Probabilistic simulation of mesoscopic “Schrödinger cat” states

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Abstract
We carry out probabilistic phase-space sampling of mesoscopic Schrödinger cat quantum states, demonstrating multipartite Bell violations for up to 60 qubits. We use states similar to those generated in photonic and ion-trap experiments. These results show that mesoscopic quantum superpositions are directly accessible to probabilistic sampling, and we analyze the properties of sampling errors. We also demonstrate dynamical simulation of super-decoherence in ion traps. Our computer simulations can be either exponentially faster or slower than experiment, depending on the correlations measured.

The calculation of quantum dynamics for large quantum systems is exponentially hard if carried out through direct solutions of Schrödinger’s equation. In analyzing this problem, Feynman realized that probabilistic methods could potentially solve this problem. Analyzing this further, he asked: “Can quantum systems be probabilistically simulated by a classical computer?” [1], and gave the answer “If . . . there’s no hocus-pocus, the answer is certainly, No!” Feynman continued, “This is called the hidden-variable problem: it is impossible to represent the results of quantum mechanics with a classical universal device”. His argument apparently rested on the assumption that Bell inequalities [2] could not be violated using probability distributions [3, 4]; the remainder of his paper analyzed Clauser’s two-photon Bell state experiment [5] to illustrate the point.

Here we investigate Feynman’s claim that probabilistic simulation of quantum systems is impossible by providing, we believe, an important explicit counterexample. We carry out a probabilistic simulation of the moments of an extreme Schrödinger cat quantum superposition state: namely, the $N$-partite Greenberger-Horne-Zeilinger (GHZ) state [6], that has been shown to violate multipartite Bell inequalities for all $N$ [7]. For $N = 2$, this corresponds to the Bell state example given in Feynman’s argument. We investigate the scaling behavior of probabilistic sampling with the number of particles $N$ through direct simulation of the multipartite Bell violations. To achieve this, we employ the
positive phase-space distributions of quantum optics [8, 9, 10, 11] for our calculations. These have statistical moments which correspond to those measured in Bell violations.

Our study conveys the qualification necessary for Feynman’s argument to be strictly correct. Probabilistic simulation of quantum systems by classical computer cannot be ruled out, based on the hidden variable problem. Indeed, our results show that probabilistic quantum simulation methods are promising. What is ruled out is only probabilistic simulation based on the hidden variables of classical realism, where the trajectories in phase space are constrained to correspond to the real values obtained if the spins, positions and momenta of the particles were actually measured. In our simulations, the variables associated with the simulation are necessarily nonclassical: as in weak measurements [12, 13], their values extend outside the allowed eigenvalue range.

The methods we use are applied to the multi-qubit GHZ states with up to 60 spins (i.e. \( N = 60 \)), demonstrating macroscopic entanglement [14]. As well as being nonclassical, the quantum states we simulate have Hilbert space dimension \( 10^{15} \) times larger than the 6 qubit universal quantum computers [15] available currently. We show that these methods can simulate the dynamics of super-decoherence [16], which is relevant to a range of new, mesoscopic quantum devices.

Our mesoscopic Schrödinger cat state simulations correspond to states generated in recent ion-trap experiments with \( N \) qubits or ions [17]. These states violate a genuine multipartite Bell inequality, which means that it is impossible to confine the Bell violation to just part of the system. We regard this as a worst-case scenario for probabilistic simulations, as it not only demonstrates a mesoscopic superposition, but gives the largest possible violation of a Bell inequality. Such inequalities require the measurement of all possible correlation functions at the highest order available. We find two distinct scaling laws for the total computational difficulty, as measured by the number of samples required to obtain a given sampling error.

For low order correlations, the number of samples required decreases with system-size. By contrast, to obtain all \( N \)-th order correlations, an exponential increase is found with a \( 2^{2N/3} \) power law, due to increased sampling errors. However, as the distinct correlation operators don’t commute, an experimentalist would need \( 2^N \) measurements, which is exponentially greater still. Surprisingly, therefore, a simulation which calculates all observables simultaneously can be exponentially faster than an experiment. This classical parallelism more than compensates for the sampling error in a probabilistic simulation.

We first recall the definition of a Bell inequality. This is a constraint on observable correlations of a physical system that obeys a local hidden variable theory (LHV) [2, 5]. In the multipartite case, the LHV theory must generate measurements by \( N \) spatially separated observers, obtained from random samples of a parameter \( \lambda \). The measured values are functions of local detector settings and the hidden parameter \( \lambda \). The value observed by the \( j \)-th observer with detector setting \( a_j \) is \( X_j(a_j, \lambda) \). All correlations are obtained from a prob-
Probabilistic calculation of the form:

\[ C(X) = \int_{\Lambda} \left[ \prod_{j} X_j(\lambda, a_j) \right] P(\lambda) d\lambda \quad (1) \]

Here \( X_j \) are experimental values, usually encoded as either 1 or −1 in a binary experiment. These assumptions lead to inequalities that any LHV correlations must satisfy. Genuine multipartite Bell inequalities are the strongest Bell violations known, ruling out LHV explanations for any subset of the observations. Quantum mechanics is known to violate these inequalities, thus ruling out LHV theories. But can one simulate these violations using probabilistic methods equivalent to quantum mechanics?

In order to simulate Bell violations for multipartite spin or qubit states, we use the SU(2)-Q distribution, which is well-suited to this type of Hilbert space \([8, 18]\). Here one defines

\[ Q(z) = Tr \left[ \hat{\rho} \hat{P}(z) \right], \quad (2) \]

where \( \hat{P}(z) \) is proportional to a coherent state projection operator. This has the form of nonorthogonal, universal POVM \([19]\), with a corresponding physical measurement strategy \([20]\). The Q function calculation for a spin expectation value is a sampled, probabilistic average over a complex function \( \sigma_x(z) \):

\[ \langle \hat{\sigma}_x^1 \rangle = \langle \sigma_x(z_1) \rangle_Q = \frac{3}{2} \int d^{2N} z \left( \frac{z_1 + z_1^*}{1 + |z_1|^2} \right) Q(z). \quad (3) \]

Full computational details and sampling methods will be given elsewhere.

To understand the ultimate scaling properties of such probabilistic techniques, we have simulated the \( N \)-th order correlations that violate multipartite Bell inequalities. These are found in quantum states that display Bell violations with \( N \) observers, not just two. The most well-known examples are the multimode entangled Greenberger-Horne-Zeilinger (GHZ) states \([6]\), generalized to \( N \) spins by Mermin\([7]\) so that they are an example of an extreme macroscopic superposition or “Schrödinger Cat”. We considered GHZ states which describe \( N \) spin-\( \frac{1}{2} \) particles or qubits:

\[ |\Phi\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\ldots\uparrow\rangle + e^{i\phi} |\downarrow\ldots\downarrow\rangle \right). \quad (4) \]

Here \( |\uparrow\rangle \) and \( |\downarrow\rangle \) denote spin-up or spin down particles in the \( z \)-direction. As well as being of deep significance in quantum physics, such mesoscopic states have been generated in recent ion-trap experiments \([16, 17, 21]\). Quantum Bell inequality violations are obtained on measuring an operator \( \hat{A} \) which is defined as a linear combination of \( 2^N \) distinct \( N \)-th order correlation functions:

\[ \hat{A} = \prod_{j=1}^{N} (\hat{\sigma}_x^j + i\hat{\sigma}_y^j). \quad (5) \]
For odd \( N \) we follow Mermin [7] and take \( \phi = \pi/2 \), measuring \( F = \Im \langle \hat{A} \rangle \), while for even \( N \) we follow Ardehali [22] and take \( \phi = \pi \), measuring \( F = -\Re \langle \hat{A} \rangle \). Genuine multipartite Bell violations are known to exist for these states, which imply that the observed correlations cannot be explained by a nonlocality shared among \( N-1 \) or fewer qubits. To test for genuine multipartite Bell nonlocality, we adopt the hybrid local-nonlocal LHV model introduced by Svetlichny [23] and Collins et al. [24].

The difference between the SU(2) Q representation, compared to an LHV theory, can be illustrated by considering the case of \( N = 2 \), where simplifying the Ardehali inequality will give rise to the corresponding quantum mechanical expectation value:

\[
F = -\langle \hat{\sigma}_1^x \hat{\sigma}_2^x \rangle + \langle \hat{\sigma}_1^y \hat{\sigma}_2^y \rangle = -\langle \sigma_1^x \sigma_2^x \rangle_Q + \langle \sigma_1^y \sigma_2^y \rangle_Q.
\]  

(6)

The correlation between real parts of the values of two factors for one of the terms is plotted in Fig. 1(a), and the correlation between the two terms of (6) is plotted in Fig. 1(b). Note that the SU(2) representation does not limit the values of \( \text{Re} \sigma_1^x \) and \( \text{Re} \sigma_2^x \) to the range \([-1, 1] \), as would happen in an LHV theory; instead, they are bounded to \([-3, 3] \). This essential feature means that Bell’s theorem does not restrict our results, because the sampled values are not the same as their physical eigenvalues. This property of having a different apparent range from the operator eigenvalues, with the possibility of complex outcomes, is also shared by the theory of weak measurements [12].

The high-dimensional multipartite state (4) can be readily sampled using probabilistic random number generators together with the Q-function. These samples can then be used to calculate required expectation values (Fig. 2(a)). In the graph, the red dashed line is the minimum correlation required to demonstrate a Bell violation. Since the calculation is essentially a parallel one, we employed graphical processor unit (GPU) technology to calculate many samples in parallel, with a number of qubits ranging from \( N = 2 \) to \( N = 60 \). This corresponds to measurement of a quintillion (\( 10^{18} \)) distinct sixtieth order correlation functions. Bell violations were verified in all cases, while genuine multipartite violations of LHV requiring all \( N \) observers to participate, with \( F_{\text{sample}}/F_{\text{QM}} > 1/\sqrt{2} \), were verified for \( N < 50 \).

To understand the source of sampling errors, we investigated the scaling of errors with system-size for single measurements of a low-order spin correlation (Fig. 2(b)), in addition to the exponentially large numbers of measurements in the expectation values \( F \). As an example of low-order correlation we have chosen the total number of “spin-ups” \( N_\uparrow = \frac{1}{2} \sum_{j=1}^N (\hat{\sigma}_j^z + 1) \). Low-order correlations were easily calculated with decreasing sampling errors as \( N \) increases.

In contrast to this, high-order correlations showed an exponentially increasing sampling error. The relative error in \( F \) scales as \( 2^{N/3} \), so that the time taken at constant error scales as \( 2^{2N/3} \). Hence, probabilistic sampling scales more favorably than experiment, which would take time proportional to \( 2^N \) due to the use of exponentially many measurement settings. Single high-order correlations might be faster, depending on experimental noise levels.
Figure 1: Correlations for the different parts of the quantity (6), in case of an SU(2) Q representation with two observers and $10^8$ samples.
Figure 2: Violations for multi-particle GHZ states. (a) Simulated Mermin violation using SU(2)-Q representation. The values of expectations and errors are normalized by the quantum mechanical prediction for the corresponding $N$. The horizontal grey dashed line gives the quantum prediction. The error bars show the sampled result and estimated sampling errors at each value of $N$. The red dash-dotted line is the LHV prediction, which gives a Bell violation when above this line. Genuine multipartite Bell violations occur for $F_{\text{sample}}/F_{\text{QM}} > 1/\sqrt{2}$. (b) Relative errors for $F$ (blue line) and first order correlation, or total number of “spin-ups” (green dashed line) using SU(2)-Q representation. The dotted reference line shows the point at which the sampling errors would give scaling properties as slow as an experimental measurement.
These results are unexpected and interesting. Sampling errors in low order correlations are insensitive to scaling up to mesoscopic sizes. These are the most commonly measured quantities, and there is no barrier to sampling these, despite Bell violations and even mesoscopic superpositions. However, correlations of the same order as the system size can be exponentially hard to sample in the case of Schrödinger cat-like states. Yet even in this case, the probabilistic strategy gives advantages. It generates exponentially many non-commuting measurement results in parallel, which can result in scaling that is exponentially faster than with direct measurements. We emphasize that these scaling results are specific to the GHZ case, and will change as the quantum state is changed.

In this paper, we have focused on the specific issue of whether one can probabilistically sample the observables of a quantum state that violates a Bell inequality. The larger problem of carrying out quantum dynamical simulations was not treated, but encouraging results are known. As an example, we consider the question of dynamical noise and decoherence in ion traps, which is an important issue in the observation of mesoscopic quantum effects [25]. The experimentally observed magnetic field noise found in ion-trap experiments can be easily added to our calculations using a simple model. Following Monz et al. [16], we assume a delta-correlated noise such that $\langle \Delta B(t) \Delta B(t') \rangle = \Delta B_0^2 \delta(t - t')$, with an interaction Hamiltonian of the form:

$$\hat{H} = \frac{\mu \Delta B(t)}{2} \sum_{j=1}^{N} \hat{\sigma}_z^j.$$  \hfill (7)

We find that this can also be readily simulated dynamically. This was achieved by multiplying an independent noise term $\exp(i \epsilon N \hat{z}_j)$ by the value corresponding to the operator $A$ in each of the samples after every time step $\Delta t$. Here
\[ \epsilon = \mu \Delta B_0 \sqrt{\Delta t/\hbar} \] defines the speed of the decoherence, and \( \zeta_j \) is a Gaussian random number such that \( \langle \zeta_j \zeta_{j'} \rangle = \delta_{jj'} \). This is shown in Fig. 3, which demonstrates the experimentally observed quadratic super-decoherence as \( N \) increases.

Other examples of dynamical quantum correlations have been treated using phase-space methods, including quantum soliton dynamics [26], interacting quantum fields [27] equivalent to \( \sim 10^6 \) qubits and the Dicke superfluorescence model [28]. These simulated correlations are in general agreement with experimental observations [29]. This shows the wide range of potential applicability of these techniques. However, the optimal dynamical methods and overall questions of efficiency are not yet known. We emphasize that these examples have limitations. Our results show that probabilistic methods are not ruled out, rather than giving an optimum recipe for dynamical quantum simulations.

In summary, we show that low order quantum correlations are the simplest to obtain with probabilistic sampling. Higher order correlations in GHZ states can also be simulated, but with greater difficulty. While these require exponentially many samples to reduce errors to acceptable levels, they do not require exponentially large memory resources. In his paper, Feynman proposed the development of universal quantum computers to solve this problem, and these could potentially carry out simulations [30]. However, this proposed hardware is currently limited in size to 6 qubits or less [15], and has proved difficult to scale to large size. It remains fundamentally useful to obtain theoretical predictions with software that doesn’t require new technology, both for practical and scientific reasons. After all, if we wish to test quantum theory on mesoscopic scales, we cannot assume that our hardware strictly obeys quantum mechanics on large scales.

Importantly, we demonstrate that probabilistic digital algorithms on existing hardware can simulate mesoscopic quantum superpositions much larger than any current experiment. Such technologies are proposed for quantum secret-sharing [31] and high-precision atom interferometers [32], amongst others. Digital simulations could therefore have a direct application both to fundamental physics, and to the design and implementation of these devices. Our demonstration that mesoscopic Bell violations can be treated probabilistically will lead to further developments. The fact that our simulations can be exponentially faster than direct measurements is a surprising consequence of the classical parallelism inherent in this computational strategy. While Feynman might regard our approach as ‘hocus-pocus’, it is certainly probabilistic.

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