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Research Proposal - Raman Spectroscopy on dairy yogurt products

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Abstract
This is a research proposal on the topic of applying the (quantum) optical process of Raman (scattering) spectroscopy on specific specimen, in this case yogurt and dairy products, to analyse, monitor, differentiate, and time-series analysis with the aid of machine learning, quantum optics knowledge and deep learning model in the process.

1 Introduction
It is widely considered for spectroscopy, and **Raman spectroscopy** specifically, to be an important field of study and tools of analysis. The need for accurate detection, material fingerprinting, non-destructive probing, drug detections, medicine and pathological diagnosis, and various on-field examination requires tools of Raman spectroscopy and its properties in major applications. It is then natural that we can use Raman spectroscopy at large, with control environment or not, and with specimens of different kinds for application purpose in monitoring, analysis, probing, time-dependent evolution analysis, and much more. In the past, this archetype of application is fairly limited to clinical trial or in-lab analysis, because of its cost, difficulties in identifying structures and chemical compounds reliably. Furthermore, the testing dataset is also a problem, and classical approximation techniques prove to have not so optimal results to be applied, especially in more complex notions and systems. However, with the advancements of capabilities of machine learning, this is now perhaps accessible and applicable to a wide arrays of previous proposed ideas, and by large much more available.

2 Motivation
The main idea for this proposal stems from the fact of choosing products and specimen of interest that fit the criteria of (a) availability of the product, (b) cost-effectiveness and application range, (c) ability to utilize specific Raman vibrational knowledge, plus physics simulation techniques and (d) applicable of machine learning applications. Yogurt and dairy-based product fit these criteria because of their popularity, demands and distribution, hence easy to acquire samples and testing. Because of its popularity and widespread usage, it is also cost-effective per sample availability. Yogurt is also a very specific and complex fermented product, which means the chemical and biological information available of a sample is nontrivial, and hence is resourceful for any potential analysis; the fermentation process also proves to be an effective testing ground for certain application, such as monitoring and controlling the states of the fermentation process, reverse-engineering from a sample of yogurt how the fermentation process went, and so on. Finally, yogurt and dairy products can be referred to a very specific class of vibrational modes. For example, Proteins in general yogurt is dominant in the *amide bands* C=O stretch, and hence induce different vibration. Different information are encoded in different regions of the vibrational spectrum and scattering, for example, deuteration, which is useful for tracking lipids or exchangeable hydrogens (spectrum shift and contrast vs H sample), can be applied to extract reasonable information about lipids and chemical compositions (Xue et al. [2012]), and so on. From such brief analysis, we can conclude that this is a particularly interesting avenue of research application.

For Raman spectroscopic classical and deep learning applications, we can refer to Qi et al. [2023], Li et al. [2022], Ren et al. [2023], Poppe [2024], et al. [2000s], Fuentes et al. [2023], Ibtehaz et al. [2023], Gu et al. [2024], Moores et al. [2018], Härkönen et al. [2020], Han and Ram [2018], Chen et al. [2024], Nair et al. [2024], Brevi et al. [2024], Liu et al. [2023, 2017], Song et al. [2024] for numerous architectural applications throughout the time. Of such topic, utilizing deep learning mostly comes with CNN, Bayesian network, or the state-of-the-art PINNs. Tradeoffs are from ease of use, adaptability, maintenance, complexity, accuracy metric, computational costs, and more, but CNN is still the mainstream choice at-hand. Most of such application are non-structural, aside from PINNS, which still lead to potential difficulty in applying at-hand such method to complex analysis. Specifically, even for PINNs, the models are inherently very restricted (if not outright useless, *for now*) unless it stays in the PDE configuration that it was designed to. **Discontinuous behaviours** are hard to approximated using PINNs, which sometimes fails. This is one of the main standpoint of differential system which is dynamic in parameters but not in structure. Other drawbacks simply point to the fact that it is **much more expensive, intensive** and less **interpretable** than usual, which does not help for some of the structural features that is required of the purpose.

3 Avenue of research

Here, we propose a study of applying *Raman spectroscopy* and *Deep learning architectures*, with encoded *physics knowledge design* for analysis, monitoring, and time-series state analysis of yogurt-based and dairy products. This research is based on observation of various possible previous works from Czaja et al. [2018], Karacaglar et al. [2019], Kolesov [2021], Zhang et al. [2020] and Silva et al. [2021]. Details of application includes some very specific, basic-to-advanced application residing on how the data is extrapolated of the application platform.

1. **Monitoring and extrapolation of data**: For yogurt, we can apply and try the usage of bare bone, sample-aware machine learning application to detect, analyse and identify properties and important monitoring parameters of a specified yogurt sample class. This can be done with timescale t in range, for example, during best-use duration, or standard 6—8 months in different conditions. Practical application to this can include toxin identification and indication for time evolution of particular sample, quality fluctuation and surface dynamic of a sample feature. It can also be used for more advanced analysis of *chemical penetration* and sample purity analysis, and hence good for non-destructive identification of chemicals in unsafe products of interest. This can couple with structural data to then identify what kind of condition, process are there that can produce such mixture.

2. **Structural analysis** We can use optical properties of quantum system in complex molecular structure to examine and extract resourceful information about the environment, state of the yogurt and the underlying process, for example, protein degradation, compound breakdowns and takeover, and various other culture information. This can be used to examine and explore the fermentation process, different production process and end-result, to determine and extrapolate structural information about the system of yogurt formation (the chemical, environment, bacteria, protein, probiotics and else).

3. **Time-series analysis**: Specifically on time-series application (of which we have mentioned previously), evolution and variation of sample overtimes, through various measures, environment, factors and else can help with determining which factor and effect potentially lead to adverse outcome, for example, spoiling during transportation, sanitary issues, molecular designs of preservatives, et cetera, food-related consumer issues (poisoning, diarrhea, etc) during dynamic situation (outside of lab situation).

Some more novel applications can be listed, such as devising new yogurt type or configuration, more correct specification and guideline for products, and so on. For machine learning application, we propose accordingly application thereof.

1. **Regression analysis, PCA, CNN & RamanNET, classifications**: We use different models, including regression and PCA models to extrapolate reasonable data, or using already available spectral dataset to encode spectrum-based patterns reproduction and interaction for usage in classification model for identifying and analysis of unique and characteristics components of the sample. *RamanNET*, a variation of CNN, can also be used taking advantage of spectral data type.

2. **Knowledge base/graph, neural network, and expert systems**: To encode sufficient and

specific knowledge, we would like to also encode chemistry and physics knowledge bias to the system. This requires designing a knowledge graph system, such similar to how an expert system is formed. Furthermore, incorporation this to modern structure and application require general framework of neural network architectures, and so on, to facilitate such complex operational consideration.

3. **Dual-simulation and Physics-informed NN** (PINN): A step-up of application in the above section, modifying and dual-comparing with existing simulation results and system, and also providing physics-aware neural network architectural design such as PINN provides a particularly large avenue of data and model-theoretic approach.

Such application requires further inquiry and detailed specifications if this proposal comes to pass, for example, data availability, data processing work, data interpretation, computational resources, design implementation and blueprints, structural analysis of models, outcome and learning principles (reinforcement learning or more advanced learning method), and so on. There is also the question of cost, computational resources of requirement, time resource availability, and so on. With such, the layout of multiple application on the same framework, of specific target helps in branching out and providing several options for utilization.

A Appendix - Normal market analysis of yogurt products

For reference purpose, we performed some market analysis of well-known, typical yogurt products and their archetype. This includes Nutifood [2022a,c,b], OpenFoodFacts [2024], MyNetDiary [2025], Kitchenomics [2022]. It is to be noted that more extensive and detail researches are required for such specific chemical and probiotic/bacteria culture and environment of certain types of yogurt, and also several more factors for analysis on law-abiding numerical values, available in databases of government agencies.

Product	Pack	Price (VND)	Price (USD)	Nutrition (per 100 g)	Declared cultures / probiotics	Shelf life / notes / source
Vinamilk — spoonable yogurt (popular 4x100 g pack)	4 x 100 g	25,500	\$0.97	Protein ≈ 3.2 g; Fat ≈ 3 g	ST; LB (standard yogurt starters; manufacturer marketing mentions "live cultures")	Shelf life ≈ 45 days (store 2-8°C). Source: Vinamilk product pages / retailers.
Moc Chau — spoonable cup	100-120 g	12,000	\$0.46	Protein ≈ 3.0-3.6 g; Fat ≈ 2-4 g (variant-dependent)	ST; LB; some variants list BB-12 or LA-5 (probiotic lines)	Fresh-style lines: 7-10 days; packaged lines commonly longer. Source: Moc Chau listings.
Nutifood (Nuvi) — drinkable probiotic yogurt	180 mL bottle	10,000	\$0.38	Protein ≈ 2.5-4 g (drinkable formulations vary)	ST; LB; marketed probiotic blends (manufacturer claims high CFU counts on some SKUs)	Refrigerated shelf life: multiple weeks; check bottle label for exact date. Source: Nutifood product pages.
Dutch Lady — YoMost (drinkable)	170 mL bottle	7,500 (example per bottle from 4-pack)	\$0.28	Protein ≈ 2.5-3.5 g	ST; LB (formulation varies by SKU)	Refrigerated shelf life (weeks); check label and retailer. Source: Dutch Lady Vietnam.
Yakult (original small bottle)	65 mL bottle	8,000	\$0.30	Protein ≈ 1-1.5 g	*Lactobacillus casei* Shirota (probiotic)	Typical shelf life 30 days refrigerated; source: Yakult Vietnam / local listings.
TH True — spoonable yogurt (TH True Milk brand)	100 g cup	11,000	\$0.42	Protein ≈ 3 g (varies by product)	ST; LB (some probiotic lines advertised)	Shelf life typically 30-45 days for packaged lines; store chilled. Source: TH True product pages.
Moc Chau — wholesale carton (example)	48 x 100 g (carton)	294,000	\$11.14	(per 100 g similar to spoonable entries above)	ST; LB; variant-dependent probiotic additives on some SKUs	Example wholesale/retail carton snapshot — useful for bulk pricing estimates.

B Appendix - Cost of Raman Spectroscopy

While incomprehensive of facilities provided, we prompted to do an estimate on typical university or facilities Raman spectroscopic process, this is shown in the next table, of which we sort them into the price tag of the instrument itself, sample preparation costs, and so on. This is particularly important because we have to somehow account for computational cost and sample availability, especially for machine learning application.

Category	Purchase / Range	Typical University Core (hourly)	Typical Commercial Per-sample / Service	Examples / Notes
Handheld / Portable Raman	\$10,000 – \$50,000	N/A (often not hosted in cores)	Screening service: \$50 – \$250[1]	Examples: Thermo FirstDefender, Metrohm/B&W Tek handhelds; good for field screening and ID
Benchtop (non-microscope)	\$20,000 – \$150,000	\$30 – \$120 / hr (instrument use)	Routine ID: \$75 – \$400; min. fees \$150 – \$300	Preconfigured 785 nm systems often \$17k–\$45k; fiber-probe options add cost
Raman Microscope / Confocal	\$150,000 – \$500,000+	\$60 – \$200+ / hr (mapping/confocal rates higher)	Mapping/confocal jobs: \$200 – \$2,000+ depending on area & depth	High-performance mapping, multiple lasers, automated stages; objectives and stages add cost
Used / Refurbished	\$10,000 – \$70,000 (wide variance)	Depends on the instrument and facility	Per-job pricing comparable to benchtop or bespoke quotes	Good value if specs match needs; check warranty / laser age
University Core: basic access	(facility-owned; no purchase by user)	\$20 – \$150 / hr (internal vs external / mapping vs simple scans)	Sample-prep fees often \$20 – \$100 extra	Many cores offer limited training; some include tech assistance in the rate
Commercial contract lab (single-sample)	N/A	N/A	\$50 – \$800 per sample (routine ID to in-depth mapping); common minimum \$150–\$300	Turnaround, rush fees, and interpretation reports increase cost
Consumables	\$100s per item annually	Billed separately or included in facility fee	Sample substrates, cuvettes, fiber probe tips billed per item	Typical: objectives \$500–\$3,000; probes \$500–\$5,000; low-fluorescence slides/substrates cost extra
Service / Maintenance	Service contracts: \$2,000 – \$20,000 / yr (depends on system)	Often covered by facility budget; may be charged to projects	Per-incident repairs or laser replacement expensive	Laser replacement or alignment services major cost drivers; annual calibration recommended
Accessories that increase cost	Mapping stages, extra excitation lasers, cryostats, cooled detectors	May be charged as separate-use or premium-hour rates	Adds to per-sample analysis time and cost	Each accessory can add \$5,000 – \$100,000 depending on complexity
Training - Initial user training (1–3 hr typical)	Tech assistance billed \$40 – \$120 / hr if provided	Consulting / interpretation: \$50 – \$200 / hr	Some cores include basic training; commercial labs bill for consulting	
Sample preparation complexity	Minimal (bulk solids): low cost; complex (bio, thin films, cross-sections): higher	Prep time often billed separately	Prep fees \$20 – \$300+ depending on method	Fluorescence mitigation, substrate cleaning, and safety (biohazard) add cost
Typical turnaround times	Immediate (handheld) to weeks (special mapping)	N/A	Rush fees common (expedite)	Mapping and depth profiling substantially increase total time and cost
Geographic / vendor variations	Prices depend on country, vendor, reseller, and currency	Facility rates and commercial quotes vary regionally	Import/shipping/customs can add to cost	Always request detailed quotes and service terms

[1] Screening price examples are illustrative; some service providers offer flat-rate screening under \$100 while specialized IDs may cost substantially more.
The ranges above are indicative, compiled from vendor brochures, university core rate pages, and commercial analytical-lab price lists. Actual prices change over time and vary with location and service level.
When budgeting, include: shipping for mailed samples, customs & duties (if international), hazardous/biohazard handling fees, software license costs, and potential training or consulting fees.

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