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Spectroscopy with Undetected Photons for Biomedical Diagnostics in Mid-Infrared

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Sensing and detection in the mid-infrared (MIR) range are crucial, as many molecules exhibit characteristic absorption bands [1]. However, traditional techniques like Fourier Transform Infrared (FTIR) spectroscopy rely on costly lasers, complex and noisy detectors often requiring cryogenic cooling, all of which limit their applicability [2]. To address these limitations, we propose a quantum spectroscopy approach based on spontaneous parametric down-conversion (SPDC), where a single pump photon is converted into a pair of time-space correlated photons, one in the MIR (idler) and its partner in the near-infrared (NIR) or visible range (signal) [3]. Because of their strict energy-momentum correlations, detecting the signal photon provides full information about the idler's properties. This enables MIR spectral analysis without direct detection and measuring molecular absorption and refractive index using standard silicon-based devices.

Simulations using a 660 nm pump laser and an AgGaS₂ crystal confirmed phase matching for photon pairs with signal photons ranging from 732 to 743 nm and idler photons spanning 5.88 to 6.66 μm , covering the Amide I and II protein absorption bands. Quantum spectroscopy simulations were performed both without and with the sample, incorporating experimental FTIR spectra of biomarkers such as bovine serum albumin (BSA) and NT-proBNP. The resulting interference patterns showed clear differences between the absence and presence of the sample, revealing sample-specific signatures detectable in the NIR range. Comparisons between different protein samples demonstrated distinct spectral patterns, highlighting the technique's ability to discriminate biomolecules based on unique fingerprints. Temperature-dependent FTIR measurements revealed changes in protein secondary structure, which were successfully reproduced in quantum simulations, showing sensitivity to subtle biochemical variations.

This study demonstrates the feasibility of quantum MIR spectroscopy as a compact, cost effective, room-temperature alternative to conventional MIR methods, with potential for early disease detection, real-time biomarker monitoring, and broader applications in various disciplines.

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