Positron Annihilation With Quantum Monte Carlo

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Experimental use of positron annihilation spectroscopy requires a strong theoretical background for drawing conclusions from the measurements and making a link between the atomic structures of the defects detected and the indirect information in the measured spectra. The most widely used method for making theoretical simulations of positron annihilation is density functional theory (DFT) [1]. While it is proven to be highly practical, there is demand for more accurate methods. This is why we have developed a Quantum Monte Carlo (QMC) [2] method for simulating positrons in solids. QMC does not require the approximation of multiple functionals, and it is able to sample directly two-body quantities, as well as expectation values in the momentum space. The trial wave functions are in a localized blip basis. With QMC, the electron-positron wavefunction is first optimized with variational Monte Carlo method (VMC), after which it is passed forward for the extremely accurate diffusion Monte Carlo simulation (DMC).

At the moment, we have obtained accurate predictions of the lifetimes of positrons in diamond phase-carbon and -silicon and wurtzite aluminium nitride. We are also studying correlation between electrons and a positron in the crystals as a function of location in real space by sampling enhancement factors, and examining how correlations play a role in annihilation events. In the future we may also simulate the Doppler broadening spectrum of annihilating electron-positron pair.

[1] Tuomisto, Filip, and Ilja Makkonen. "Defect identification in semiconductors with positron annihilation: experiment and theory." Reviews of Modern Physics 85 (2013)
[2] Foulkes, W. M. C., et al. "Quantum Monte Carlo simulations of solids." Reviews of Modern Physics 73 (2001)

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