



LETTER

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Sampling general N-body interactions with auxiliary fields

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Abstract – We present a general auxiliary field transformation which generates effective interactions containing all possible N -body contact terms. The strength of the induced terms can analytically be described in terms of general coefficients associated with the transformation and thus are controllable. This transformation provides a novel way for sampling 3- and 4-body (and higher) contact interactions non-perturbatively in lattice quantum Monte Carlo simulations. As a proof of principle, we show that our method reproduces the exact solution for a two-site quantum mechanical problem.

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Introduction. – The introduction of auxiliary fields, *e.g.*, via the Hubbard-Stratonovitch (HS) transformation [1,2], as a means of linearizing the interaction term of the Hamiltonian in terms of its density operator is common practice in many areas of theoretical physics, and is particularly prevalent in condensed matter and nuclear physics [3,4]. Upon linearization of the theory, the problem becomes that of many particles undergoing one-body interactions with the fluctuating background auxiliary field. In occupation number formalism, the problem becomes very similar to that of *non-interacting* (amongst themselves) particles, which in some cases can be evaluated via steepest-descent methods (*e.g.*, 1D Ising model). At the very least, the transformation greatly facilitates numerical treatment of the many-body problem [5–8]. In path integral formalisms that involve Grassmann fields, the transformation is essential as it reduces the Lagrangian to terms bilinear in fermionic fields, which can subsequently be integrated out exactly via Grassmann Gaussian integration (*e.g.*, bosonization of fermionic theories [9]). The HS transformation is ideal for theories that initially have 2-body interactions (*i.e.*, terms quadratic in the density operator). In principle many-body interactions can be linearized through recursive application of the HS transformation, but at the cost of introducing numerous auxiliary fields. Also, in the framework of time-dependent mean-field theory, ref. [10] worked out how the HS transformation can be utilized to describe many-body interactions through a non-linear effective interaction.

In contrast, in this letter we present a way to linearize the effective interaction and provide explicit derivations for this transformation. A transformation that naturally includes 3-body interactions, for example, would be beneficial for studying ultra-cold gases of polar molecules, where 3-body (and higher) interactions can be tuned to become dominant [11,12].

In this letter we detail a generalization of the HS transformation that includes two-body and all possible *higher* contact interactions that involves only one auxiliary field. The standard HS transformation can be viewed as a particular limit of this general transformation. Our transformation, in principle, induces all possible n -body interactions $\lambda^{(n)}\hat{\rho}^n$ where $\hat{\rho}$ is the density operator. The coefficients $\lambda^{(n)}$, which are known as low-energy coefficients (LECs) in an Effective Field Theory framework, are analytically determined and controllable through a set of accompanying coefficients c_j that control the coupling of the density operator with the j -th power of the auxiliary field in the linearized theory. The numerical implementation of this transformation is trivial as the sampling of the fields can be obtained from known distributions. For 2-flavor fermionic systems (*e.g.*, nucleons), this transformation allows for complete control of contact interactions up to 4-body in nature.

Formalism. – Consider the following integral which is intended to correspond to the interacting part of a

partition function at a single space-time point

$$\mathcal{Z}_{c,N} \equiv \int_{-\infty}^{\infty} d\phi P_N(\phi) \exp \left\{ - \sum_{j=1}^{2N-1} c_j \phi^j \hat{\rho} \right\}, \quad (1)$$

where $P_N(\phi)$ is the normalized probability distribution

$$P_N(\phi) = \frac{N}{\Gamma\left(\frac{1}{2N}\right)} e^{-\phi^{2N}}. \quad (2)$$

Here, ϕ is an auxiliary field which couples to the fermionic density operator¹ $\hat{\rho} = \sum_f \bar{\psi}_f \psi_f$, where $f = 1, \dots, F$ runs over the different fermion species at a given site, $N \geq 1$ and the coefficients c_j can be complex in general. Also, in order for the integral to converge, the leading exponent is not allowed to be odd in ϕ . Because the density operators at different spacetime points commute, we present only the derivation for a single point.

The argument of the exponential in (1) describes interaction vertices with an incoming and outgoing fermionic field (the density operator) and from one to $(2N-1)$ auxiliary fields associated with interaction strength c_j . The integral is normalized such that $\mathcal{Z}_{c,N} \rightarrow 1$ for $c_j \rightarrow 0$. The result of the integration over the largest exponent of ϕ times another polynomial in ϕ is given by

$$\int_{-\infty}^{\infty} d\phi e^{-\phi^{2N}} \phi^{2k} = \frac{\Gamma\left(\frac{1+2k}{2N}\right)}{N} \xrightarrow{N \rightarrow \infty} \frac{2}{1+2k}, \quad \forall k \in \mathbb{N}_0, N \in \mathbb{N}. \quad (3)$$

It is sufficient to only consider polynomials in even powers of ϕ because of the symmetry of the integration – odd powers vanish.

In this work we identify the integral $\mathcal{Z}_{c,N}$ with an effective action consisting of general $2k$ -fermionic field vertices

$$\mathcal{Z}_\lambda \equiv \exp \left\{ - \sum_{k=1}^{\infty} \lambda^{(k)} \hat{\rho}^k \right\}. \quad (4)$$

To emphasize different notations in the following context: an object with upper index without parenthesis denotes the power of an object (*e.g.*, $\hat{\rho}^k$), while an object with upper index within parenthesis corresponds to a label for the object within a given set (*e.g.*, $\lambda^{(k)}$). We expand $\mathcal{Z}_{c,N}$ and \mathcal{Z}_λ in powers of the density operator $\hat{\rho}$ and systematically match order-by-order, relating the auxiliary field interactions to the induced many-body forces. Using

¹In this work we concentrate on central interactions. It would be an interesting exercise to extend the framework to more general interactions corresponding to quantum number dependent densities like $\hat{\rho}_i \equiv \bar{\psi} \Gamma_i \psi$ by introducing an auxiliary field ϕ_i for each matrix component i . Eventually, the coupling coefficients c_j must be replaced by tensors structures to form scalar quantities. As an example, Γ_i could represent a Pauli spin matrix for nucleon degrees of freedom. However, this task is beyond the scope of this work.

Faà di Bruno's formula [13] we find that

$$\mathcal{Z}_{c,N} = \sum_{M=0}^{\infty} \mathcal{Z}_{c,N}^{(M)} \hat{\rho}^M, \quad (5)$$

$$\mathcal{Z}_{c,N}^{(M)} = \sum_{k=\lceil M/2 \rceil}^{\lfloor (2N-1)M/2 \rfloor} \frac{\Gamma\left(\frac{1+2k}{2N}\right)}{\Gamma\left(\frac{1}{2N}\right)} \sum_{\vec{m} \in \mathcal{M}_{NM}^{(2k)}} \prod_{j=1}^{2k} \left[\frac{(-c_j)^{m_j}}{m_j!} \right], \quad (6)$$

where the sum runs over the set

$$\mathcal{M}_{NM}^{(2k)} = \left\{ \vec{m} \in \mathbb{N}_0^{2k} \left| \left(\sum_{j=1}^{2k} j m_j = 2k \right) \wedge \left(\sum_{j=1}^{2k} m_j = M \right) \wedge (j \geq 2N \Rightarrow m_j = 0) \right. \right\}, \quad (7)$$

and

$$\mathcal{Z}_\lambda = \sum_{M=0}^{\infty} \mathcal{Z}_\lambda^{(M)} \hat{\rho}^M, \quad \mathcal{Z}_\lambda^{(M)} = \sum_{\vec{m} \in \mathcal{M}^{(M)}} \prod_{k=1}^M \left[\frac{(-\lambda^{(k)})^{m_k}}{m_k!} \right] \quad (8)$$

where the sum in $\mathcal{Z}_\lambda^{(M)}$ is over the set

$$\mathcal{M}^{(M)} = \left\{ \vec{m} \in \mathbb{N}_0^M \left| \sum_{k=1}^M k m_k = M \right. \right\}. \quad (9)$$

As the highest coefficient $\lambda^{(k)}$ (in terms of k) in (8) is given by $\lambda^{(M)}$ and is also linear in exactly this coefficient (because if $m_M = 1$ then $m_{j \neq M} = 0$), one can recursively determine all coefficients $\lambda^{(M)}$ for $M > 0$ by

$$\mathcal{Z}_\lambda^{(M)} = -\lambda^{(M)} + \mathcal{Z}_\lambda^{(M)} \Big|_{\lambda^{(M)} \rightarrow 0} = \mathcal{Z}_{c,N}^{(M)}, \quad \mathcal{Z}_\lambda^{(1)} \Big|_{\lambda^{(1)} \rightarrow 0} = 0. \quad (10)$$

Note that one can prove by induction that each coefficient $\lambda^{(M)}$ is proportional to a sum where each term is a products of M fermion auxiliary-field coefficients²: $\lambda^{(M)} \propto c_{j_1} \cdots c_{j_M}$. Furthermore, when matching both expansions in eq. (10), in general it is not possible to guarantee that terms at higher orders M , with M larger than the number available coefficients $M > (2N-1)$, agree. Thus, one can only guarantee that forces are correctly induced up to order $(2N-1)$ and therefore one must pick N large enough to reproduce all relevant forces; *e.g.*, $(2N-1) \geq F$. If this is the case, then any normal ordered matrix elements with expansion coefficients in eqs. (6) and (8) with $M > (2N-1)$ must evaluate to zero and thus the matrix elements of the expansions agree to all orders.

In table 1 we show the coefficients of the induced forces up to the order of four-body forces ($M = 4$) for three different choices of N .

²Because each fermion-auxiliary field interaction has exactly one incoming and outgoing fermion line, a diagram with M incoming and outgoing fermion lines (and without fermion loops) must be proportional to exactly M vertices and thus M different c_j coefficients.

Table 1: We show the results of the matching for $N = 1$, $N = 2$, and $N = \infty$ with all $c_{j>3} = 0$. The first column is the Hubbard-Stratonovich case, which produces only a two-body interaction. We repeatedly used $\Gamma(x) = (x-1)\Gamma(x-1)$ to simplify many $N = 2$ coefficients, and use the shorthand $\gamma_{3,1} = \Gamma(3/4)/\Gamma(1/4)$. We provide a *Mathematica* notebook useful for the generating the $\lambda^{(M)}$ for a given N in the Supplementary Material `N.Body.Forces.nb` (see also the file `N.Body.Forces-readme.md`).

	$N = 1$	$N = 2$	$N = \infty, c_{j>3} = 0$
$\lambda^{(1)}$	0	$\gamma_{3,1}c_2$	$\frac{1}{3}c_2$
$\lambda^{(2)}$	$-\frac{1}{4}c_1^2$	$-\left(\frac{1}{8} - \frac{\gamma_{3,1}^2}{2}\right)c_2^2 - \frac{1}{4}c_1c_3 - \frac{1}{2}\gamma_{3,1}c_1^2 - \frac{3}{8}\gamma_{3,1}c_3^2$	$-\frac{1}{6}c_1^2 - \frac{2}{45}c_2^2 - \frac{1}{5}c_1c_3 - \frac{1}{14}c_3^2$
$\lambda^{(3)}$	0	$\left(\frac{1}{8} - \frac{\gamma_{3,1}^2}{2}\right)c_1^2c_2 + \left(\frac{5}{32} - \frac{3\gamma_{3,1}^2}{8}\right)c_2c_3^2$ $+ \frac{1}{2}\gamma_{3,1}c_1c_2c_3 + \frac{1}{3}\gamma_{3,1}^3c_2^3$	$\frac{2}{45}c_1^2c_2 + \frac{8}{2835}c_3^3 + \frac{8}{105}c_1c_2c_3 + \frac{2}{63}c_2c_3^2$
$\lambda^{(4)}$	0	$\left(\frac{\gamma_{3,1}^2}{8} - \frac{1}{96}\right)c_1^4 - \frac{\gamma_{3,1}^3}{2}c_1^2c_2^2 - \left(\frac{3}{64} - \frac{3\gamma_{3,1}^2}{16}\right)c_1^2c_3^2$ $-\frac{\gamma_{3,1}}{8}c_1c_3^3 - \left(\frac{1}{8} - \frac{\gamma_{3,1}^2}{2}\right)c_1c_2^2c_3 - \frac{\gamma_{3,1}+3\gamma_{3,1}^3}{8}c_2^2c_3^2$ $-\left(\frac{1}{192} - \frac{\gamma_{3,1}^4}{4}\right)c_2^4 - \left(\frac{15}{512} - \frac{9\gamma_{3,1}^2}{128}\right)c_3^4$	$\frac{1}{180}c_1^4 + \frac{4}{14175}c_2^4 + \frac{1}{105}c_1^3c_3 - \frac{52}{10395}c_2^2c_3^2 - \frac{5}{7644}c_3^4$ $-\frac{4}{945}c_1^2c_2^2 + \frac{13}{3150}c_1^2c_3^2 - \frac{16}{1575}c_1c_2^2c_3 - \frac{1}{1155}c_1c_3^3$

To avoid numerical-sign problems, one hopes to find a set of c_j that are all real for a given set of $\lambda^{(1)} \dots \lambda^{(M)}$. Identifying when this is possible is known as the truncated Hamburger moments problem [14,15], and the solution is to consider the square matrices

$$\Lambda_{ij}^{(k)} = (i+j)! \times Z_{\lambda}^{(i+j)}, \quad (11)$$

where i and j start at 0 and each go to k . When the determinants of all the $\Lambda^{(k)}$ are positive for k from 1 to $\lceil M/2 \rceil$, a set of entirely real c_j may be found. When M is odd, one may include $\lambda^{(M+1)}$ and adjust it to help satisfy the positivity conditions. The determinants of the first $\Lambda^{(k)}$ for the first two k are

$$\begin{aligned} \det \Lambda^{(1)} &= -2\lambda^{(2)}, \\ \det \Lambda^{(2)} &= -4 \left(4 [\lambda^{(2)}]^3 + 9 [\lambda^{(3)}]^2 - 12\lambda^{(2)}\lambda^{(4)} \right), \end{aligned} \quad (12)$$

and we see that requiring the determinant of $\Lambda^{(1)}$ to be positive means requiring an attractive two-body force, a familiar result from the Hubbard-Stratonovich case.

Numerical results. – To demonstrate the efficacy of our transformation, we consider a system of 3 different fermion species f interacting on a two-site model (with sites $\{0, 1\}$) with the following Hamiltonian:

$$\hat{H} = \kappa \left(-3 \sum_{f=1}^3 \sum_{\langle i,j \rangle} \hat{a}_{f,i} \hat{a}_{f,j}^\dagger + \lambda^{(2)} \sum_{i \in \{0,1\}} \hat{\rho}_i^2 + \lambda^{(3)} \sum_{i \in \{0,1\}} \hat{\rho}_i^3 \right), \quad (13)$$

where $\hat{a}_{f,i}^\dagger$ ($\hat{a}_{f,i}$) is a creation (annihilation) operator for a fermion of species f at site i and $\hat{\rho}_i = \sum_f \hat{a}_{f,i}^\dagger \hat{a}_{f,i}$

is the number operator at site i . Here the sum over $\langle i, j \rangle \in \{(0,1), (1,0)\}$ represents nearest neighbor hoppings between the two sites, and κ is a dimensionful parameter that sets the dynamical scale of our problem. As is evident in (13), $\lambda^{(2)}$ and $\lambda^{(3)}$ represent the size of two- and three-body interactions (relative to κ), respectively, and are dimensionless. A positive (negative) value of $\lambda^{(i)}$ indicates a repulsive (attractive) interaction. We quote results in units of κ . The two-site model can be diagonalized and its spectrum directly determined from its eigenvalues. We use the transfer matrix formalism [5] to obtain this spectrum³. With the spectrum in hand, we compare these results with those obtained from a stochastic lattice projection calculation [5] where the introduction of auxiliary fields via our transformation is needed. A detailed description of these calculations is in preparation [16]. In what follows, we give a succinct description.

The projection method extracts the lowest-energy level E in the spectrum of the system via

$$E = - \lim_{\tau \rightarrow \infty} \partial_\tau \log Z[\tau, \Psi_T], \quad (14)$$

where Z is given by

$$\begin{aligned} Z[\tau, \Psi_T] &\equiv \langle \Psi_T | e^{-\tau: \hat{H}} | \Psi_T \rangle \\ &= \int \left(\prod_x d\phi_x P_N(\phi_x) \right) \mathcal{K}[\tau, \vec{\phi}, c_j, \Psi_T], \end{aligned} \quad (15)$$

Ψ_T is an initial trial wave function, and $\vec{\phi}$ indicates the collection of all ϕ over x , all space (both sites) and time from 0 to τ .

³We compare the spectrum obtained from the transfer matrix (instead of direct diagonalization of the Hamiltonian) since it incorporates lattice discretization effects. This enables a direct comparison with our lattice projection calculations.

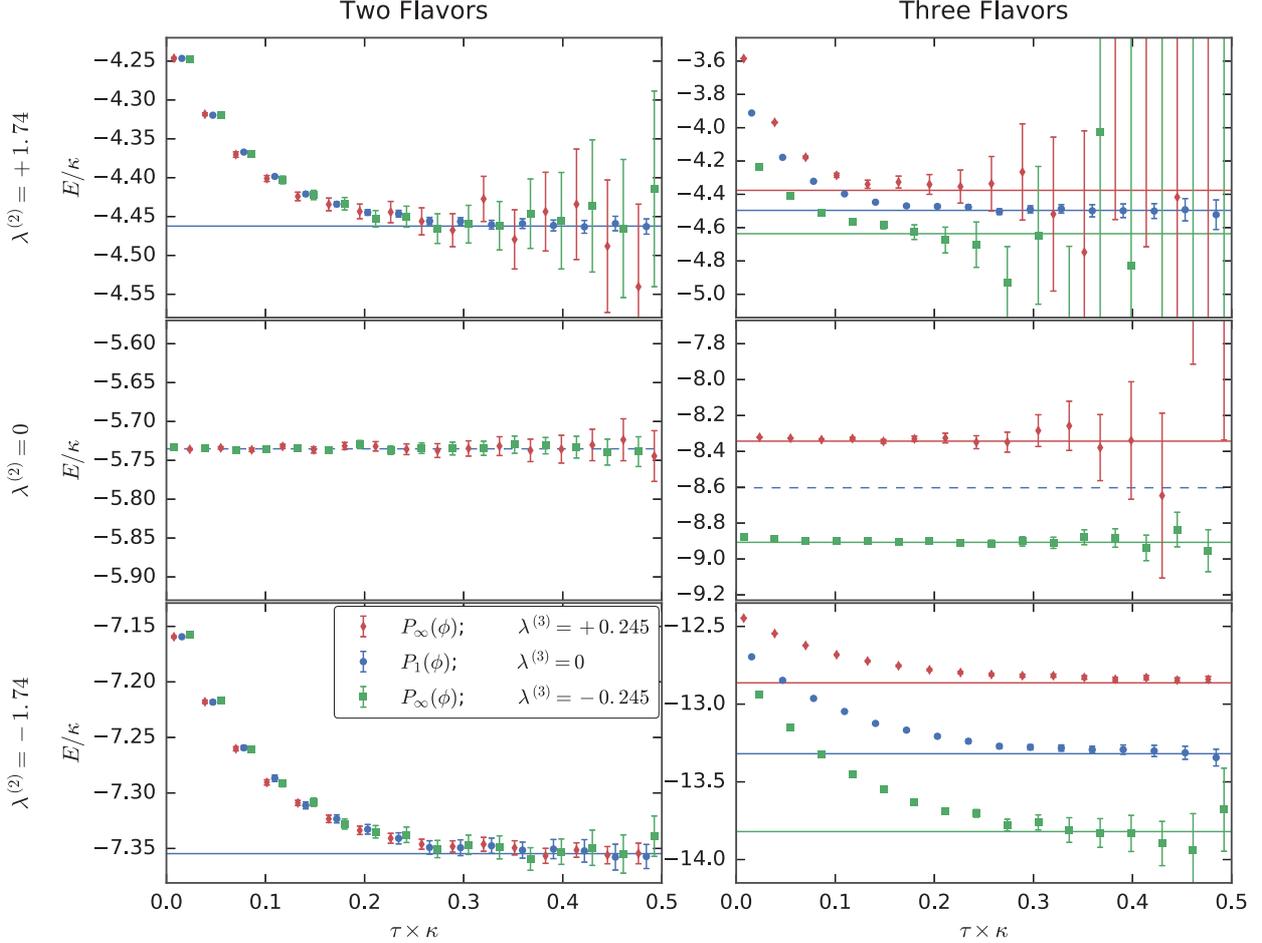


Fig. 1: (Colour online) $E(\tau)/\kappa$ for different systems. All systems were studied with 2×10^8 measurements. Some systems show a signal-to-noise problem and others yield an easy extraction of a constant plateau in the long-time limit. The left panels all show two-fermion systems and the corresponding right panels show the three-fermion systems with the same parameters. In the top (middle) [bottom] two panels we show a system with repulsive (absent) [attractive] two-body forces. Red (blue) [green] points correspond to repulsive (absent) [attractive] three-body forces. The blue points were sampled according to the HS distribution P_1 and the other points according to P_∞ . The data in the middle two panels were generated with P_∞ and coefficients $c_j = 0$ for $j > 3$ tuned to exactly cancel the two-body force, and we show dashed lines for the corresponding non-interacting energies.

After discretizing time $\tau \rightarrow a_\tau N_\tau$, the exponential of the normal ordered Hamiltonian gets replaced by the normal ordered exponential of the Hamiltonian—the so-called transfer matrix [5]. This introduces a quadratic error in the time discretization

$$e^{-a_\tau \hat{H}} = : e^{-a_\tau \hat{H}} : + \mathcal{O}(a_\tau^2). \quad (16)$$

In the last step of the (15) we have applied our transformation with its associated probability distribution $P_N(\phi)$ at each spacetime point and introduced \mathcal{K} which is a functional of ϕ and depends explicitly on the coefficients c_j , the trial wave function Ψ_T , and the time separation τ . The form of $P_N(\phi)$ depends on the order N of the transformation that is applied. For the work presented here, we consider the two extreme cases

$$N = 1, \quad P_1(\phi) = \frac{1}{\sqrt{\pi}} \exp(-\phi^2), \quad (17)$$

$$N = \infty, \quad P_\infty(\phi) = \begin{cases} 1/2, & |\phi| < 1, \\ 0, & \text{otherwise.} \end{cases} \quad (18)$$

The case $N = 1$ corresponds to the Gaussian distribution of the original Hubbard-Stratonovich transformation (and thus only $\lambda^{(2)}$ is non-zero), whereas for $N = \infty$ we have uniform sampling and in principle all allowed many-body contact interactions. In the $N = \infty$ case, there are in principle an infinite number of c_j —we set them all to zero for $j > 3$.

As our trial wave function for multifermion systems $|\Psi_T\rangle$ we pick a direct product state of single-particle ground-state wave functions, $|\psi_f\rangle = \frac{1}{\sqrt{2}}[a_{f,0}^\dagger - a_{f,1}^\dagger]|0\rangle$ for each flavor f . The direct product structure allows us to write the functional \mathcal{K} in (15) as

$$\mathcal{K}[\tau, \vec{\phi}, c_j, \Psi_T] = \left(K^{-1}[\tau; \vec{\phi}, c_j] \right)^\alpha, \quad (19)$$

where α is the number of fermion types and

$$K^{-1}[\tau; \vec{\phi}, c_j] = \frac{1}{2} \left(K^{-1}[0, \tau; 0, 0; \vec{\phi}, c_j] - K^{-1}[0, \tau; 1, 0; \vec{\phi}, c_j] - K^{-1}[1, \tau; 0, 0; \vec{\phi}, c_j] + K^{-1}[1, \tau; 1, 0; \vec{\phi}, c_j] \right), \quad (20)$$

After introducing a time discretization $\tau = a_\tau t$, the K matrix is given by

$$K[i, t; i', t'; \vec{\phi}, c_j] \equiv \delta_{i, i'} \delta_{t, t'} + a_\tau \delta_{\langle i, i' \rangle} \delta_{t, t'+1} + \delta_{i, i'} \delta_{t, t'+1} (c_1 \phi_{i, t} + c_2 \phi_{i, t}^2 + c_3 \phi_{i, t}^3 - 1). \quad (21)$$

Here we have used the fact that we let $c_j = 0$ for $j > 3$. We attach the indices i and t on the auxiliary field to indicate that there exists auxiliary fields for each spatial and temporal point.

Because we work with discretized time, we analyze the discretized version of eq. (14),

$$E(\tau) \equiv -\frac{1}{a_\tau} \log \left(\frac{Z[\tau + a_\tau, \Psi_T]}{Z[\tau, \Psi_T]} \right) \quad (22)$$

and search for constant plateaus at long times to numerically determine the $\tau \rightarrow \infty$ limit.

In fig. 1 we show the numerical results of $E(\tau)/\kappa$ for combinations of $\lambda^{(M)}$ where $\lambda^{(2)} \in \{\pm 1.74, 0.0\}$ and $\lambda^{(3)} \in \{\pm 0.245, 0.0\}$ for two and three-fermion systems. For calculations with $\lambda^{(3)} = 0.0$, ϕ was sampled according to the HS distribution P_1 and all other calculations sampled according to P_∞ . The solid lines correspond to the exact answers from diagonalization of the transfer matrix, and the dashed lines correspond to non-interacting energies. We note that for all two-fermion calculations, both $N = 1$ and $N = \infty$ calculations agree with each other, regardless of the value of $\lambda^{(3)}$, since the 3-body interaction plays no role. Furthermore, with $\lambda^{(2)} = 0.0$ but non-zero $\lambda^{(3)}$, the two-fermion system reproduces the non-interacting result. In the three-fermion system, the effects of $\lambda^{(3)}$ are apparent and agree well with exact diagonalization.

Note that the coefficients c_j can be complex in general. The bottom row of fig. 1 (with negative $\lambda^{(2)}$, corresponding to an attractive two-body force) satisfies the determinant conditions and has the cleanest statistical results since we have chosen a set of only real c coefficients. The other rows have statistical fluctuations that are harder to tame, which is unsurprising as they violate the determinant conditions and have complex c coefficients. A quantitative analysis will be given in [16], as well as an analysis of signal-to-noise behavior for the different systems.

Discussion. – The Hubbard-Stratonovitch transformation has been a useful tool for making analytic and numerical progress in problems of physical interest, and is a special case of the transformation described in this work. Our transformation, which uses a self-interacting auxiliary field, allows for the direct inclusion of controllable many-body forces into numerical calculations.

Choosing a degree of auxiliary field self-interaction fixes the sampling distribution and limits the types of fermion/auxiliary-field interaction vertices. These interactions in turn generate a slew of N -body forces. Sampling a Gaussian distribution for the auxiliary field recovers the original HS transformation, while uniform sampling in principle allows for the independent control of all possible N -body forces, while intermediate distributions yield correlated forces.

We have demonstrated that on a two-site model, different sampling techniques reproduce the exact results in a variety of cases, correctly handling all combinations of attractive, repulsive, and absent two-body forces with attractive and repulsive three-body forces. While even the agreement of the one-body energies found with the different methods is nontrivial, the agreement of the two-body systems between methods and the agreement of the three-body systems with exact results indicate a reliable understanding and definite control over many-fermion interactions.

Similar to the situation of the original HS transformation with repulsive two-body interactions, there exist certain combinations of many-body forces which are only achievable with complex c_j . Such cases are in general susceptible to numerical-sign problems for any auxiliary field distribution [15], though this is not guaranteed and in some systems can be avoided [17,18]. Because the c coefficients appear non-linearly in the higher-body λ coefficients, there is not a unique set of c 's that yield a particular set of λ 's, but one may still use the determinant conditions (eqs. (11) and (12)) to check whether a set of forces described by a set of λ 's suffers from a sign problem arising from complex c_j .

It would be interesting to consider sampling by more generic functions such as $P_N(\phi) = \exp(-\sum_n \alpha^{(n)} \phi^n)$ with multiple tuneable ϕ self-interactions, or cases where ϕ is restricted to only a finite set of values, such as ± 1 . For field-theoretic applications, it may prove fruitful to understand how the renormalization of different $\lambda^{(M)}$ control renormalization of the parameters c_j .

We expect our transformation to be useful in a variety of physical systems where many-body interactions are important. Numerical applications may include density functional theory approaches to nuclear physics [19], the non-perturbative inclusion of multinucleon forces into NLEFT which might unlock precision characterizations of halo nuclei, the study of systems near the Efimov threshold such as cold atoms (see refs. [20,21] and references therein), systems at high density, and any other system where contact interactions need stochastic implementation.

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