

Contributions of George J. Papadopoulos*

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I review some of the scientific work of George Papadopoulos. The main emphasis is on his works on path integrals and their applications. The review is closed by an excursus on polaron physics, where the path-integral approach has been proven to be the method of excellence.

Key words: quantum dynamics; path-integral method; Dirac electron; magnetic field; polarons

1. Preface

Discussions with George Papadopoulos, more often than not, ended up with reflections on Thales, Pythagoras, Plato, Aristotle, Archimedes... (Fig. 1). I therefore cannot resist the temptation to illustrate my present review of some of George's work with references to Ancient Greece. I had the pleasure to interact with George over longer periods. On this occasion, I wish George many new creative achievements in the coming period.

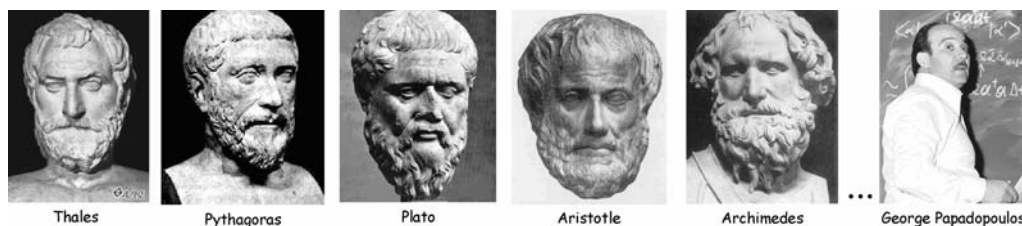


Fig. 1. Prolonging the timeline of theoretical studies from Ancient Greece

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2. Path integrals and their applications

Path integrals and their applications in quantum, statistical and solid state physics have been the subject of the book [1], co-authored by George Papadopoulos. Among the original contributions by George, his excursions on quantum dynamics and path integrals must be mentioned. The path integral for the partition function, which determines the free energy, is calculated over closed paths. See Figure 2 for an example of an (intricate-) closed path.

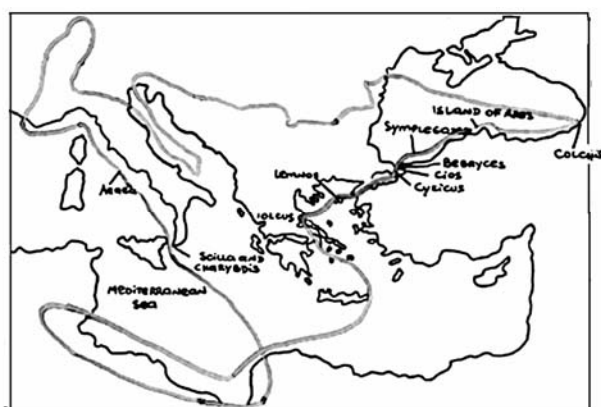


Fig. 2. *Beginning with thee, O Phoebus, I will recount the famous deeds of men of old, who, at the behest of King Pelias, down through the mouth of Pontus and between the Cyanean rocks, sped well-benched Argo in quest of the golden fleece.* (Apollonius Rhodius, *Argonautica*)
(map from <http://lukio.vimpeli.fi/italia/argoviag.htm>)

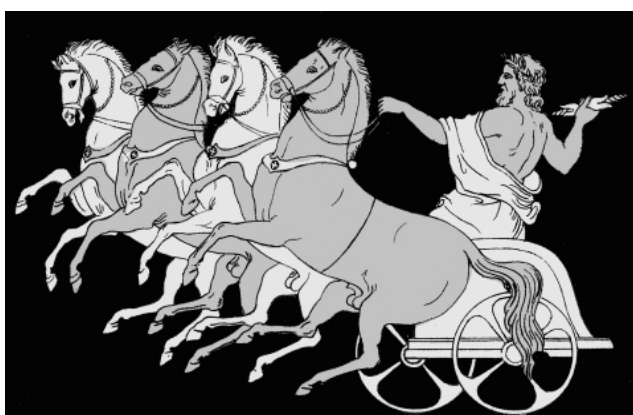


Fig. 3. *And therein were fashioned two chariots, racing, and the one in front Pelops was guiding, as he shook the reins, and with him was Hippodameia at his side, and in pursuit Myrtilus urged his steeds, and with him Oenomaus had grasped his couched spear, but fell as the axle swerved and broke in the nave, while he was eager to pierce the back of Pelops.* (Apollonius Rhodius, *Argonautica*) (The Chariot of Zeus, from *Stories from the Greek Tragedians* by Alfred Church, 1879.
http://en.wikipedia.org/wiki/Image:The_Chariot_of_Zeus,_Project_Gutenberg_eText_14994.png)

He treated the quantum dynamics of dissipative Lagrangians, proposed a systematic approach for the derivation of the path-integral propagator for a constrained particle described by a dissipative Lagrangian [3]. In Figure 3, an early illustration of the effect of dissipation is presented. As friction heated the axle of Oenomaus' chariot, the wax linchpins melted, and when the wheels eventually fell off, the whole chariot broke apart.

Further, George developed a path integral description of an electron gas in a random potential [4] and analyzed functional integrals with applications in polymer physics and in the study of spin-Bose systems.

Feynman's path-integral method had already been successful in tackling many quantum-mechanical problems. Although, in principle, there was nothing to prevent the application of the method to obtain a formal expression for the propagator of the Dirac equation, in practice a variety of mathematical difficulties had prevented direct actual calculations. In 1976 George co-authored a paper [5] in which the propagator for a free fermion and for a fermion in a magnetic field was directly derived in the path-integral formalism. The propagator for a Dirac electron in a constant magnetic field was indirectly obtained by evaluating a world-line (space-time path) integral. The corresponding spectrum was then extracted from an auxiliary propagator.

3. A spectrum of scientific activities

The works of George span a broad spectrum of his fruitful scientific activities. Problems of relativistic physics remained one of George's key interests over his scientific career. He and his co-authors provided a useful approximation to treat the Dirac equation with a confining scalar potential and a fourth component of the vector potential of rectangular shape [6]. They also demonstrated the analytic advantages of those potentials [7]. Figure 4 shows Prometheus subjected to a "confining potential".

Several works of George and his co-workers deal with the interaction of light with matter. He analyzed the interaction of radiation with atoms [8], light-scattering properties of linear polymers, energy exchange between parametric modes in a nonlinear optical medium, the energetics of a system consisting of radiation and a two-level atom in an ideal resonant cavity [9], the amplitude and phase of the acoustic effect.

Another field of his research interests is in the physics of tunneling, where he provided important ingredients for the understanding of time-dependent quantum tunneling via crossover processes [10] and of photon induced tunneling oscillations in a double quantum well [11].

George and his co-authors also extensively applied fundamental theoretical approaches to problems of materials physics. For example, they characterized polycrystalline polyamine copper dinitrate complexes [12] and iron oxide pigments: hematite, goethite and magnetite [13] using photoacoustic, EPR and electrical conductivity investigations.



Fig. 4. *Thou firmament of God, and swift-winged winds,
Ye springs of rivers, and of ocean waves
That smile innumerable! Mother of us all,
O Earth, and Sun's all-seeing eye, behold,
I pray, what I, a God, from Gods endure.*

(Aeschylus, *Prometheus Bound*, <http://www.bartleby.com/8/4/1.html>)

(Picture by P. P. Rubens, from <http://www.artprints-on-demand.co.uk/noframes/rubens/prometheus.htm>)

4. Polarons

The polaron concept is of interest, not only because it describes the particular physical properties of an electron in polar crystals and ionic semiconductors, but also because it is an interesting field-theoretical model consisting of a fermion interacting with a scalar boson field.

A conduction electron (or hole) together with its self-induced polarization in a polar crystal forms a quasiparticle, which is called a polaron [14–17]. Properties of polarons have attracted increasing attention due to their relevance to physics of conjugated polymers, colossal magnetoresistance perovskites, high- T_c superconductors, layered MgB_2 superconductors, fullerenes, quasi-1D conductors, semiconductor nanostructures.

A conduction electron repels the negative ions and attracts the positive ions (Fig. 5). A self-induced potential arises, which acts back on the electron and modifies its physical properties. The polaron coupling constant was introduced by Fröhlich [16]:

$$\alpha = \frac{e^2}{\hbar} \sqrt{\frac{m_b}{2\hbar\omega_{LO}}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)$$

where ω_{LO} is the long-wavelength frequency of a longitudinal optical (LO) phonon; ϵ_∞ and ϵ_0 are, respectively, the electronic and the static dielectric constants of the polar crystal, m_b is the electron (hole) band mass.

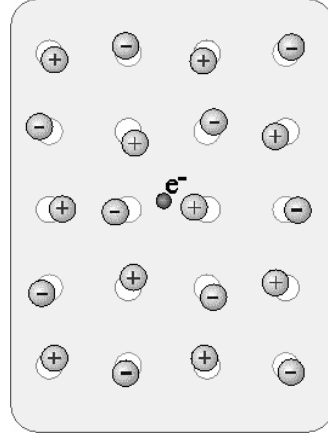


Fig. 5. An artist's view of a polaron (from Ref. [18])

Feynman's all-coupling path-integral treatment [19, 20] is based on his suggestion to formulate the polaron problem in the Lagrangian form of quantum mechanics and then to eliminate the phonon field from the propagator. As a result, the polaron problem is formulated [19] as an equivalent one-particle problem in which the interaction, non-local in time or "retarded", is between the electron and itself:

$$\langle 0, \beta | 0, 0 \rangle = \int D\mathbf{r}(\tau) \exp \left[-\frac{1}{2} \int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{\alpha}{2^{3/2}} \int_0^\beta \int_0^\beta \frac{e^{-|\tau-\sigma|}}{|\mathbf{r}(\tau) - \mathbf{r}(\sigma)|} d\tau d\sigma \right]$$

with $\beta = 1/(k_B T)$.

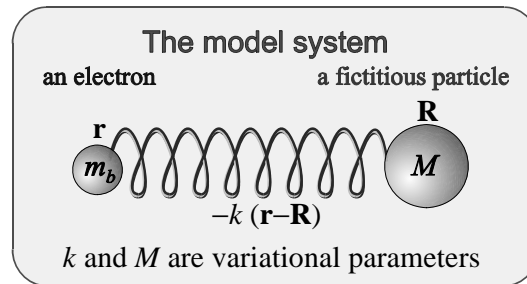


Fig. 6. The Feynman model system for a variational study of the polaron

Feynman introduced a variational principle for path integrals to study the polaron. He simulated the interaction between the electron and the polarization modes by a harmonic interaction between a hypothetical particle and the electron (Fig. 6).

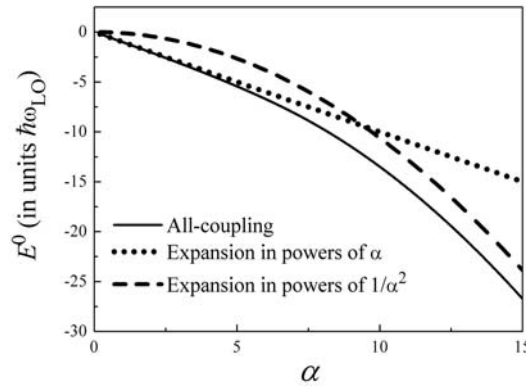


Fig. 7. Feynman-polaron energy as a function of α : the all-coupling theory

Applying the variational principle for path integrals resulted in an upper bound for the polaron self-energy at all α , which at weak and strong coupling gave quite accurate limits (see Fig. 7). Feynman obtained a smooth interpolation between weak and strong coupling for the ground-state energy. Over the years, the Feynman polaron model remained in many respects the most successful approach to this problem.

At zero temperature and in the weak-coupling limit, the optical absorption is due to the elementary polaron scattering process, schematically shown in Fig. 8. An incoming photon is absorbed by a polaron. The polaron emits a phonon during the absorption process and takes recoil energy from the incident light.

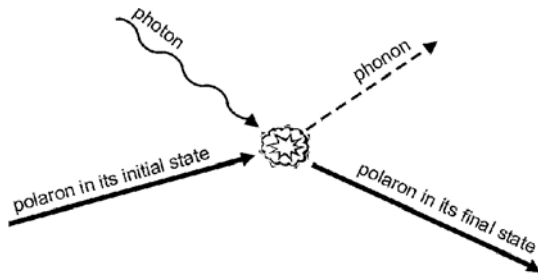


Fig. 8. Elementary polaron scattering process (from Ref. [21], © 2003 by the American Institute of Physics)

In the weak-coupling limit ($\alpha \ll 1$), the polaron absorption coefficient at zero temperature can be expressed in terms of elementary functions in two limiting cases [23, 24]:

- at high densities

$$\Gamma(\omega) = \frac{1}{\epsilon_0 n c} \frac{2^{1/2} N^{2/3} \alpha}{(3\pi^2)^{1/3}} \frac{e^2}{(\hbar m_b \omega_{LO})^{1/2}} \frac{\omega-1}{\omega^3} \Theta(\omega-1)$$

- and at low densities

$$\Gamma(\omega) = \frac{1}{\epsilon_0 n c} \frac{2 N e^2 \alpha (\omega - 1)^{1/2}}{3 m_b \omega_{LO}} \frac{1}{\omega^3}$$

where ω is the frequency of the incident light represented in units of ω_{LO} .

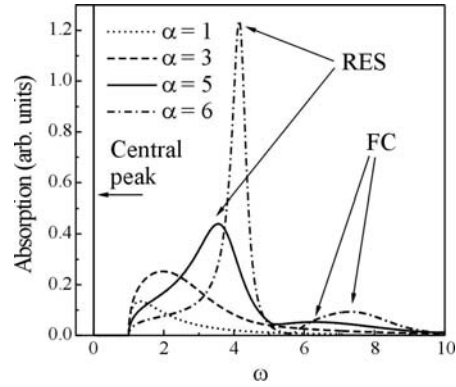


Fig. 9. Polaron optical absorption spectra at zero temperature, calculated within the path integral method [24, 25] for various values of α . A δ -like central peak is schematically shown by a vertical line (from Ref. [21], © 2003 by the American Institute of Physics)

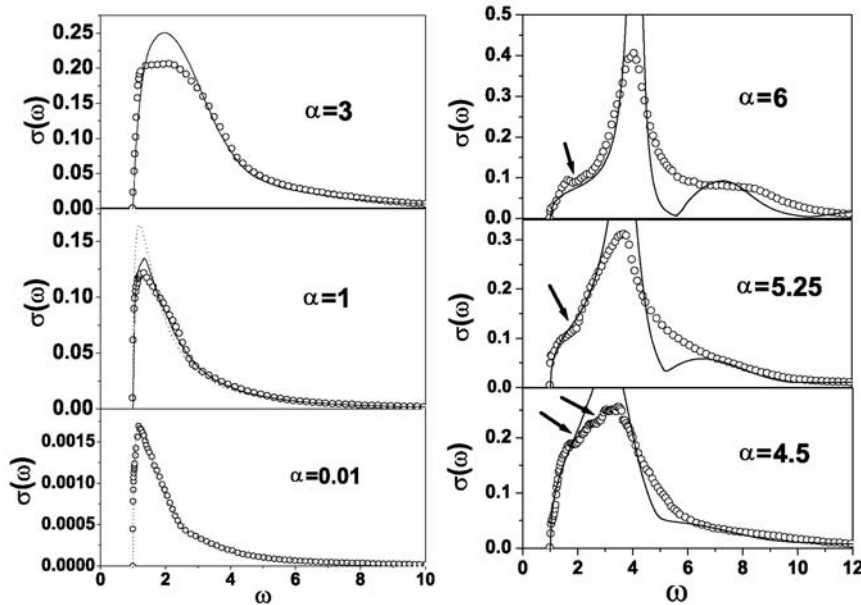


Fig. 10. Left-hand panel: Optical conductivity spectra for the weak-coupling regime (open circles) compared to the second-order perturbation theory (dotted lines) and arbitrary-coupling path-integral theory [24] (solid lines). Right-hand panel: Optical conductivity spectra for the intermediate coupling regime (open circles) compared to the arbitrary-coupling path-integral theory (DSG [24]), (solid lines). Arrows point to the anomalies in absorption spectra arising at the two- and three-phonon thresholds (from. Ref. [26], © 2003 by the American Physical Society)

The optical absorption of single large polarons at arbitrary coupling has been derived using the path-integral method [24, 25] (Fig. 9). At larger coupling, $\alpha \geq 5.9$, the polaron can undergo transitions toward a relatively stable internal excited state called the “relaxed excited state” (RES). The RES peak in the spectrum also has a phonon sideband, which is related to a Franck–Condon- (FC)-type transition. For α ranging from ~ 4 to ~ 7 , the RES peak is very intense compared with the FC peak.

Calculations of the optical conductivity for the Fröhlich polaron performed within the diagrammatic Quantum Monte Carlo method [26] (Fig. 10), fully confirm the results of the path-integral variational approach [24] at $\alpha \leq 3$. In the intermediate coupling regime $3 < \alpha < 6$, the low-energy behaviour and the position of the maximum of the optical conductivity spectrum of Ref. [26] follow well the prediction of Ref. [24]. There are the following qualitative differences between the two approaches in the intermediate and strong coupling regime: in Ref. [26], the dominant peak broadens and the second peak does not develop, giving instead rise to a flat shoulder in the optical conductivity spectrum at $\alpha = 6$. This behaviour can be attributed to the optical processes with participation of two or more phonons. The RES peaks calculated in [24, 25] tend to become too narrow as α increases. The nature of the excited states of a polaron needs further study.

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