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Calculating recombination rates and biexciton binding/antibinding in core-shell dots and nano-rods[1]

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Predicting radiative lifetimes and photoluminescence (PL) emission energies from electron-hole recombination in nano structures is complicated by correlation. Quantum correlations—particularly the attraction between the recombining electron and hole—reduce the PL emission energy but also modify the wave functions, enhancing recombination rates. Interactions with spectator particles can also affect energies and lifetimes, though sometimes the sign of these changes is non-intuitive. Path-integral quantum Monte Carlo (PI-QMC) is a wave-function free computational quantum approach that can easily handle interactions between several electrons and holes in a nanostructure. We present an application to core-shell dots and nano-rods, where proper treatment of correlation is necessary to understand the binding/antibinding transition in the biexciton [1]. The imaginary-time paths provide further insights into the properties of the electron-hole states. We show how changing the topology of the paths can be used to calculate recombination rates and give insights into the recombination process. Fluctuations in the paths are used to calculate responses to electric and magnetic fields. These calculations are performed with the open source pi-qmc code available on GitHub and as a community resource on the nanoHUB.

[1] P. G. McDonald, E. J. Tyrrell, J. Shumway, J. M. Smith, and I. Galbraith, Phys. Rev. B 86, 125310, (2012).

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