \right)}$, where the nondiagonal part of the nonlinear interaction is generated by the spin density vector and spin-singlet density $U_f^{\dagger}[\hat{\psi}] \equiv e^{-i\left(-\gamma \frac{\mathbf{F} \cdot \mathbf{f}}{\hbar^2} \right)} e^{-i\left(\frac{g_3}{2} \hat{\mathbf{N}}^0 \hat{\mathbf{N}}^0 \right)}$, and where the spin magnitude is $F = \sqrt{F^2_x + F^2_y + F^2_z}$. The quantum algorithms for $U_o$ (20) and $U_f[\hat{\psi}]$ (31) are known and well tested. The quantum algorithm for $U_f^{\dagger}[\hat{\psi}]$ for $f = 1, 2$ (34) is new and has performed successfully in recent numerical tests of soliton-soliton collisions and interacting non-Abelian quantum vortices.

Free massive fermion

The unitary quantum lattice gas algorithm for evolving a 2-spinor field

$$\hat{\psi}(x) = \begin{pmatrix} \psi^L(x) \\ \psi^R(x) \end{pmatrix}, \quad (19)$$

where spacetime points $x = (x, t)$ and spatial points $x$ on a three-dimensional cubical grid (30). One can begin to construct the quantum algorithm to model a free nonrelativistic massive fermion by using a number operator $N^c = \frac{1}{2}(1 - \sigma_z)$, which is idempotent ($N^c)^2 = N^c$. The unitary operator generated by this number operator is

$$c \equiv e^{i\frac{\pi}{4} N^c} = 1 + (e^{i\frac{\pi}{4}} - 1) N^c = \frac{1}{2} \begin{pmatrix} 1 & 1+i \\ 1-i & 1+i \end{pmatrix}, \quad (20)$$

and it is applied at every point $x$ by the local map: $\hat{\psi}(x) = C \hat{\psi}(x) \rightarrow \hat{\psi}(x)$. The displacements of the spin up (+1) and spin down (−1) components the 2-spinor field are implemented by stream operators:

$$S_{\Delta x, 1} \equiv e^{\hbar \Delta x \nabla} = n + e^{\Delta x \nabla} n h = \begin{pmatrix} e^{\Delta x \nabla} & 0 \\ 0 & 1 \end{pmatrix}, \quad (21a)$$

$$S_{\Delta x, -1} \equiv e^{\hbar \Delta x \nabla} = h + e^{\Delta x \nabla} n = \begin{pmatrix} 1 & 0 \\ 0 & e^{\Delta x \nabla} \end{pmatrix}, \quad (21b)$$

where $n = \frac{1}{2}(1 - \sigma_z)$ and $h = \frac{1}{2}(1 + \sigma_z)$. These number and hole operators (used as generators in (21)) are also idempotent, i.e. $n^2 = n$ and $h^2 = h$. For $\sigma = \pm 1$, the operators (21) can be written in manifestly unitary form $S_{\Delta x, \sigma} \equiv e^{iN^c \Delta x \mathbf{p}/\hbar}$, where $N^c \equiv \frac{\mathbf{p}}{2\hbar} + \frac{\mathbf{p}}{2\hbar}$, expressed in terms of the quantum mechanical momentum operator $\mathbf{p} \equiv -i\hbar \nabla$. The unitary stream and collide operators are the basic building blocks of any quantum lattice gas algorithm. With the appropriate boundary conditions, the application of (21) on a quantum state $|\Omega\rangle$ is guaranteed to conserve the total number density

\(^1\) A relativistic representation of SO(3,1) requires a 4 dimensional representation, requiring 4x4 Dirac matrices and a 4-spinor field.
\[ \int d^3x \langle \Omega | \hat{\psi}^\dagger(x) \hat{\psi}(x) | \Omega \rangle. \]

Consider the product operator

\[ I_{x\sigma} = S_{-\Delta x, \sigma} C^\dagger S_{\Delta x, \sigma} C \]

(22a)

\[ = \frac{1}{2} \begin{pmatrix} 1 + e^{-\sigma \Delta x \cdot \nabla} & -i + ie^{\sigma \Delta x \cdot \nabla} \\ -i + ie^{\sigma \Delta x \cdot \nabla} & 1 + e^{\sigma \Delta x \cdot \nabla} \end{pmatrix}. \]

(22b)

The ordering of operators in (22) is not unique since \([S_{-\Delta x, \sigma} C^\dagger S_{\Delta x, \sigma}] = 0\). One defines a symmetrized operator \(U_{x\sigma} \equiv I_{32} I_{x\sigma}\), where the identity \(\cosh z = \frac{1}{2} \sinh z = 1 - 2 \sinh^2(z/2)\). A suitable evolution operator to model a quantum particle’s motion in three spatial dimensions may be constructed by a product of such fully symmetrized operators, one for each orthogonal Cartesian direction

\[ U_0 \equiv U_x U_y U_z. \]

(23)

Only the spinor field \(\hat{\psi}(x, t)\) is stored on a computer simulation at one time—the method is a time-explicit method. Yet, from a theoretical point of view, the many-body state operator of the total entire system is actually a tensor product of all the 2-spinor field operators over all the grid points

\[ \hat{\Psi}(t) \equiv \bigotimes_{x \in \text{grid}} \hat{\psi}(x, t). \]

(24)

Likewise, the system’s evolution operator is a tensor product over all the local unitary operators

\[ U_{\text{gas}}^0 = \bigotimes_{x \in \text{grid}} U_0, \]

(25)

which is a matrix of size \(2^{2V} \times 2^{2V}\), where volume of the grid is \(V = L^3\) for grid size \(L\) with two qubits per point encoding \(\psi\) on the qubit array. The system evolution equation for a quantum gas is

\[ \hat{\Psi}(t + \tau) \equiv U_{\text{gas}}^0 \hat{\Psi}(t). \]

(26)

\(U_{\text{gas}}^0\) encodes the basic algorithm to model a quantum gas of particles confined to a lattice [31].

The quantum system governed by (31) is a quantum lattice gas, which in this case is a quantum gas of particles confined to a spacetime lattice. The qubit array is arranged in a cubical grid. The system evolution equation (26) can be expressed in differential point form as the equation of motion is

\[ i\hbar \partial_t \hat{\psi}(x) = -\sigma_x \frac{\hbar^2}{2m} \nabla^2 \hat{\psi}(x), \]

(27)

which is the nonrelativistic limit of the Weyl-Dirac equation for a free fermion in the chiral representation. That is, (26) is used to numerically represent (27) on a qubit array. Defining the massive bosonic (pairing) field as

\[ \varphi(x) = \frac{1}{\sqrt{2}} \left( \hat{\psi}^L(x) + \hat{\psi}^R(x) \right), \]

(28)

the equation of motion for the \(\varphi\) operator is

\[ i\hbar \partial_t \varphi(x) = -\frac{\hbar^2}{2m} \nabla^2 \varphi(x). \]

(29)

Let \(|\Omega^{(1)}\rangle\) denote a single particle quantum state. In the 1-body sector of the Hilbert space, the expectation value of (29) with respect to \(|\Omega^{(1)}\rangle\) becomes the well known Schrödinger wave equation for a free quantum particle with wave function \(\varphi(x) = \langle \Omega^{(1)} | \varphi(x) | \Omega^{(1)} \rangle\)

\[ i\hbar \partial_t \varphi(x) = -\frac{\hbar^2}{2m} \nabla^2 \varphi(x). \]

(30)

Understanding the behavior of quantum lattice gases on supercomputers allows us to better understand ultracold quantum gases, and this work bridges the gap between quantum computing and analog quantum simulation. The connection between quantum computing and ultracold quantum gases becomes more apparent in the following representations of BECs. Yet, to model a BEC the \(\varphi^4\) nonlinear terms in (2) and (3) must be represented in terms of separate unitary operators that multiply the righthand side of (26).

**Scalar BEC model**

The number density operator for the bosonic field in the quantum lattice gas is

\[ \hat{\rho}(x) = \varphi^\dagger(x) \varphi(x) \]

(31)

\[ = \frac{1}{2} \left( \varphi^\dagger L(x) + \varphi^\dagger R(x) \right) \left( \varphi^L(x) + \varphi^R(x) \right). \]

(32)

To model a scalar BEC, one can add a nonlinear interaction potential \(U(\hat{\rho})\) by representing it as the time-component of the 4-vector potential in the Abelian U(1) gauge group. \(U(\hat{\rho}) = g_0 \hat{\rho}/2\) in the Hartree-Fock approximation, where the coupling parameter is \(g_0 = \hbar^2 \pi a/m + \cdots\) for scattering length \(a\). The unitary evolution operator for the scalar BEC is

\[ U_{\text{BEC}}[\varphi] \equiv e^{-i \frac{U(\hat{\rho})}{\hbar} - \frac{\mu}{m} \nabla^2} U_{\text{gas}}^0, \]

(33)

where the particle mass is \(m = m_o/2\), and the chemical potential is \(\mu\). \(U_{\text{BEC}}[\varphi]\) represents the basic quantum lattice gas algorithm [31, 33] used to numerically model a scalar BEC. The equation of motion for \(\varphi\) is

\[ i\hbar \partial_t \varphi(x) = -\frac{\hbar^2}{2m} \nabla^2 \varphi(x) + (g \varphi^L(x) \varphi(x) - \mu) \varphi(x). \]

(34)

The expectation value of (34), in the mean-field limit, becomes the well known Gross-Pitaevskii (GP) equation [32, 36] for a spin-0 BEC superfluid

\[ i\hbar \partial_t \varphi(x) = -\frac{\hbar^2}{2m} \nabla^2 \varphi(x) + (g \varphi^*(x) \varphi(x) - \mu) \varphi(x). \]

(35)
Spinor BEC models

To model a spinor BEC, the quantum state (19) is given a hyperfine spin-indexed 4-spinor field

\[ \hat{\psi}_m(x) = \left( \begin{array}{c} \hat{\psi}^L_m(x) \\ \hat{\psi}^R_m(x) \end{array} \right), \tag{36} \]

where the hyperfine level is \( m \in [-f, f] \) for a spin-\( f \) BEC. In this way, the spin-1/2 field \( \hat{\psi} \) is promoted to multiplet fermionic field (13). That is, the fermionic field in the Zeeman hyperfine manifold can be expressed as a direct sum

\[ \hat{\psi} = \bigoplus_{m=-f}^{f} \hat{\psi}_m = \left( \begin{array}{c} \hat{\psi}_f^L \\ \hat{\psi}_f^R \\ \vdots \\ \hat{\psi}_{-f}^L \\ \hat{\psi}_{-f}^R \end{array} \right), \tag{37} \]

which is a multiplet probability amplitude field with \( 2(2f+1) \) components. For a spin-\( f \) multiplet field, the diagonal part of the evolution operator for the spinor BEC can also be expressed as a direct sum

\[ U^d[\hat{\psi}] = \bigoplus_{m=-f}^{f} U^\text{BEC}[\hat{\psi}_m], \tag{38} \]

which is a matrix of size \( 2(2f+1) \times 2(2f+1) \). In the low-energy and low-momentum limits, the resulting non-relativistic equation of motion for each Zeeman level is

\[ i\hbar \partial_t \hat{\psi}_m = \sigma_x \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu + g_0 \hat{\psi}^\dagger \hat{\psi} \right) \hat{\psi}_m, \tag{39} \]

where \( \hat{\psi}_m = (\hat{\psi}_m^L, \hat{\psi}_m^R)^T \) for \( m \in [-f, f] \). Equivalently, this can be written for the full fermionic field (37) as a tensor product over the levels in the Zeeman manifold

\[ i\hbar \partial_t \hat{\psi} = 1_{2f+1} \otimes \sigma_x \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu + g_0 \hat{\psi}^\dagger \hat{\psi} \right) \hat{\psi}. \tag{40} \]

Finally, to model the spinor GP equations (10) for a non-Abelian superfluid, nonlinear unitary interactions are appropriately added to the product (38) to model, for example, either an \( f = 1 \) or \( f = 2 \) spinor BEC. The quantum algorithmic procedures for doing this for the spin-1 and spin-2 cases are described next.

A spin \( f = 1 \) matrix representation of the SU(2) Lie algebra \([f_i, f_j] = i\hbar \epsilon_{ijk} f_k\) is

\[ f_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad f_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad f_z = \hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{41} \]

Since the cube of the generator is proportional to the generator itself \( (\hat{F} \cdot f)^3 = (F_x^2 + F_y^2 + F_z^2) \hat{F} \cdot f = F^2 \hat{F} \cdot f \), the nondiagonal interaction is generated by a tri-idempotent number operator \((N^2 \neq N \text{ and } N^3 = N)\)

\[ N = \frac{\hat{F} \cdot f}{\hbar} = \frac{1}{F} \begin{pmatrix} F_x & F_x+iF_y & F_x-iF_y \\ F_x+iF_y & 0 & F_y+F_z \\ F_x-iF_y & F_y+F_z & 0 \end{pmatrix} \tag{42a} \]

\[ N^2 = \frac{1}{F^2} \begin{pmatrix} F_x^2+F_y^2+F_z^2 & (F_x+iF_y)^2 & (F_x-iF_y)^2 \\ (F_x+iF_y)^2 & F_x^2 & F_y^2+F_z^2 \\ (F_x-iF_y)^2 & F_y^2+F_z^2 & F_x^2 \end{pmatrix}. \tag{42b} \]

For a spin-1 BEC, \( U_{f=1}[\hat{\varphi}] \) on the righthand side of (18) can be analytically expanded to all orders

\[ U_{f=1}[\hat{\varphi}] = 1 + \left( \cos \left( \frac{g_1 F_T}{\hbar^2} \right) - 1 \right) \hat{N}^2 - i \sin \left( \frac{g_1 F_T}{\hbar^2} \right) \hat{N} \tag{43a} \]

\[ = 1 - \frac{g_1^2 T^2}{2\hbar^4} \hat{N}^2 \sin^2 \left( \frac{g_1 F_T}{2\hbar^2} \right) - i \frac{g_1 T}{\hbar^2} \hat{N} \sin \left( \frac{g_1 F_T}{2\hbar^2} \right). \tag{43b} \]

Therefore, the equation of motion for the spin-1 BEC is modeled by the quantum algorithm (expressed in split unitary operator form)

\[ \hat{\psi}(\mathbf{x}, t + \tau) = U_{f=1}[\hat{\psi}] U^d[\hat{\psi}] \hat{\psi}(\mathbf{x}, t), \tag{44} \]

where

\[ U_{f=1}[\hat{\varphi}] = U_{f=1}[\hat{\varphi}] \otimes 1. \tag{45} \]

A spin \( f = 2 \) matrix representation of the SU(2) Lie algebra \([f_i, f_j] = i\hbar \epsilon_{ijk} f_k\) is
\[ f_x = h \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{1}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{1}{2}} & 0 & 1 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad f_y = h \begin{pmatrix} 0 & -i & 0 & 0 & 0 \\ i & 0 & -i\sqrt{\frac{1}{2}} & 0 & 0 \\ 0 & i\sqrt{\frac{1}{2}} & 0 & -i & 0 \\ 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & i & 0 \end{pmatrix}, \quad f_z = h \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}. \] (46)

The number operator generating the evolution is
\[ N \equiv \hat{F} \cdot f = \frac{1}{\hbar} \begin{pmatrix} 2F_x & F_x - iF_y & 0 & 0 & 0 \\ F_x + iF_y & F_x & \sqrt{2}(F_x - iF_y) & 0 & 0 \\ 0 & \sqrt{2}(F_x + iF_y) & \sqrt{2}(F_x - iF_y) & 0 & 0 \\ 0 & 0 & 0 & F_x - iF_y & F_x + iF_y \\ 0 & 0 & 0 & -F_x - iF_y & F_x - iF_y \end{pmatrix}. \] (47)

Since the number operator (47) is neither idempotent nor tri-idempotent, there is no closed-form expansion of \( U_{f_{1/2}}^{\text{nd}}[\hat{F}, \varphi] \) to all orders using a generalized Euler identity. Nevertheless, the spin-density part of the nondiagonal evolution operator \( U_{f_{1/2}}^{\text{nd}}[\hat{F}, \varphi] = e^{-i\left(\frac{\varphi}{\hbar} F\right)} \) expanded to lowest order
\[ U_{f_{1/2}}^{\text{nd}}[\hat{F}, \varphi] = \left( \begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right) - i \frac{g_1 \tau}{\hbar^2} \left( \begin{array}{cccccc} 0 & 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) + \cdots \] (48)

can be used for analytical matching purposes. That is, although there are no known spin-2 representations of \( SU(2) \) that can be exactly summed to infinite order, it is possible to perform an infinite-order expansion that is an analytical continuation of \( U_{f_{1/2}}^{\text{nd}}[\hat{F}, \varphi] \) that matches (48) at lowest order. Using such an analytical continuation, one is free to choose the value of \( g_1 \) to be order unity for modeling nonperturbative quantum matter. Consider the set of number operators, rendered in the spin-1/2 subspaces \( m = 2, 1 \) and \( m = -1, -2 \)
\[ f_x^{(1/2)} = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad f_y^{(1/2)} = \frac{\hbar}{2} \begin{pmatrix} 0 & -i & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad f_z^{(1/2)} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \] (49)

and in the spin-1 subspace \( m = 1, 0, -1 \)
\[ f_x^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad f_y^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad f_z^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \] (50)

Spin-2 spin-density interaction dynamics may be generated by a spin-1/2 nonlinear tri-idempotent number operator \( \left( N_{(2)}^{(1/2)} \neq N_{(1/2)} \right) \) and \( N_{(3/2)}^{(1/2)} = N_{(1/2)} \)
\[ \left[ F_{(1/2)} \right] \equiv \frac{2(\hat{F}_{(1/2)}) \cdot f_{(1/2)}}{h F_{(1/2)}} = \frac{1}{F_{(1/2)}} \begin{pmatrix} F_{(1/2)}^{(1/2)} & F_{(1/2)}^{(1/2)} & 0 & 0 & 0 \\ F_{(1/2)}^{(1/2)} & F_{(1/2)}^{(1/2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \right. \] (51)

and a spin-1 nonlinear tri-idempotent number operator \( \left( N_{(2)}^{(1)} \neq N_{(1)} \right) \) and \( N_{(3)}^{(1)} = N_{(1)} \)
\[ \left[ F_{(1)} \right] \equiv \frac{\hat{F}_{(1)} \cdot f_{(1)}}{h F_{(1)}} = \frac{1}{F_{(1)}} \begin{pmatrix} F_{(1)}^{(1)} & 0 & 0 & 0 & 0 \\ 0 & F_{(1)}^{(1)} & 0 & 0 & 0 \\ 0 & 0 & F_{(1)}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & F_{(1)}^{(1)} & 0 \\ 0 & 0 & 0 & 0 & F_{(1)}^{(1)} \end{pmatrix}, \quad \right. \] (52)
One can employ a unitary decomposition of the spin-2 spin-density dynamics as a product of spin-1/2 and spin-1 dynamics, i.e., $e^{-i \frac{g_1 \hat{F}_d}{\hbar} / h} \approx e^{-i \frac{g_1 \hat{F}_{1/2}^d}{\hbar}} N_{(1/2)}[\hat{F}_{1/2}] / h - i \frac{g_1 \hat{F}_d}{\hbar} N_{(1)}[\hat{F}_1] / h$. So to match \textsuperscript{18}, an expansion of $U_{f=2}^{\text{nd}}[\hat{F}, \hat{\varphi}]$ about $g_1$ may be written as

$$U_{f=2}^{\text{nd}}[\hat{F}, \hat{\varphi}] \approx e^{-i \frac{g_1 \hat{F}_{1/2}^d}{\hbar}} N_{(1/2)}[\hat{F}_{1/2}] - i \frac{g_1 \hat{F}_d}{\hbar} N_{(1)}[\hat{F}_1]$$

where continuation in the small $g_1$ regime is ensured by choosing $\hat{F}_{1/2} = (F_x, F_y, 2F_z)$ and $\hat{F}_1 = (\sqrt{3}F_x, \sqrt{3}F_y, 3F_z)$. This nonperturbative analytical continuation becomes exactly computable by employing generalized Euler identities

$$U_{f=1/2}^{\text{nd}}[\hat{F}_{1/2}, \hat{\varphi}] = e^{-i \frac{g_1 \hat{F}_{1/2}^d}{\hbar}} N_{(1/2)}[\hat{F}_{1/2}] = 1 - g_1^2 \frac{\tau^2}{2h^2} N_{(1/2)}^2 \sin \frac{2g_1 \hat{F}_{1/2}^d}{\hbar^2} - i \frac{g_1 \tau}{h} N_{(1/2)} \sin g_1 \hat{F}_{1/2}^d / 2h^2$$

$$U_{f=1}^{\text{nd}}[\hat{F}_1, \hat{\varphi}] = e^{-i \frac{g_1 \hat{F}_d}{\hbar}} N_{(1)}[\hat{F}_1] = 1 - g_1^2 \frac{\tau^2}{2h^2} N_{(1)}^2 \sin \frac{2g_1 \hat{F}_d}{\hbar^2} - i \frac{g_1 \tau}{h} N_{(1)} \sin g_1 \hat{F}_d / 2h^2.$$ 

So the closed-form infinite expansions \textsuperscript{18,3} can be used to handle the $g_1 \sim 1$ regime while retaining unitarity of the matrix representation of

$$U_{f=2}^{\text{nd}}[\hat{F}, \hat{\varphi}] \approx U_{f=1/2}^{\text{nd}}[\hat{F}_{1/2}, \hat{\varphi}] U_{f=1}^{\text{nd}}[\hat{F}_1, \hat{\varphi}].$$

For the $f = 2$ case, let us define the matrix $N^{00}$

$$N^{00} = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

which is an involution operator. In turn, we may calculate the value of $\hat{A}_{00}(\mathbf{x}, \mathbf{x'})$ as

$$\hat{A}_{00}(\mathbf{x}, \mathbf{x'}) = \hat{\varphi}(\mathbf{x}) N^{00} \hat{\varphi}(\mathbf{x'})$$

$$= \frac{1}{\sqrt{5}} \begin{pmatrix} \hat{\varphi}_2(\mathbf{x}) \hat{\varphi}_2(-\mathbf{x}') + \hat{\varphi}_2(\mathbf{x}) \hat{\varphi}_2(-\mathbf{x}') - \hat{\varphi}_{1}(\mathbf{x}) \hat{\varphi}_{-1}(\mathbf{x}') - \hat{\varphi}_{-1}(\mathbf{x}) \hat{\varphi}_{1}(\mathbf{x}') + \hat{\varphi}_0(\mathbf{x}) \hat{\varphi}_0(\mathbf{x'}) \end{pmatrix}. $$

If we define the 2-point spin-singlet density operator $\hat{N}^{00}(\mathbf{x}, \mathbf{x'})$ implicitly as

$$\frac{\delta(\hat{A}_{00}(\mathbf{x}, \mathbf{x'}) \hat{\varphi}(\mathbf{x}))}{\delta \hat{\varphi}^\dagger(\mathbf{x'})} \equiv \hat{N}^{00}(\mathbf{x}, \mathbf{x'}) \hat{\varphi}(\mathbf{x}),$$

then this number operator may be formally written as

$$\hat{N}^{00}(\mathbf{x}, \mathbf{x'}) = \frac{\delta \hat{A}_{00}^\dagger(\mathbf{x}, \mathbf{x'})}{\delta \hat{\varphi}^\dagger(\mathbf{x'})} \frac{\hat{A}_{00}(\mathbf{x}, \mathbf{x'})}{\hat{\varphi}(\mathbf{x})},$$

\textsuperscript{59}
This completes the description of the quantum lattice gas representation of non-Abelian spinor BECs.

**CONCLUSION**

A closed-form analytical expansion of the non-diagonal part (spin density coupling) of the hyperfine interaction of a non-Abelian superfluid (zero-temperature spinor-2 BEC) was presented. Spin-2 BEC theory possesses non-Abelian gauge symmetry, so spin-2 quantum matter in its strong coupling regime is not amenable to perturbative treatment. Yet, it is possible to analytically continue the representation into the nonperturbative (strong-coupling) regime \( g_1 \sim 1 \) by matching the
nondiagonal collide operators in the perturbative (weak-coupling) regime \( g_1 \ll 1 \).

In the many-body sector (e.g. for spin-2 BECs containing particle-particle entangled states) \( \delta \) can also serve as an efficient quantum algorithm for future implementation on a Feynman quantum computer \( \delta \). In principle on a Feynman quantum computer, such quantum algorithms can be a more precise tool for studying spinor BEC dynamics. It can exceed the utility of analog quantum simulators based on ultracold quantum gases of alkali atoms because of the absence of experimental noise and related decoherence effects in spinor BEC experiments relying on engineered Hamiltonians.

In the single-body sector and in the low-energy limit, the quantum algorithm on the analytically-continued spin-density interaction \( \delta \) is congruent to spin-2 GP equations, which is a representation of the spin-2 BEC at zero temperature, and can serve as an accurate unitary algorithm for supercomputer implementation today. Numerical quantum simulations of the \( f = 2 \) spinor BEC based on quantum algorithm \( \delta \) applied to the time-dependent interaction of non-Abelian quantum vortices will be presented in a subsequent communication.

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