is simply a Gaussian. To determine coefficients $\rho_p^{[i']}$ and $\Sigma_{pq}^{[i']}$ from the initial density matrix on cluster $[i']$, we demand (cluster index $[i']$ suppressed)

$$\mathrm{Tr}[\hat{\rho}\hat{X}_q] = \int \prod_p \mathrm{d}x_p x_q \mathcal{W}(\{x\}), \tag{12}$$

$$\mathrm{Tr}[\hat{\rho}(\hat{X}_q\hat{X}_r + \hat{X}_r\hat{X}_q)] = 2\int \prod_p \mathrm{d}x_p x_q x_r \mathcal{W}(\{x\}) \tag{13}$$

such that the moments match to second order.

2. Discrete Wigner function

While the Gaussian approximation of the Wigner function described above is quite general, it neglects the moments beyond the second order. dTWA, on the other side, can capture all moments of the single-spin observables for initial states that factorize between individual spins [35]. In the following, we briefly recapitulate the derivation dTWA's sampling to introduce the notation and then generalize the method to clusters of spins.

The key idea behind the dTWA is to replace the Gaussian approximation of the Wigner function with a discrete Wigner function defined via a discrete set of phase-point operators $\hat{\mathbf{A}}^{\otimes n} = \bigotimes_i^N \hat{A}^{[i]}$ where $\hat{A}^{[i]}$ are discrete phase-point operators that span the SU(2) phase space of the ith spin. These are usually defined as $\hat{A}^{[i]}_{p,q} = [\mathbb{1} + \mathbf{r}(p,q)\cdot\hat{\sigma}]/2$, $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_z, \hat{\sigma}_z)$ are the Pauli matrices, and $\mathbf{r}(p,q)$ denotes suitable combinations thereof (cf. [34,35,37]): $\mathbf{r}(0,0) = (1,1,1)$, $\mathbf{r}(0,1) = (-1,-1,1)$, $\mathbf{r}(1,0) = (1,-1,-1)$, and $\mathbf{r}(1,1) = (-1,1,-1)$. In case the wave function factorizes, the Wigner function of the system is then given simply by the product of single-spin Wigner function given by $w^{[i]}(p,q) = \langle \hat{A}_{(p,q)}\rangle/2$. Crucially, for all spin states pointing along one axis each value of $w^{[i]}(p,q)$ is positive and, since they sum to 1, one can interpret them as probability distribution to sample from. A schematic illustration is provided in Fig. 2.

Considering a system of n_c clusters of n spins each, we again seek to describe the state by a discrete Wigner function. The main difference to before is that each local Hilbert space is represented by a copy of SU(D), where $D = 2^n$. In analogy to before, we introduce the phase-point operators $\hat{\mathbf{A}}^{\otimes n_c} = \bigotimes_{i'}^{n_c} \hat{A}_n^{[i']}$ with $\hat{A}_n^{[i']} = (\mathbb{1}_D + \mathbf{r}_n^{[i']}\cdot\mathbf{X}_n)/D$, where $\mathbf{r}_n^{[i']} = (r_1^{[i']}, \ldots, r_{D^2-1}^{[i']})_i$ represents a vector of $D^2 - 1 = 4^n - 1$ real-valued parameters and $\mathbf{X}_n$ corresponds to a vector of the operators of the operator basis for a cluster of n spins as used in cTWA. Note, we can construct the operator basis $\mathbf{X}_n$ for n spins iteratively from an operator basis $\mathbf{X}_1$ for a single spin by taking tensor products $\mathbf{X}_n = (\mathbf{X}_1 \otimes \mathbb{1}, \mathbb{1} \otimes \mathbf{X}_{n-1}, \mathbf{X}_1 \otimes \mathbf{X}_{n-1})$. One can construct $\mathbf{r}_n$ analogously:

$$\mathbf{r}_n(\mathbf{p},\mathbf{q}) = [\mathbf{r}_1(p_1,q_1), \mathbf{r}_{n-1}(\tilde{\mathbf{p}},\tilde{\mathbf{q}}), \mathbf{r}_1(p_1,q_1)\otimes\mathbf{r}_{n-1}(\tilde{\mathbf{p}},\tilde{\mathbf{q}})] \tag{14}$$

with $\mathbf{p},\mathbf{q} \in \{0,1\}^n$ and $\tilde{\mathbf{p}}$ ($\tilde{\mathbf{q}}$) denoting the vector derived from $\mathbf{p}$ ($\mathbf{q}$) by dropping the first element. Suppressing the index n from now on, the Wigner function of a cluster is defined as before to be $w^{[i']}(\mathbf{p},\mathbf{q}) = \langle \hat{A}_{(\mathbf{p},\mathbf{q})}\rangle/D$. If the quantum wave function factorizes between spins within a cluster, the Wigner function also factorizes and the result is essentially equivalent

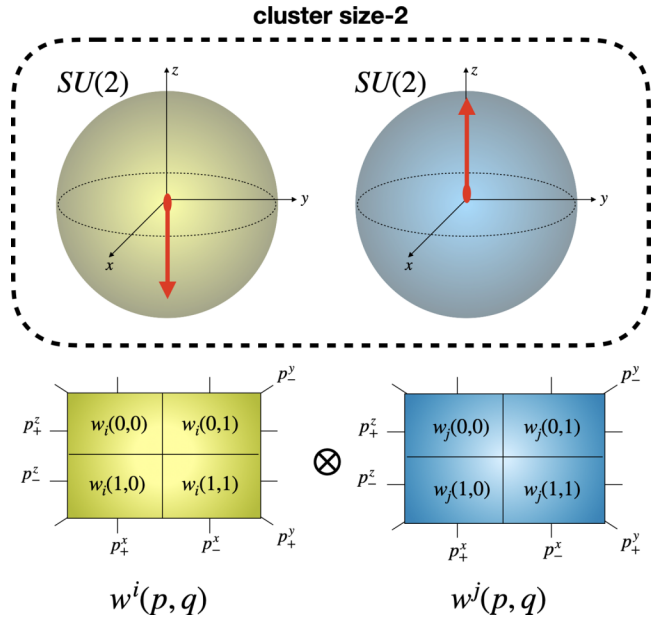

FIG. 2. A schematic of the discrete cluster truncated Wigner approximation. Considering a cluster of two spins, the individual Hilbert spaces (depicted as Bloch spheres) combine to the Hilbert space of the cluster. Shown below is a representation of the single-spin discrete Wigner functions in the spirit of [35]. The probabilities of a spin pointing along the $\pm x$, $\pm y$, and $\pm z$ directions are computed by summing over the vertical, diagonal, and horizontal lines, respectively. For product states within a cluster, one can simply take the tensor product of single-spin discrete Wigner functions to obtain Wigner functions for the cluster. In the case of clusters of size 2, the resulting Wigner function is four dimensional and contains 16 phase points.

to the single-spin case:

$$w^{[i']}(\mathbf{p},\mathbf{q}) = \prod_i \langle \hat{A}_{(p_i,q_i)}\rangle/2 = \prod_i w^{[i]}(p_i,q_i). \tag{15}$$

The key difference is in the phase-point vectors $\mathbf{r}_n(\mathbf{p},\mathbf{q})$ connected to this Wigner function which now also encompass a much larger operator basis. In summary, if the initial wave function factorizes between spins, one can simply sample the initial values for the single-spin operators and compute the initial values for operators acting on multiple spins by appropriate products. For a more detailed description of the sampling process, see Appendix A.

As a concrete example, consider a cluster of two spins in a Néel state $|\uparrow\downarrow\rangle$. To generate a sample, one draws the four values for $\langle\hat{X}_1\rangle$, $\langle\hat{Y}_1\rangle$, $\langle\hat{X}_2\rangle$, and $\langle\hat{Y}_2\rangle$ randomly from $\{-1,1\}$ and sets $\langle\hat{Z}_1\rangle = -\langle\hat{Z}_2\rangle = 1$. Then the rest of the correlators are computed from the products of these, e.g., $\langle\hat{X}_1\hat{Y}_2\rangle = \langle\hat{X}_1\rangle\langle\hat{Y}_2\rangle$ and so on. This means that the initial spin vectors are randomly drawn from one of the 16 spin configurations. All other states on the Bloch sphere can be sampled using the same configurations, followed by an appropriate rotation.

C. Clustering strategies

The cTWA necessitates a choice of clustering of the spins. While in ordered systems, it makes sense to simply choose