

Supplementary Material: On the exact continuous mapping of fermions

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ABSTRACT

In Sec. 1, we briefly review the necessary background of the Schwinger theory of angular momentum and demonstrate how it is exact at the matrix element level but not the operator level. In Sec. 2, we provide a derivation of how one can use the JW transformation and the Schwinger theory of angular momentum to obtain a fermion-to-boson map that exactly reproduces the matrix structure of the many-fermion problem. Importantly, in this section, we demonstrate that all the spurious excitations that arise as a result of the Schwinger mapping are eliminated when the physical basis is used to evaluate the matrix elements, which ensures that *both* the forward and backward fermion-to-spin-to-fermion transformations are well defined. In Sec. 3, we show that, for the purpose of obtaining an exact and practical Cartesian mapping of fermionic operators, two alternative spin-to-boson transformations that one may consider suffer from serious deficiencies.

Schwinger theory of angular momentum: spin-boson isomorphism at the matrix element level

In this section we demonstrate and stress how the Schwinger theory of angular momentum provides an isomorphic representation of the spin algebra at the matrix element level, but *not* at the operator level. The Schwinger boson representation¹ expresses spin 1/2 operators in terms of two coupled bosons per spin degree of freedom,

$$\sigma_j^+ = |1_j\rangle\langle 0_j| \quad \xleftrightarrow{\text{Schwinger}} \quad \hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha}, \quad (\text{S1a})$$

$$\sigma_j^- = |0_j\rangle\langle 1_j| \quad \xleftrightarrow{\text{Schwinger}} \quad \hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta}, \quad (\text{S1b})$$

$$\mathbf{1}_j = |1_j\rangle\langle 1_j| + |0_j\rangle\langle 0_j| \quad \xleftrightarrow{\text{Schwinger}} \quad \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} + \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} \quad (\text{S1c})$$

$$\sigma_j^z = |1_j\rangle\langle 1_j| - |0_j\rangle\langle 0_j| \quad \xleftrightarrow{\text{Schwinger}} \quad \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} - \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha}, \quad (\text{S1d})$$

where the coupled bosons follow regular bosonic commutation relations,

$$[\hat{b}_{j\alpha}, \hat{b}_{k\beta}^\dagger] = \delta_{j,k} \delta_{\alpha,\beta}, \quad (\text{S2a})$$

$$[\hat{b}_{j\alpha}, \hat{b}_{k\beta}] = 0. \quad (\text{S2b})$$

The quotation marks around the map symbol in Eqs. (S1) connecting the spin operators and the coupled bosons are used to stress the fact that, on the operator level, this transformation only recovers the correct result when double and higher-order (joint and individual) excitations of the α and β modes corresponding to a given spin index j are excluded. To demonstrate this point, consider the commutation and anticommutation relations of spin operators: similar to bosons, spins on different sites commute,

$$[\tilde{\sigma}_j, \tilde{\sigma}_k] = 0, \quad (\text{S3})$$

where $\tilde{\sigma}_j \in \{\sigma_j^+, \sigma_j^-, \sigma_j^z\}$ and $j \neq k$; in contrast, unlike bosons, spins on the same site obey the following commutation and anticommutation relations,

$$[\sigma_j^+, \sigma_j^-] = \sigma_j^z, \quad (\text{S4a})$$

$$[\sigma_j^z, \sigma_j^\pm] = \pm 2\sigma_j^\pm, \quad (\text{S4b})$$

and

$$\{\sigma_j^+, \sigma_j^-\} = \mathbf{1}_j. \quad (\text{S5})$$

Using the Schwinger boson representation in Eq. (S1), one can easily recover the spin commutation relations, Eqs. (S3) and (S4). However, the anticommutation relation in Eq. (S5) is only approximately recovered,

$$\{\sigma_j^+, \sigma_j^-\} \xrightarrow{\text{Schwinger}} \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} + \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} + 2\hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} \hat{b}_{j\beta} = \mathbf{1}_j + \mathcal{O}_j(2), \quad (\text{S6})$$

where, $\mathcal{O}_j(n)$ denotes terms containing n^{th} order excitations for the j^{th} index. This result is obtained by placing the boson creation and annihilation operators in a *normal-ordered* form, i.e., where the creation operators lie to the left. These high-order excitations could be joint α and β mode excitations, such as the double excitation $\hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} \hat{b}_{j\beta}$, or individual mode excitations, such as the second order excitation $\hat{b}_{j\gamma}^\dagger \hat{b}_{j\gamma}^\dagger \hat{b}_{j\gamma} \hat{b}_{j\gamma}$, where $\gamma \in \{\alpha, \beta\}$. Hence, Eq. (S6) shows that the Schwinger boson representation only recovers the algebra of spin operators on the joint single-excitation subspace for the j^{th} bosonic modes (the subspace for the j^{th} coupled bosons consisting of the states where the α mode is in the ground state while the β mode is in the first excited state, and vice versa).

Before demonstrating how to evaluate the matrix element of an arbitrary product of spin operators in their Schwinger boson representation, as given by Eqs. (S1), we note a few consequences of the properties of spins. First, any operator or many-spin wavefunction can be decomposed into a sum of spin factorizable terms. Second, given the commutation relation of different spins in Eq. (S3), the order in which these spins components are placed does not matter. This implies that the evaluation of the matrix elements of an operator with contributions from a limited number of spins requires operations with respect to those spins. To illustrate this point, consider performing a trace over an operator $O = \prod_{j=1}^M \hat{O}_j$ using the 2^M many-spin basis, $|\mathbf{n}\rangle$, where $\mathbf{n} = |n_1, \dots, n_M\rangle$ and $n_j \in \{0, 1\}$,

$$\sum_{\{\mathbf{n}\}} \langle \mathbf{n} | \hat{O} | \mathbf{n} \rangle = \prod_{j=1}^M \left[\sum_{n_j \in \{0,1\}} \langle n_j | \hat{O}_j | n_j \rangle \right]. \quad (\text{S7})$$

This simple illustration demonstrates the desirable property of traces of spin operators using the many-spin basis that it is factorizable into traces over one spin operators. Because the Schwinger theory of angular momentum maps distinct spins to distinguishable bosons, this desirable property is conserved.

We now show how the original spin basis over which traces can be taken can be mapped to a restricted bosonic basis, which is normally called the physical basis. The Hilbert space of spin j consists of two states, $\{|1_j\rangle, |0_j\rangle\}$, which is used to restrict the Hilbert space of the Schwinger bosons,

$$|1_j\rangle \mapsto |n_{j,\alpha} = 0, n_{j,\beta} = 1\rangle, \quad (\text{S8})$$

$$|0_j\rangle \mapsto |n_{j,\alpha} = 1, n_{j,\beta} = 0\rangle. \quad (\text{S9})$$

Using this mapped basis, it is clear that excitations of order $\mathcal{O}(n \geq 2)$, which arise from the larger Hilbert space of unrestricted bosons, do not contribute to matrix elements of spin operators in the Schwinger representation.

Therefore, *the Schwinger boson representation for spins only represents an exact isomorphism at the level of matrix elements evaluated using the “physical” single-excitation basis of the bosons corresponding to the j spin.*

Mapping Fermions to Schwinger-bosons: Proof of Exactness at the Matrix Element Level

In this section, we show how one can map fermionic creation and annihilation operators to bosonic ones, and thereby Cartesian phase space variables, by sequentially exploiting the JW transformation and the Schwinger theory of angular momentum, and demonstrate that the resulting map constitutes an exact isomorphism that reproduces the matrix structure of the many-fermion problem.

Using the Schwinger representation in Eq. (S1) to express the JW transformed fermionic creation and annihilation operators in Eqs. (2)-(3), we map fermionic operators to boson and Cartesian phase space operators,

$$\hat{c}_j \xrightarrow{\text{“}\mapsto\text{”}} \hat{F}(0, j) \hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta} = \frac{1}{2} \hat{F}(0, j) (\hat{q}_{j\alpha} - i\hat{p}_{j\alpha}) (\hat{q}_{j\beta} + i\hat{p}_{j\beta}), \quad (\text{S10a})$$

$$\hat{c}_j^\dagger \xrightarrow{\text{“}\mapsto\text{”}} \hat{F}(0, j) \hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha} = \frac{1}{2} \hat{F}(0, j) (\hat{q}_{j\beta} - i\hat{p}_{j\beta}) (\hat{q}_{j\alpha} + i\hat{p}_{j\alpha}), \quad (\text{S10b})$$

where

$$\hat{F}(j, k) \quad \mapsto \quad \prod_{l=\min[j+1, k+1]}^{\max[j-1, k-1]} f(\hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} - \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha}) = \prod_{l=\min[j+1, k+1]}^{\max[j-1, k-1]} f\left(\frac{1}{2}[\hat{q}_{l\alpha}^2 + \hat{p}_{l\alpha}^2 - \hat{q}_{l\beta}^2 - \hat{p}_{l\beta}^2]\right). \quad (\text{S11})$$

As in case of the Schwinger transformation, we keep the quotation marks around the map symbol connecting the fermionic operators and the bosonic representation in Eqs. (S10) and (S11) to indicate that this transformation can be expected to recover the correct fermionic algebra on the joint single excitation subspace of the coupled α and β bosons per fermionic index j . For more complex operators, $\hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\})$, constructed from products of fermionic creation and annihilation operators, the Schwinger mapped version will in general contain such higher order excitations,

$$\hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) \xrightarrow{JW} \hat{O}(\{\hat{\sigma}_j\}) \xrightarrow{\text{Schwinger}} \hat{O}(\{\hat{b}_{j\beta}^\dagger, \hat{b}_{j\beta}, \hat{b}_{j\alpha}^\dagger, \hat{b}_{j\alpha}\}). \quad (\text{S12})$$

Equations (S10)-(S12) thus provide the procedure to start from an arbitrary operator composed of fermionic creation and annihilation operators, transition via the JW transformation to an equivalent expression in terms of spin operators, and then use the Schwinger representation to render the JW-transformed fermionic operator in a bosonic form (which can, in turn, be mapped to a Cartesian representation as shown in the main paper).

In the following subsections, we show that the final step of the fermion-to-spin-to-boson transformation in Eq. (S12) does not introduce spurious terms that would prevent the inverse boson-to-spin-to-fermion transformation. To do this, we demonstrate that the deviations from the exact fermionic operator-level map that arise due to the Schwinger representation occur exclusively in the unphysical space of high-lying excitations and are naturally excluded when using the physical basis.

Emergence of unphysical excitations in the fermion-to-boson map

Here, we demonstrate that arbitrary products of spin operators in the Schwinger representation *always* lead to the correct mapped spin operators on the single-excitation manifold but that these are generally accompanied with spurious additional high-order excitations. In this subsection our goal is not to eliminate these high-lying excitations (which will be done in Sec. 2.2 by using the physical basis), but rather to show that the Schwinger representation always leads to the correct spin behavior on the single-excitation manifold and only results in deviations in subspaces corresponding to higher order excitations. Essential to this is that, in the Schwinger representation, unphysical excitations are never able to return to the single-excitation manifold. One can understand this by observing that the Schwinger representation of the basic spin operators (ladder operators), $\sigma_j^+ \mapsto \hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha}$ and $\sigma_j^- \mapsto \hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta}$, requires that as the α mode is excited, the β mode must be de-excited, and vice versa.

To illustrate this point in more detail, one can start by recognizing that the powers $n \geq 2$ of the mapped operators in Eqs. (S1), take the form

$$[\sigma_j^+]^n \xrightarrow{\text{Schwinger}} [\hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha}]^n = 0 + \mathcal{O}_j(n), \quad (\text{S13a})$$

$$[\sigma_j^-]^n \xrightarrow{\text{Schwinger}} [\hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta}]^n = 0 + \mathcal{O}_j(n), \quad (\text{S13b})$$

$$[\mathbf{1}_j]^n \xrightarrow{\text{Schwinger}} [\hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} + \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha}]^n = \mathbf{1}_j + \mathcal{O}(2) + \dots + \mathcal{O}(n), \quad (\text{S13c})$$

$$[\sigma_j^z]^n \xrightarrow{\text{Schwinger}} [\hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} - \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha}]^n = \begin{cases} \mathbf{1}_j + \mathcal{O}(2) + \dots + \mathcal{O}(n) & \text{for } n \text{ even} \\ \sigma_j^z + \mathcal{O}(2) + \dots + \mathcal{O}(n) & \text{for } n \text{ odd} \end{cases}. \quad (\text{S13d})$$

As Eqs. (S13a)-(S13d) show, powers of the spin operators lead to the correct contribution in the single-excitation manifold with additional unphysical high-order excitations. Similarly, products of arbitrary powers of the Schwinger-mapped spin polarization and the spin ladder operators also recover the correct result on the single-excitation manifold accompanied by additional unphysical higher-order excitations,

$$[-\sigma_j^z]^n \sigma_j^+ \xrightarrow{\text{Schwinger}} [\hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta}]^n \hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha} = (-1)^n \sigma_j^+ + \mathcal{O}_j(2) + \dots + \mathcal{O}_j(n), \quad (\text{S14a})$$

$$\sigma_j^+ [-\sigma_j^z]^n \xrightarrow{\text{Schwinger}} \hat{b}_{j\beta}^\dagger \hat{b}_{j\alpha} [\hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta}]^n = \sigma_j^+ + \mathcal{O}_j(2) + \dots + \mathcal{O}_j(n), \quad (\text{S14b})$$

$$[-\sigma_j^z]^n \sigma_j^- \xrightarrow{\text{Schwinger}} [\hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta}]^n \hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta} = \sigma_j^- + \mathcal{O}_j(2) + \dots + \mathcal{O}_j(n), \quad (\text{S14c})$$

$$\sigma_j^- [-\sigma_j^z]^n \xrightarrow{\text{Schwinger}} \hat{b}_{j\alpha}^\dagger \hat{b}_{j\beta} [\hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta}]^n = (-1)^n \sigma_j^- + \mathcal{O}_j(2) + \dots + \mathcal{O}_j(n), \quad (\text{S14d})$$

Equations (S13) and (S14) further demonstrate that the Schwinger representation correctly captures the spin algebra on the single-excitation manifold and that no operation arising from any product of mapped spin operators can cause an unphysical

excitation to return to the physical single-excitation subspace. In other words, the product of an unphysical excitation of order n , $\mathcal{O}_j(n)$ of the type appearing in Eqs. (S13)-(S14) and any mapped spin operator $\tilde{\sigma}_j \in \{\sigma_j^+, \sigma_j^-, \sigma_j^z, \mathbf{1}_j\}$ always leads to an excitation of similar order or higher,

$$\begin{aligned}\tilde{\sigma}_j(\hat{b}_{j\beta}^\dagger, \hat{b}_{j\beta}, \hat{b}_{j\alpha}^\dagger, \hat{b}_{j\alpha})\mathcal{O}_j(n) &= \mathcal{O}_j(n) + \mathcal{O}_j(n+1), \\ \mathcal{O}_j(n)\tilde{\sigma}_j(\hat{b}_{j\beta}^\dagger, \hat{b}_{j\beta}, \hat{b}_{j\alpha}^\dagger, \hat{b}_{j\alpha}) &= \mathcal{O}_j(n) + \mathcal{O}_j(n+1).\end{aligned}\tag{S15}$$

Thus, as stated above, an unphysical high-order excitation ($n \geq 2$) can *never* return to the physical single-excitation subspace.

Equations (S13), (S14), and (S15) thus establish that the correct spin structure is always recovered from any arbitrary product of boson-mapped spin operators, and that the only deviation from the correct spin algebra arises in the generation of high-order excitations (which are removed upon using the physical basis in the following subsection). This allows one to show that the backward Schwinger transformation of the boson-mapped fermionic operator in Eq. (S12) is well defined as long as the higher order excitations are removed, i.e.,

$$\hat{\mathcal{O}}(\{\hat{c}_j^\dagger, \hat{c}_j\}) \xrightarrow{JW} \hat{\mathcal{O}}(\{\tilde{\sigma}_j\}) \xrightarrow{\text{Schwinger}} \hat{\mathcal{O}}(\{\hat{b}_{j\beta}^\dagger, \hat{b}_{j\beta}, \hat{b}_{j\alpha}^\dagger, \hat{b}_{j\alpha}\}) \xrightarrow{\text{Schwinger}} \hat{\mathcal{O}}(\{\tilde{\sigma}_j\}) + \mathcal{O}(2) + \dots \tag{S16}$$

Equation (S16) demonstrates that the fermion-to-spin-to-boson transformation presented in this section has a well defined backward transformation, granted that high order excitations are neglected.

A simple example that illustrates this point is the fermionic anticommutation relations after mapping individual creation and annihilation operators to the boson representation using Eqs. (7)-(8),

$$\begin{aligned}\{\hat{c}_j, \hat{c}_k^\dagger\} &\mapsto \{\hat{F}(0, j)\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta}, \hat{F}(0, k)\hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha}\} \\ &= \delta_{j,k}\hat{F}(0, j)^2 \left[\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta}\hat{b}_{j\beta}^\dagger\hat{b}_{j\alpha} + \hat{b}_{j\beta}^\dagger\hat{b}_{j\alpha}\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} \right] + (1 - \delta_{j,k})\hat{F}(0, \min[j, k])^2\hat{F}(j, k) \\ &\quad \times \left[\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} \left(\theta(j-k)(\hat{b}_{k\alpha}^\dagger\hat{b}_{k\alpha} - \hat{b}_{k\beta}^\dagger\hat{b}_{k\beta}) + \theta(k-j)(\hat{b}_{j\alpha}^\dagger\hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger\hat{b}_{j\beta}) \right) \hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} \right. \\ &\quad \left. + \hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} \left(\theta(j-k)(\hat{b}_{k\alpha}^\dagger\hat{b}_{k\alpha} - \hat{b}_{k\beta}^\dagger\hat{b}_{k\beta}) + \theta(k-j)(\hat{b}_{j\alpha}^\dagger\hat{b}_{j\alpha} - \hat{b}_{j\beta}^\dagger\hat{b}_{j\beta}) \right) \hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} \right] \\ &= \delta_{j,k}\hat{F}(0, j)^2 \left[\mathbf{1}_j + \mathcal{O}_j(2) \right] + (1 - \delta_{j,k})\hat{F}(0, \min[j, k])^2\hat{F}(j, k) \\ &\quad \times \left[\theta(j-k) \left[\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta}(-\hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} + \mathcal{O}_k(2)) + (\hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} + \mathcal{O}_k(2))\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} \right] \right. \\ &\quad \left. + \theta(k-j) \left[(-\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} + \mathcal{O}_j(2))\hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} + (\hat{b}_{j\alpha}^\dagger\hat{b}_{j\beta} + \mathcal{O}_j(2))\hat{b}_{k\beta}^\dagger\hat{b}_{k\alpha} \right] \right] \\ &= \delta_{j,k}\hat{F}(0, j)^2 \left[\mathbf{1}_j + \mathcal{O}_j(2) \right] + (1 - \delta_{j,k})\hat{F}(0, \min[j, k])^2\hat{F}(j, k) \left[\theta(j-k)\hat{a}_j^\dagger\hat{b}_j\mathcal{O}_k(2) + \theta(k-j)\hat{b}_k^\dagger\hat{a}_k\mathcal{O}_j(2) \right],\end{aligned}\tag{S17}$$

where, choosing $f(\sigma_j^z) = -\sigma_j^z$ for simplicity and using Eq. (S13d), it is clear that

$$\hat{F}(j, k)^{2n} = \prod_{l=\min[j, k]}^{\max[j, k]} \left[\mathbf{1}_l + \mathcal{O}_l(2) + \dots + \mathcal{O}_l(2n) \right], \tag{S18a}$$

$$\hat{F}(j, k)^{2n+1} = \prod_{l=\min[j, k]}^{\max[j, k]} \left[-\sigma_l^z + \mathcal{O}_l(2) + \dots + \mathcal{O}_l(2n+1) \right]. \tag{S18b}$$

Importantly, the last line of Eq. (S17) reduces to the fermionic anticommutation relations, $\{\hat{c}_j, \hat{c}_k^\dagger\} = \delta_{j,k}$, in the single-excitation limit, i.e., when $\mathcal{O}(n) \rightarrow 0$ for $n \geq 2$. Following the same approach shown in this example to interrogate the bosonic representation of more complex products of fermionic operators, one recovers the correct spin representation at the single-excitation level with additional high-order excitations. As shown in the next subsection, these unphysical excitations are eliminated when using the physical basis.

Removal of unphysical excitations in the fermion-to-boson map via use of the physical basis

Here we show that the spurious high-order excitation operators generated as a consequence of the fermion-to-boson transformation in Sec. 2.1 can be rigorously removed by using the physical basis in the evaluation of matrix elements. Specifically, it is easy to confirm that, while the fermion-to-boson map in Eq. (S12) is not exact on the operator level due to its generation of unphysical, high-order excitations, use of the physical basis renders the map an exact isomorphism at the matrix element level,

$$\langle \tilde{\mathbf{n}} | \hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{JW} \langle \tilde{\mathbf{n}} | \hat{O}(\{\tilde{\sigma}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{Schwinger} \langle \mathbf{n} | \hat{O}(\{\hat{b}_{j\beta}^\dagger, \hat{b}_{j\beta}, \hat{b}_{j\alpha}^\dagger, \hat{b}_{j\alpha}\}) | \mathbf{n}' \rangle, \quad (\text{S19})$$

where the lack of the quotation marks around the map symbol denotes that the map is exact for the evaluation of matrix elements. Here the physical basis in the boson representation is determined by the fermionic basis. To establish this relationship, one can transform the fermionic many-body basis $|\tilde{\mathbf{n}}\rangle$, to the analogous spin basis, $|\tilde{\mathbf{n}}\rangle$, and finally into the appropriate boson basis $|\mathbf{n}\rangle$. Here, $\tilde{\mathbf{n}} \equiv \{\tilde{n}_1, \tilde{n}_2, \dots, \tilde{n}_M\}$ is the *ordered* set of fermion occupation numbers, $\tilde{\mathbf{n}} \equiv \{\tilde{n}_1, \tilde{n}_2, \dots, \tilde{n}_M\}$ is the (not necessarily ordered) set of spin “occupation” numbers, and $\mathbf{n} \equiv \{n_{1\beta}, n_{1\alpha}, n_{2\beta}, n_{2\alpha}, \dots, n_{M\beta}, n_{M\alpha}\}$ is the (not necessarily ordered) set of analogous boson occupation numbers.

Because of the central role that the physical basis plays in the present transformation, its origin merits further consideration. The physical basis originates from the consideration, first, of the Schwinger representation of spin 1/2 operators as coupled bosons. A spin, like the single-particle orbital in a fermionic problem, has a Hilbert space with only two states. For simplicity, and because of the intuitive connection to possible states of a fermionic single-particle orbital, we label these two states as occupied and unoccupied. To identify these two states in the Schwinger boson representation, which fixes the physical basis, it is sufficient to consider the expression for the unit operator in the Schwinger representation, Eq. (S1c). Being the unit operator, when one evaluates its diagonal matrix elements in the physical basis, one must recover the value 1. Hence,

$$1 = \langle \tilde{n}_j | \mathbf{1}_j | \tilde{n}_j \rangle \xrightarrow{Schwinger} \langle n_{j\beta}, n_{j\alpha} | \hat{b}_{j\beta}^\dagger \hat{b}_{j\beta} | n_{j\beta}, n_{j\alpha} \rangle + \langle n_{j\beta}, n_{j\alpha} | \hat{b}_{j\alpha}^\dagger \hat{b}_{j\alpha} | n_{j\beta}, n_{j\alpha} \rangle = 1, \quad (\text{S20})$$

which must hold whether the spin, and therefore fermionic single-particle orbital, is in its occupied or unoccupied state, $\tilde{n}_j = 1, 0$. Setting $\tilde{n}_j = 1$ requires one to choose which of the two boson modes, α or β , should mirror the fermionic occupation number. Here, we have chosen the β mode to reflect the fermionic occupation number, which requires that the α mode have the opposite behavior, i.e., that its occupation be anticorrelated to the fermionic occupation of the single-particle orbital. This choice dictates that the relationship between the fermionic and bosonic occupation numbers corresponding to a single-particle orbital index, j , is given by $n_{j\beta} = \tilde{n}_j$ and $n_{j\alpha} = 1 - \tilde{n}_j$, where $\tilde{n}_j \in \{0, 1\}$. Thus, these considerations can be used to clarify the origins of the physical basis in which one obtains two coupled bosons, α and β , with anticorrelated excitation numbers constrained to the single-excitation subspace.

An important consequence of the physical basis arises when considering the transition to Cartesian phase space. Once one has obtained the mapped bosonic Hamiltonian using the mapping procedure outlined Eqs. (S10)-(S11), one can formulate the problem in phase space by replacing the bosonic creation and annihilation operators with their phase space counterparts given in Eq. (9). For manipulations in Cartesian phase space, it is necessary to use the resolution of the identity in continuous space to obtain expressions that can be evaluated using trajectories, such as in path integral, quantum-classical and semiclassical approaches. However, the expression for the resolution of the identity in phase space for bosons in this transformation needs to be modified to reflect that only the ground and first excited states are allowed,

$$\mathbf{1}_{j\gamma} = \int dq_{j\gamma} \mathcal{P}_{j\gamma} |q_{j\gamma}\rangle \langle q_{j\gamma}| \mathcal{P}_{j\gamma}, \quad (\text{S21a})$$

$$= \int dp_{j\gamma} \mathcal{P}_{j\gamma} |p_{j\gamma}\rangle \langle p_{j\gamma}| \mathcal{P}_{j\gamma}, \quad (\text{S21b})$$

where

$$\mathcal{P}_{j\gamma} = \sum_{n=0}^1 |n_{j\gamma}\rangle \langle n_{j\gamma}| \quad (\text{S22})$$

is the projection operator onto the physical subspace, consisting of the ground and first excited harmonic oscillator energy eigenstates, of the j^{th} γ -mode boson and $\gamma \in \{\alpha, \beta\}$. Here it is worth noting the similarity between this Hilbert space restriction and that which must be imposed when working with spin coherent states² and when using the MMST transformation to map discrete states for the path integral treatment of nonadiabatic problems.^{3,4} This constraint on the Hilbert space ensures that use of the resolution of the identity does not introduce errors associated with excursions into the unphysical space of higher excitations of the mapped bosons.

Since the matrix elements of high-order excitations, i.e., operators that contain multiple creation or annihilation operators corresponding to the same mode, exactly disappear when using the physical basis defined above, $\langle \mathbf{n} | \mathcal{O}(n \geq 2) | \mathbf{n}' \rangle = 0$, it is clear that Eq. (S19) must be valid. Thus, the fermion-to-boson map in Eqs. (S10) and (S11) is strictly exact when the basis used for the evaluation of matrix elements and traces is restricted to the single-excitation subspace per fermion index j .

Alternative spin mapping approaches

In this section, we analyze the feasibility of using alternative spin-to-boson maps, namely the Holstein-Primakoff⁵ and Matsubara-Matsuda⁶ transformations, for the derivation of fermion-to-Cartesian phase space maps. In particular, we show that, while the Holstein-Primakoff transformation can generally be used in lieu of the Schwinger theory of angular momentum, it introduces undesirable nonlinearities in the form of the square root of the shifted occupation number operator, $(1 - \hat{b}^\dagger \hat{b})^{1/2}$. In the case of the Matsubara-Matsuda transformation, we first demonstrate that, when applied to the mapping of discrete states, it yields the MMST transformation. However, we then show that the Matsubara-Matsuda transformation *cannot* be used to obtain an exact means of mapping fermionic creation and annihilation operators to bosonic ones (and, consequently, to phase space variables, using Eq. (9)) when combined with the JW transformation. Nevertheless, we demonstrate how it can be used to obtain an *approximate* fermion-to-boson map and analyze how such a map could be used with appropriate constraints to investigate the quantum statics and dynamics of the many-fermion problem.

Holstein-Primakoff representation

In the Holstein-Primakoff transformation,⁵ one uses a single boson for each spin index j , by expressing the α boson in the Schwinger mapping in terms of the β boson⁷ by using the completeness relation of the joint Hilbert space, Eq. (S1c),

$$\sigma_j^+ \xrightarrow{HP} \hat{b}_j^\dagger (1 - \hat{b}_j^\dagger \hat{b}_j)^{1/2}, \quad (\text{S23a})$$

$$\sigma_j^- \xrightarrow{HP} (1 - \hat{b}_j^\dagger \hat{b}_j)^{1/2} \hat{b}_j, \quad (\text{S23b})$$

which implies that

$$\sigma_j^z \xrightarrow{HP} 2\hat{b}_j^\dagger \hat{b}_j - 1, \quad (\text{S24a})$$

$$\mathbf{1}_j \xrightarrow{HP} 1 + \mathcal{O}_j(2). \quad (\text{S24b})$$

It is straightforward to confirm that the Holstein-Primakoff transformation, like the Schwinger representation, exactly recovers the spin commutation relations, Eq. (S3) on the operator level, but recovers the spin anticommutation relations, Eq. (S5), accompanied by unphysical excitations. Also similar to the Schwinger representation, the Holstein-Primakoff transformation recovers the correct spin algebra on the matrix element level when the Hilbert space of the mapped bosons is restricted to the subspace consisting of the ground and first excited states of each boson. Hence, following the same argument made in the context of the Schwinger representation in Sec. 2.2, the fermion-to-boson (and then to phase space variables) map obtained using the JW transformation followed by the Holstein-Primakoff transformation is exact on the matrix element level when the physical basis is used to evaluate matrix elements and traces. Hence, this allows us to derive a fermion-to-boson and therefore Cartesian phase space operator transformation, which is exact on the matrix element level, that takes the form,

$$\hat{c}_j \mapsto \hat{F}(0, j) (1 - \hat{b}_j^\dagger \hat{b}_j)^{1/2} \hat{b}_j = \frac{1}{2} \hat{F}(0, j) (3 - \hat{q}_j^2 - \hat{p}_j^2)^{1/2} (\hat{q}_j + i\hat{p}_j), \quad (\text{S25a})$$

$$\hat{c}_j^\dagger \mapsto \hat{F}(0, j) \hat{b}_j^\dagger (1 - \hat{b}_j^\dagger \hat{b}_j)^{1/2} = \frac{1}{2} \hat{F}(0, j) (3 - \hat{q}_j^2 - \hat{p}_j^2)^{1/2} (\hat{q}_j - i\hat{p}_j), \quad (\text{S25b})$$

where

$$\hat{F}(j, k) \mapsto \prod_{l=\min[j+1, k+1]}^{\max[j-1, k-1]} f(2\hat{b}_j^\dagger \hat{b}_j - 1) = \prod_{l=\min[j+1, k+1]}^{\max[j-1, k-1]} f(\hat{q}_j^2 + \hat{p}_j^2 - 2). \quad (\text{S26})$$

In this case, the physical basis in the boson representation corresponds to the physical basis of the β mode in transformation obtained using the Schwinger representation, i.e., $\tilde{n}_j = n_j$, where $\tilde{n}_j \in \{0, 1\}$ is the fermionic occupation number for the j^{th} single-particle orbital. For the Cartesian representation of the transformation in Eqs. (S25)-(S26), the same considerations regarding the restriction on the Hilbert space arising from the projected resolution of the identity in Sec. 2.2 apply.

The presence of the square root in the Holstein-Primakoff transformation, however, can lead to complications, especially when combining it with an approximate treatment of the resulting Hamiltonian. Because of this, the square root term is often expanded in terms of the bosonic occupation number operator $\hat{b}_j^\dagger \hat{b}_j$,

$$(1 - \hat{b}_j^\dagger \hat{b}_j)^{1/2} = 1 - \frac{1}{2} \hat{b}_j^\dagger \hat{b}_j - \frac{1}{8} [\hat{b}_j^\dagger \hat{b}_j]^2 - \dots, \quad (\text{S27})$$

and then truncated at some low order, as in the theory of spin waves.⁸ However, truncation of this expansion renders the resulting transformation approximate. Furthermore, use of the Holstein-Primakoff representation can lead to difficulties in, for example, semiclassical treatments that require the Wigner transform of the Hamiltonian. Also, as previously noted in the context of semiclassical and quantum-classical treatments of discrete states mapped using the Holstein-Primakoff transformation,⁹ it is common for the dynamics (whether in real or imaginary time) to move the system out of the physical subspace, leading to imaginary contributions to the classical limit of the mapped Hamiltonian. However, despite these possible complications, we do not discount cases where the fermion-to-boson (and, consequently, to phase space variables) transformation provided in Eqs. (S25)-(S26) may prove advantageous.

Matsuda-Matsubara representation

A different representation of spins, called the Matsubara-Matsuda transformation,⁶ uses hard-core bosons, whose Hilbert space is restricted to the zero and one excitation subspace,

$$\sigma_j^+ \xrightarrow{\text{Mat.}-\text{Mat.}} \hat{B}_j^\dagger, \quad (\text{S28a})$$

$$\sigma_j^- \xrightarrow{\text{Mat.}-\text{Mat.}} \hat{B}_j, \quad (\text{S28b})$$

$$\mathbf{1}_j \xrightarrow{\text{Mat.}-\text{Mat.}} \hat{B}_j^\dagger \hat{B}_j + \hat{B}_j \hat{B}_j^\dagger = 1, \quad (\text{S28c})$$

$$\sigma_j^z \xrightarrow{\text{Mat.}-\text{Mat.}} \hat{B}_j^\dagger \hat{B}_j - \hat{B}_j \hat{B}_j^\dagger = 2\hat{B}_j^\dagger \hat{B}_j - 1, \quad (\text{S28d})$$

where the hard-core constraint limits the Hilbert space of a particular mode to the subspace consisting of zero and one excitations. This restriction of the Hilbert space can be captured via the commutation relation

$$[\hat{B}_j, \hat{B}_k^\dagger] = \delta_{j,k}(1 - 2\hat{B}_j^\dagger \hat{B}_j). \quad (\text{S29})$$

In other words, in contrast to the Schwinger and Holstein-Primakoff transformations, this transformation is exact at the operator level, since different bosonic modes commute, while the creation and annihilation operators of a particular hard-core bosonic mode anticommute $\{\hat{B}_j, \hat{B}_j^\dagger\} = 1$.

Application to N -level systems: Relation to the MMST transformation

Before we consider its use in the development of a fermionic map, it is informative to consider how the Matsubara-Matsuda transformation can be understood as the generator of the MMST transformation. To appreciate this, we note that an arbitrary N -level system outer product, $|j\rangle \langle k|$, can be replaced by a two-body product of spin operators that can then be mapped to hard-core bosons using the Matsubara-Matsuda transformation,

$$|j\rangle \langle k| \mapsto \sigma_j^+ \sigma_k^- = |1_j, 0_k\rangle \langle 0_j, 1_k|, \quad (\text{S30a})$$

$$\mapsto \hat{B}_j^\dagger \hat{B}_k. \quad (\text{S30b})$$

Thus, the the physical basis for the N -level system can be expressed as a many-body boson basis subject to two restrictions. The first is that of hard-core bosons themselves, which requires that for each *individual* hard-core boson, the physical Hilbert space spans only the zero and one excitation subspace. The second constraint corresponds to the fact that the physical basis for the N -level system translates to the *collective* one-excitation manifold of all possible many-body hard-core boson states, i.e., the set of many-body states where one hard-core boson is in the first excited state while the rest remain in their ground states.

To obtain a phase space description of N -level systems, one would ideally want to use the relationship between regular bosonic creation and annihilation operators and continuous position and momentum operators, Eq. (9), for hard-core boson operators. Such a replacement, however, would yield operators that are unable to recover the hard-core boson commutation relations, Eq. (S29). While such a replacement is not exact on the operator level, use of the physical basis leads to an exact isomorphism at the matrix-element level. Thus, one can replace the hard-core bosons $\{\hat{B}_j^\dagger, \hat{B}_j\}$ in Eq. (S31) with regular bosons, $\hat{b}_j^\dagger, \hat{b}_j$, yielding the MMST transformation,

$$|j\rangle \langle k| \quad \text{“} \mapsto \text{”} \quad \hat{b}_j^\dagger \hat{b}_k. \quad (\text{S31})$$

Here, like in the Schwinger boson representation of spin operators, we emphasize that the map is *not* exact at the operator level, as can be confirmed via the anticommutation relation of N -level system outer products,

$$\begin{aligned} \{|j\rangle\langle k|, |m\rangle\langle n|\} &\mapsto \{\hat{b}_j^\dagger \hat{b}_k, \hat{b}_m^\dagger \hat{b}_n\} = \delta_{km} \hat{b}_j^\dagger \hat{b}_n + \delta_{nj} \hat{b}_m^\dagger \hat{b}_k + 2\hat{b}_j^\dagger \hat{b}_m^\dagger \hat{b}_n \hat{b}_k \\ &\mapsto \delta_{km} |j\rangle\langle n| + \delta_{nj} |m\rangle\langle k| + \mathcal{O}(2). \end{aligned} \quad (\text{S32})$$

However, the map becomes exact at the matrix element level when it is used in conjunction with the physical basis to obtain the matrix elements of, for example, the propagator and, more broadly, of an arbitrary operator,¹⁰

$$\langle n | \hat{O}(\{|j\rangle\langle k|\}) | m \rangle \mapsto \langle 0_1, \dots, 1_n, \dots, 0_m, \dots, 0_N | \hat{O}(\{\hat{b}_j^\dagger \hat{b}_k\}) | 0_1, \dots, 0_n, \dots, 1_m, \dots, 0_N \rangle. \quad (\text{S33})$$

Hence, while the MMST map is not exact on an operator level, it exactly reproduces the matrix structure when used in conjunction with the physical basis.

Application to many-fermion problems

Considering the success of the MMST transformation in the treatment of nonadiabatic problems, it is desirable to consider whether the Matsubara-Matsuda transformation⁶ followed by the relaxation of the hard-core constraint can also be used to obtain an exact fermion-to-boson map.

We begin by substituting the Matsubara-Matsuda expression of spin operators, Eq. (S28) into the JW transformed expression for fermionic operators, Eqs. (2)-(3), yielding,

$$\hat{c}_j \mapsto \hat{F}(0, j) \hat{B}_j, \quad (\text{S34a})$$

$$\hat{c}_j^\dagger \mapsto \hat{F}^\dagger(0, j) \hat{B}_j^\dagger, \quad (\text{S34b})$$

where

$$\hat{F}(j, k) \mapsto \prod_{l=\min[j+1, k+1]}^{\max[j-1, k-1]} f(2\hat{B}_j^\dagger \hat{B}_j - 1). \quad (\text{S35})$$

The isomorphism between hard-core bosons and spins establishes the exact nature of the above map. However, our goal is an expression for fermionic operators in terms of continuous positions and momenta. To that end, it is desirable to replace the hard-core bosons with regular bosons, whose algebra can be easily connected with that of phase space variables, and assess the validity of the resulting transformation. Unfortunately, in contrast to the MMST transformation, we now show that the resulting map is *not* valid at the operator or matrix element level. In other words,

$$\hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) \xrightarrow{JW} \hat{O}(\{\tilde{\sigma}_j\}) \xrightarrow{Mat.-Mat.} \hat{O}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \not\rightarrow \hat{O}(\{\hat{b}_j^\dagger, \hat{b}_j\}), \quad (\text{S36a})$$

$$\langle \tilde{\mathbf{n}} | \hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{JW} \langle \tilde{\mathbf{n}} | \hat{O}(\{\tilde{\sigma}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{Mat.-Mat.} \langle \mathbf{n} | \hat{O}(\{\hat{B}_j^\dagger, \hat{B}_j\}) | \mathbf{n}' \rangle \not\rightarrow \langle \mathbf{n} | \hat{O}(\{\hat{b}_j^\dagger, \hat{b}_j\}) | \mathbf{n}' \rangle. \quad (\text{S36b})$$

Here, the physical basis of the mapped bosons, $\{\hat{b}_j^\dagger, \hat{b}_j\}$, is equivalent to that of the β boson in the fermion-to-boson transformation presented in Sec. (2.2), where $\tilde{n}_j = n_j$, where $\tilde{n}_j \in \{0, 1\}$ is the fermionic occupation number for the j^{th} single-particle orbital. We illustrate the inability of the resulting transformation to treat the many-fermion case by considering one of simplest products of mapped fermionic operators. First, we consider the expected fermionic result,

$$\begin{aligned} \langle \tilde{\mathbf{n}} | \hat{c}_j \hat{c}_k^\dagger | \tilde{\mathbf{n}}' \rangle &= \langle \tilde{\mathbf{n}} | (\delta_{j,k} - \hat{c}_k^\dagger \hat{c}_j) | \tilde{\mathbf{n}}' \rangle \\ &= \delta_{j,k} g(\tilde{\mathbf{n}}, \tilde{\mathbf{n}}') (1 - \delta_{\tilde{n}'_j, 1}) - (1 - \delta_{j,k}) g(\tilde{\mathbf{n}}, \tilde{\mathbf{n}}' | j, k) h(\tilde{\mathbf{n}}'; j, k), \end{aligned} \quad (\text{S37})$$

where

$$g(\tilde{\mathbf{n}}, \tilde{\mathbf{n}}') = \prod_{r=1}^M \delta_{\tilde{n}_r, \tilde{n}'_r}, \quad (\text{S38})$$

$$g(\tilde{\mathbf{n}}, \tilde{\mathbf{n}}' | \mathbf{m}) = \prod_{\substack{r=1 \\ r \neq m_1, m_2, \dots}}^M \delta_{\tilde{n}_r, \tilde{n}'_r}, \quad (\text{S39})$$

$$h(\tilde{\mathbf{n}}; \mathbf{j}) = \left[\prod_{r=s_1+1}^{s_2-1} (-1)^{\tilde{n}_r} \right] \left[\prod_{r=s_3+1}^{s_4-1} (-1)^{\tilde{n}_r} \right] \times \dots, \quad (\text{S40})$$

$$(\text{S41})$$

and $s_1, s_2, \dots$ correspond to $j_1, j_2, \dots$ rearranged in order of increasing magnitude.

Now we consider the matrix elements of the mapped version,

$$\begin{aligned}
\langle \mathbf{n} | \hat{F}(0, j) \hat{b}_j \hat{F}(0, k) \hat{b}_k^\dagger | \mathbf{n}' \rangle &= \delta_{j,k} \langle \mathbf{n} | \hat{F}(0, j)^2 (1 + \hat{b}_j^\dagger \hat{b}_j) | \mathbf{n}' \rangle + (1 - \delta_{j,k}) \langle \mathbf{n} | \hat{F}(0, \min[j, k])^2 \hat{F}(j, k) \\
&\quad \times \left[\theta(j - k) \hat{b}_j (1 - 2\hat{b}_k^\dagger \hat{b}_k) \hat{b}_k^\dagger + \theta(k - j) \hat{b}_j (1 - 2\hat{b}_j^\dagger \hat{b}_j) \hat{b}_k^\dagger \right] | \mathbf{n}' \rangle \\
&= \delta_{j,k} g(\mathbf{n}, \mathbf{n}') (1 + \delta_{n'_j, 1}) + (1 - \delta_{j,k}) \langle \mathbf{n} | \hat{F}(0, \min[j, k])^2 \hat{F}(j, k) \\
&\quad \times \left[\hat{b}_j \hat{b}_k^\dagger - 2\theta(j - k) \hat{b}_j \hat{b}_k^\dagger \hat{b}_k \hat{b}_k^\dagger - 2\theta(k - j) \hat{b}_j \hat{b}_j^\dagger \hat{b}_j \hat{b}_k^\dagger \right] | \mathbf{n}' \rangle \\
&= \delta_{j,k} g(\mathbf{n}, \mathbf{n}') (1 + \delta_{n'_j, 1}) \\
&\quad + (1 - \delta_{j,k}) \langle \mathbf{n} | \hat{F}(0, \min[j, k])^2 \hat{F}(j, k) \left[-\hat{b}_k^\dagger \hat{b}_j + \mathcal{O}_k(2) + \mathcal{O}_j(2) \right] | \mathbf{n}' \rangle \\
&= \delta_{j,k} g(\mathbf{n}, \mathbf{n}') (1 + \delta_{n'_j, 1}) - (1 - \delta_{j,k}) g(\mathbf{n}, \mathbf{n}' | j, k) h(\mathbf{n}'; j, k),
\end{aligned} \tag{S42}$$

where we have used the fact that

$$\begin{aligned}
\hat{F}(0, n)^2 &= \prod_{l=1}^{l=n-1} (1 - 2\hat{b}_l^\dagger \hat{b}_l)^2 \\
&= \prod_{l=1}^{l=n-1} (1 + 4\hat{b}_l^\dagger \hat{b}_l^\dagger \hat{b}_l \hat{b}_l) \\
&= 1 + \mathcal{O}(2) + \dots + \mathcal{O}(2n - 2),
\end{aligned} \tag{S43}$$

and where the physical basis assigned to the bosons $\mathbf{n}$ is equivalent to the fermion basis $\tilde{\mathbf{n}}$, i.e. $\{\tilde{n}_1 = n_1, \dots, \tilde{n}_M = n_M\}$. Hence, Eqs. (S37) and (S42) demonstrate that in general

$$\langle \tilde{\mathbf{n}} | \hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) | \tilde{\mathbf{n}}' \rangle \not\rightarrow \langle \mathbf{n} | \hat{O}(\{\hat{b}_j^\dagger, \hat{b}_j\}) | \mathbf{n}' \rangle. \tag{S44}$$

Hence, the Matsubara-Matsuda mapping, which lies at the heart of the derivation of the MMST transformation for systems with discrete states, cannot be used to obtain an analogous exact map for fermionic creation and annihilation operators.

One may understand the failure of the Matsubara-Matsuda map combined with the removal of the hard-core constraint to properly capture properties of fermion operators by considering its more fundamental failure to capture the algebra of spins. Effectively, it is impossible to construct the correct expressions for the unit and spin polarization operators, $\mathbf{1}_j$ and σ_j^z , from the ladder operators, σ_j^+ and σ_j^- , in the version of the Matsubara-Matsuda transformation where the hard-core constraint has been removed,

$$\sigma_j^+ \mapsto \hat{b}_j^\dagger, \tag{S45a}$$

$$\sigma_j^- \mapsto \hat{b}_j, \tag{S45b}$$

$$\mathbf{1}_j \mapsto \hat{b}_j^\dagger \hat{b}_j + \hat{b}_j \hat{b}_j^\dagger = 2\hat{b}_j^\dagger \hat{b}_j + 1 \neq 1, \tag{S45c}$$

$$\sigma_j^z \mapsto \hat{b}_j^\dagger \hat{b}_j - \hat{b}_j \hat{b}_j^\dagger \neq 2\hat{b}_j^\dagger \hat{b}_j - 1. \tag{S45d}$$

In contrast, the Schwinger theory of angular momentum allows both the unit and spin polarization operators, $\mathbf{1}_j$ and σ_j^z , to be constructed from the mapped ladder operators, σ_j^+ and σ_j^- , leading to expressions that recover the spin algebra on the (joint) single-excitation manifold of the α and β modes (see Eqs. (S1)).

Controlled use of the fermion-to-boson map in Matsubara-Matsuda representation

While the Matsubara-Matsuda transformation cannot be used to obtain a rigorous map connecting fermionic and bosonic operators, the resulting transformation can be used safely, granted that certain restrictions are imposed. For example, we note that for operators that contain a “small-scale” product of fermionic operators, $\hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\})$, one can use the map in Eqs. (S34)-(S35), rearrange the resulting operator product in its normal-ordered form while still in the hard-core boson representation, and then relax the hard-core boson constraint. The resulting fermionic operator, expressed entirely in terms of regular bosonic operators, will recover the exact matrix elements as the original fermionic operator,

$$\langle \tilde{\mathbf{n}} | \hat{O}(\{\hat{c}_j^\dagger, \hat{c}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{JW} \langle \tilde{\mathbf{n}} | \hat{O}(\{\tilde{\sigma}_j\}) | \tilde{\mathbf{n}}' \rangle \xrightarrow{Mat.-Mat.} \langle \mathbf{n} | \hat{O}(\{\hat{B}_j^\dagger, \hat{B}_j\})_{\text{ord}} | \mathbf{n}' \rangle \mapsto \langle \mathbf{n} | \hat{O}(\{\hat{b}_j^\dagger, \hat{b}_j\})_{\text{ord}} | \mathbf{n}' \rangle. \tag{S46}$$

In addition, because it can be expressed exclusively in terms of bosonic operators, it is straightforward to obtain a phase space formulation by rewriting the operators in terms of continuous positions and momenta using Eq. (9). Despite the apparent similarity between Eqs. (S36b) and (S46), there is one critical difference: the mapped operator $\hat{O}(\{\hat{B}_j^\dagger, \hat{B}_j\})_{\text{ord}}$ is placed in its normal-ordered form (thus the “ord” subscript) before the hard-core boson constraint is removed. For operators where the functional form requires an infinite expansion of products of fermionic creation and annihilation operators, such as the real and imaginary time propagators, performing these manipulations term by term in the expansion is impractical and ultimately amounts to solving the fermionic problem in its original complexity, which would eliminate the advantages of having a transformation to continuous phase space variables that could be directly used in path integral, quantum-classical, and semiclassical schemes.

Nevertheless, here we examine the utility of Eq. (S46) for such operators. Because of the central role of the (imaginary or real time) propagator to most problems of interest, and because its treatment illustrates the concerns that arise when using the regular bosonic form of the transformation Eqs. (S34)-(S35), we specialize our discussion to these operators.

We begin by considering the argument of the propagator, the many-fermion Hamiltonian. First, we arrange the mapped hard-core bosonic Hamiltonian in its normal-ordered form and then relax the hard-core boson constraint,

$$\hat{H}_{\text{ord}}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \quad \text{“} \mapsto \text{”} \quad \hat{H}_{\text{ord}}(\{\hat{b}_j^\dagger, \hat{b}_j\}). \quad (\text{S47})$$

To illustrate this procedure, consider the general many-fermion Hamiltonian in Eq. (1), which we map using to its hard-core boson representation using Eqs. (S34)-(S35) and arrange in its normal-ordered form,

$$\hat{H}_{\text{ord}} \mapsto \sum_{j,k} h_{j,k}(\mathbf{\Gamma}) \hat{F}(j,k) \hat{B}_j^\dagger \hat{B}_k + \frac{1}{2} \sum_{j,k,l,m} U_{jk,lm}(\mathbf{\Gamma}) \text{sgn}(j-k) \text{sgn}(l-m) \hat{F}(j,k,l,m) \hat{B}_j^\dagger \hat{B}_k^\dagger \hat{B}_m \hat{B}_l. \quad (\text{S48})$$

Once in this form, it is possible to replace the hard-core boson operators $\{\hat{B}_j, \hat{B}_j^\dagger\}$ with their regular boson counterparts $\{\hat{b}_j, \hat{b}_j^\dagger\}$ and then with their phase space expressions $\{\hat{q}_j, \hat{p}_j^\dagger\}$,

$$\begin{aligned} \hat{H}_{\text{ord}} \quad \text{“} \mapsto \text{”} \quad & \sum_{j,k} h_{j,k}(\mathbf{\Gamma}) \hat{F}(j,k) \hat{b}_j^\dagger \hat{b}_k + \frac{1}{2} \sum_{j,k,l,m} U_{jk,lm}(\mathbf{\Gamma}) \text{sgn}(j-k) \text{sgn}(l-m) \hat{F}(j,k,l,m) \hat{b}_j^\dagger \hat{b}_k^\dagger \hat{b}_m \hat{b}_l \\ & = \sum_{j,k} h_{j,k}(\mathbf{\Gamma}) \frac{1}{2} \hat{F}(j,k) (\hat{q}_j - i\hat{p}_j) (\hat{q}_k + i\hat{p}_k) \\ & \quad + \frac{1}{2^3} \sum_{j,k,l,m} U_{jk,lm}(\mathbf{\Gamma}) \text{sgn}(j-k) \text{sgn}(l-m) \hat{F}(j,k,l,m) (\hat{q}_j - i\hat{p}_j) (\hat{q}_k - i\hat{p}_k) (\hat{q}_m + i\hat{p}_m) (\hat{q}_l + i\hat{p}_l). \end{aligned} \quad (\text{S49})$$

where

$$\hat{F}(j,k) \quad \text{“} \mapsto \text{”} \quad \prod_{l=\min[j+1,k+1]}^{\max[j-1,k-1]} f(2\hat{b}_l^\dagger \hat{b}_l - 1) = \prod_{l=\min[j+1,k+1]}^{\max[j-1,k-1]} f(\hat{q}_l^2 + \hat{p}_l^2 - 2), \quad (\text{S50})$$

and its multi-index generalization, $\hat{F}(\mathbf{s})$, is given by Eq. (14). We again place quotation marks around the map sign in Eqs. (S47)-(S50) to emphasize that this action is only valid to obtain the matrix elements of the mapped Hamiltonian, but not for use in additional manipulations at the operator level. We now consider the propagator and note that while the normal-ordered hard-core bosonic form of the propagator can be replaced with its regular bosonic counterpart, the same cannot be said when only the Hamiltonian is in its normal-ordered form

$$\langle \mathbf{n} | \left(\exp \left[-a \hat{H}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \right] \right)_{\text{ord}} | \mathbf{n}' \rangle \quad \mapsto \quad \langle \mathbf{n} | \left(\exp \left[-a \hat{H}(\{\hat{b}_j^\dagger, \hat{b}_j\}) \right] \right)_{\text{ord}} | \mathbf{n}' \rangle, \quad (\text{S51a})$$

$$\langle \mathbf{n} | \exp \left[-a \hat{H}_{\text{ord}}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \right] | \mathbf{n}' \rangle \quad \not\mapsto \quad \langle \mathbf{n} | \exp \left[-a \hat{H}_{\text{ord}}(\{\hat{b}_j^\dagger, \hat{b}_j\}) \right] | \mathbf{n}' \rangle, \quad (\text{S51b})$$

where $a \in \{\beta, \pm i\tau\}$, corresponding to the imaginary and real time propagators, respectively. One can prove that the mapping in Eq. (S51b) is not exact by noting that the matrix elements of the hard-core and regular bosonic Hamiltonians raised to a power $n \geq 2$ yield different results,

$$\langle \mathbf{n} | \left[\hat{H}_{\text{ord}}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \right]^n | \mathbf{n}' \rangle \neq \langle \mathbf{n} | \left[\hat{H}_{\text{ord}}(\{\hat{b}_j^\dagger, \hat{b}_j\}) \right]^n | \mathbf{n}' \rangle. \quad (\text{S52})$$

Therefore, the matrix elements of the expansion of the propagator are only exact up to first order in the Hamiltonian. However, since this approach has accuracy to first order, when the (real or imaginary) time, a , in the propagator is sufficiently small,

$$\langle \mathbf{n} | \exp \left[a \hat{H}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \right] | \mathbf{n}' \rangle_{\text{ord}} \approx \langle \mathbf{n} | \left[1 - a \hat{H}_{\text{ord}}(\{\hat{b}_j^\dagger, \hat{b}_j\}) \right] | \mathbf{n}' \rangle \quad (\text{S53})$$

Given this, it may be possible to use this map by decomposing the propagator in a path integral scheme where one splits the propagator into P time slices and then inserts the projector corresponding to the mapped physical subspace,

$$\langle \mathbf{n} | \left(\exp \left[-a \hat{H}(\{\hat{B}_j^\dagger, \hat{B}_j\}) \right] \right)_{\text{ord}} | \mathbf{n}' \rangle \approx \lim_{P \rightarrow \infty} \prod_{k=1}^P \langle \mathbf{n} | \left(\exp \left[-(a/P) \hat{H}_{\text{ord}}(\{\hat{b}_j^\dagger, \hat{b}_j\}) \right] \mathcal{P} \right)^P | \mathbf{n}' \rangle \quad (\text{S54})$$

where

$$\mathcal{P} = \prod_{j=1}^M \mathcal{P}_j = \prod_{j=1}^M \sum_{n_j=0}^1 |n_j\rangle \langle n_j|. \quad (\text{S55})$$

This way of restricting the physical subspace in a path integral scheme by imposing a constraint on the resolution of the identity in phase space has been used in the similar problem of deriving path integral expressions for systems with discrete states mapped using the MMST transformation.^{3,4} Moreover, we emphasize that once the many-fermion Hamiltonian is written in terms of bosonic creation and annihilation operators, the transformation to Cartesian positions and momenta only requires substituting these operators with their phase space expressions given in Eq. (9).

Hence, as we have shown above, *although the fermion-to-boson transformation that results from using the JW and regular boson form of the Matusubara-Matsuda transformations does not constitute an isomorphism at the operator or matrix element levels, it could potentially be used in a controlled manner within the path integral framework to derive expressions in the short timestep limit that can be used to study the statics and dynamics of many-fermion systems.*

References

1. Schwinger, J. On Angular Momentum. In Biedenharn, L. C. & Dam, H. V. (eds.) *Quantum theory of angular momentum*, 229–279 (Academic Press, New York, 1965). DOI 10.2172/4389568.
2. Klauder, J. R. Coherent State Quantization of Constraint Systems. *Ann. Phys.* **254**, 419 (1997). DOI 10.1006/aphy.1996.5647.
3. Ananth, N. & Miller, T. F. Exact quantum statistics for electronically nonadiabatic systems using continuous path variables. *J. Chem. Phys.* **133**, 234103 (2010). DOI 10.1063/1.3511700.
4. Ananth, N. Mapping variable ring polymer molecular dynamics: A path-integral based method for nonadiabatic processes. *J. Chem. Phys.* **139**, 124102 (2013). DOI 10.1063/1.4821590.
5. Holstein, T. & Primakoff, H. Field dependence of the intrinsic domain magnetization of a ferromagnet. *Phys. Rev.* **58**, 1098 (1940). DOI 10.1103/PhysRev.58.1098.
6. Matsubara, T. & Matsuda, H. A Lattice Model of Liquid Helium, I. *Prog. Theor. Phys.* **16**, 569 (1956). DOI 10.1143/PTP.16.569.
7. Mattis, D. C. *The Theory of Magnetism I. Statics and Dynamics* (Springer-Verlag, New York, 1988).
8. Auerbach, A. *Interacting Electrons and Quantum Magnetism* (Springer-Verlag, New York, 1998).
9. Thoss, M. & Stock, G. Mapping approach to the semiclassical description of nonadiabatic quantum dynamics. *Phys. Rev. A* **59**, 64 (1999). DOI 10.1103/PhysRevA.59.64.
10. Stock, G. & Thoss, M. Semiclassical Description of Nonadiabatic Quantum Dynamics. *Phys. Rev. Lett.* **78**, 578 (1997). DOI 10.1103/PhysRevLett.78.578.