What SQD Is Trying to Exploit

Sample-based quantum diagonalization (SQD) is designed to exploit the *structure and sparsity* of quantum states when represented as bitstrings (computational basis states). The method leverages the fact that, for many physically relevant quantum systems (such as ground states of molecular Hamiltonians), the true eigenstate is often *sparse* in the computational basis: only a small fraction of all possible bitstrings have significant amplitude in the wavefunction[1].

Key Properties Being Exploited

- **Sparsity of the Target Eigenstate:**
  SQD is most efficient when the target quantum state (e.g., a ground state) is sparse in the computational basis, meaning that only a relatively small number of bitstrings (basis states) have non-negligible probability amplitude[1]. This allows the algorithm to focus computational resources on the most important components of the wavefunction.
- **Sampling from Quantum Circuits:**
  The bitstrings sampled from a quantum circuit represent the most significant determinants (Slater determinants or Fock states) in the eigenstate of interest. By collecting these samples, SQD constructs a subspace spanned by these important bitstrings, which is then used for classical diagonalization[1].
- **Robustness to Quantum Noise:**
  Because SQD operates on samples (bitstrings) rather than full wavefunctions, it can be robust to certain types of quantum noise. Even if some samples are corrupted, as long as the majority reflect the true structure of the state, the method can still succeed[1].
- **Efficient Representation of Large Hamiltonians:**
  SQD can handle Hamiltonians with millions of interacting terms, as it only requires knowledge of matrix elements between the sampled bitstrings, not the full Hamiltonian matrix[1].

What Properties of Bitstrings Are Used?

- **Bitstring as Fock State/Determinant:**
  Each bitstring corresponds to a specific occupation pattern of orbitals (in quantum chemistry) or spins (in spin models). The probability of sampling a given bitstring reflects its weight in the quantum state prepared by the circuit.
- **Projection and Subspace Construction:**
  The set of unique bitstrings sampled forms a basis for a low-dimensional subspace. The Hamiltonian is projected onto this subspace, and diagonalization within it yields approximations to eigenvalues and eigenstates[1].
- **Selection of Physically Relevant States:**
  Since the bitstrings with highest sampling probability are those with largest amplitude in the

target state, the method naturally selects the most physically relevant determinants, efficiently capturing the essential physics with fewer resources (when the state is sparse)[1].

Summary Table: Properties Exploited in SQD

Property of Bitstrings	How SQD Exploits It
Sparsity in computational basis	Focuses on most relevant determinants
High amplitude determinants	Samples these most frequently
Bitstring = occupation pattern	Maps directly to physical states
Subspace spanned by samples	Enables efficient classical diagonalization

Conclusion

In summary, SQD exploits the *sparsity* and *structure* of quantum states in the bitstring (computational) basis. By sampling bitstrings that represent the most significant components of the state, it constructs a compact, physically meaningful subspace for classical diagonalization—enabling efficient and robust estimation of eigenvalues and eigenstates, especially for large, complex quantum systems[1].

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1. https://docs.quantum.ibm.com/guides/qiskit-addons-sqd