Coherent-State Sampling for Vibronic Spectroscopy: Detector Benchmarking and Photon-Number-Resolution Requirements

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Photonic sampling provides a natural route to vibronic spectroscopy, where molecular transition strengths can be encoded into optical sampling statistics [1]. In this setting, single-photon detectors become a key element of spectral reconstruction, yet their impact on reconstructed molecular vibronic spectra is rarely assessed in a detector-centered way. We present coherent-state sampling for vibronic spectroscopy within the linear coupling model and use it as a benchmark for photonic detector platforms. In this framework, Huang–Rhys factors are encoded in the photon statistics of coherent states, and individual detection events correspond to state-resolved vibronic configurations [2].

Using pentacene as a test case, we compare three implementations of the same protocol: classical pseudo-random sampling, photonic sampling with a superconducting nanowire single-photon detector, and photonic sampling with a single-photon avalanche diode. We evaluate them against both the analytic sum-over-states reference within the linear coupling model and the experimental high-resolution absorption spectrum measured at 5 K. All three implementations reproduce the analytic reference with fidelity above 0.99 and show good agreement with experiment, while the comparison between detector platforms reveals how hardware imperfections influence the reconstructed spectral profile. The conventional computer simulation shows the closest agreement with the theoretical reference, while the SNSPD implementation yields closely comparable performance among the photonic platforms, and the SPAD results further illustrate the impact of detector-specific imperfections on the reconstructed spectrum.

We further use the state-resolved output of coherent-state sampling to infer the maximum photon-number resolution required per mode for different molecular systems and spectral regions, and illustrate this approach for naphthalene and anthracene. Grouping transitions by the maximum vibrational quantum number shows how the required detector resolution depends both on the molecular system and on the spectral region: low-energy features can be captured with lower photon-number resolution, whereas higher-energy spectral tails require higher photon-number resolution. For the two systems considered here, the relevant spectral structure is largely captured with resolution up to two photons per mode. More broadly, this analysis provides a practical numerical route to determining photon-number-resolution requirements for different molecules and spectral regions. Rather than targeting formal quantum advantage, this work positions coherent-state sampling as an experimentally grounded benchmark for single-photon detector platforms and as a practical route from molecular spectroscopy to detector specifications.

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References

[1] J. Huh et al., Nat. Photonics 9, 615 (2015).

[2] I. Konyshev et al., e-print arXiv:2508.03943 (2025).