Non-equilibrium transport theory for dopant arrays in silicon

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The recent development of precise phosphorus donor placement in silicon [1,2] has attracted attention to the chains and arrays of such sites. Donor arrays have already proven well suited for quantum simulation of the Extended Hubbard [3] and SSH [4] models and are of major interest for future quantum-information devices.

In the experiment, systems of a few sites are gated and studied electrically in terms of so-called stability and Coulomb-blockade diagrams obtained by measuring the current while sweeping gate voltages. The theory aims then to simulate such diagrams and provide a two-way correspondence between the physical system and the simulated model. Thus, the need for a non-equilibrium transport theory of dopant systems arises.

Our approach based on combining exact diagonalization with non-equilibrium Green's functions allows for calculating both terminal and local currents in the arrays and other observables characterizing the system. Typically, by resorting to Green's functions, one loses the information on the underlying eigenstates. Our methodology lets us preserve this knowledge and back-trace states responsible for features of interest. This gives us a way to gain more information about the transport processes than can be obtained directly from transport measurements. Thus, we can, e.g., characterize the many-body configurations that contribute to the current, determine current magnitudes for different channels, and visualize how the electron flow circumvents disturbances in the form of array randomness. We study some of these effects to better understand transport studies of experimentally realized arrays [3].

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[1] M. Fuechsle, J. A. Miwa, S. Mahapatra, H. Ryu, S. Lee, O. Warschkow, L. C. L. Hollenberg, G. Klimeck, M. Y. Simmons, *Nature Nanotech.* **7**, 242 (2012).

[2] J. Wyrick, X. Wang, R. V. Kashid, P. Namboodiri, S. W. Schmucker, J. A. Hagmann, K. Liu, M. D. Stewart, C. A. Richter, G. W. Bryant, R. M. Silver, *Adv. Funct. Mater.* **29**, 1903475 (2019).

[3] X. Wang, E. Khatami, F. Fei, J. Wyrick, P. Namboodiri, R. Kashid, A. F. Rigosi, G. W. Bryant, R. Silver, *Nature Commun.* **13**, 6824 (2022).

[4] M. Kiczynski, S. K. Gorman, H. Geng, M. B. Donnelly, Y. Chung, Y. He, J. G. Keizer, M. Y. Simmons, *Nature* **606**, 694 (2022).