Coloring the noise or cheating ones way to quantum effects

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We use a generalized form of Langevin equation in which the noise is correlated (colored) rather then being white to devise a number of very powerful sampling methods. After revising the theory that is behind our approach, we show how one can model the noise to achieve optimal sampling in ordinary and in ab-initio (Car-Parrinello) molecular dynamics. Most remarkably our sampling method can be used to introduce quantum effect at zero additional cost with respect to a standard simulation.

References

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