The problem of computing the properties of a low mass quantum particle in equilibrium in a disordered medium is considered. With the advancement of computational speed, statistical methods for sampling a complex phase space are now viable. The Feynman–Kac path integral establishes a connection between a quantum particle and classical polymer consisting of p atoms. This allows the computation of quantum mechanical equilibrium values using well-known methods devised for classical systems. Here we review the application of the path integral to the computation the properties of thermalized positron and positronium and introduce some new directions of investigation.

The subject matter considered in our work focuses on systems in which a single light particle interacts with more massive atoms and molecules. Because of its long deBroglie wavelength, the light particle obeys the laws of quantum mechanics while the translational degrees of freedom of the massive atoms can be treated classically. Examples of light particles are electrons, positrons, or positronium. This scenario is important for understanding electron transport in insulating materials, weakly ionized plasmas, and any other situation which can be modeled by an excess electron in a classical gas, liquid, or solid. It also applies to lifetime studies of positrons produced by radioactive sources which have been injected into various materials.

Depending on the density or temperature, different qualitative behaviors of the light quantum particle (hereafter qp) become manifest. At high temperature and low density (i.e., in a dilute gas) the thermalized qp has a short wavelength compared with the mean interatomic spacing and undergoes a sequence of independent, random, scatterings from the constituent atoms or molecules. As the region of the liquid-vapor critical point is approached, interesting and non-intuitive behavior occurs in low temperature systems such as helium. As the host density and temperature are varied, large changes are seen in the electron mobility and the positron and positronium annihilation rate (see Fig. 1). Near the liquid-vapor critical point, the measurements qualitatively suggest that the qp may become self-trapped in a bubble or droplet of the fluid, depending on whether the net qp-atom interaction is repulsive (bubble) or attractive (droplet). In the vicinity of the triple point, both spectroscopic and lifetime measurements suggest that the qp is...
Fig. 1. The decay rate of ortho-positronium in ethane versus the scaled density along the isotherms 34, 50, 70 and 104 °C. At all temperatures the decay rate fails to keep up with the linear extrapolation, however, as the temperature approaches the critical temperature the deviation from linearity in the decay rate becomes more pronounced. At 34 °C, very nearly the critical temperature, the decay rate attains constancy over a wide range of density values around the critical density. The density is scaled such that the critical density is one.

It is important to note that, from a theorists view, the annihilation rate is a far more ideal probe of the qp quantum states than the mobility because it is an equilibrium property. The mobility is a transport property which formally requires the construction of correlations in time, a much more difficult task. Most theorists have avoided this problem by focusing on the potential energy of the electron as an indicator of mobility. In contrast, for both positron ($e^+$) and ortho-positronium (o-Ps) the decay rate, $\lambda$, is simply proportional to the overlap of the positron with the atomic electrons. The statistical average is therefore a convolution of the qp-atom radial distribution function with the local electron density of the host atoms or molecules. Thus, for a theorist, the...