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Quantum Kinetic Theory of Multiband Electron Systems and the Future of Device Modeling

In a couple of recent works [1,2], we have established the foundations of a U(1) x SU(N) gauge invariant quantum kinetic theory of general N-bands electron systems, driven by classical electromagnetic fields slowly varying in time and space on atomic scales. In this talk, and after a brief general overview of the salient new features of this formalism, especially in linear response to an electric field, we will first illustrate its power on selected examples in spintronics. Namely, we will show how concrete calculations shed new light on the subtle interplay between quantum geometry and disorder, in modulating the spin Hall effect [3] and the spin-orbit torque effect [4]. The importance of vertex corrections, and how our quantum kinetic approach captures them with striking efficiency, will be discussed. In the second part, we will turn our focus to orbitronics [5], with the derivation of a new mechanism for out-of-equilibrium interband quantum coherence, which may explain the recent observations of current induced edge orbital accumulation in thin films of centrosymmetric normal metals [6]. In conclusion, we will open a perspective towards the development of new numerical simulation capabilities, whose theoretical underpinning is provided by our formalism, and that we believe will help bridge the current gap between microscopic material modeling (DFT-Wannier) and the needs for future device modeling at the mesoscopic scale, in a rapidly evolving “beyond CMOS” / “more than Moore” context.

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[2] T Valet, R Raimondi, Quantum Kinetic Theory of the Linear Response for Weakly Disordered Multiband Systems, arXiv:2410.08975, 2024.
[3] R. Raimondi, C. Gorini, P. Schwab, and M. Dzierzawa, Quasiclassical approach to the spin Hall effect in the two-dimensional electron gas, Phys. Rev. B, 74, 035340 (2006).
[4] D. G. Ovalle, A. Pezo and A. Manchon, Spin-orbit torque for field-free switching in C3v crystals, Phys. Rev. B, 107, 094422 (2023).
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