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Finite-size effects in transport data from Quantum Monte Carlo simulations RAIMUNDO ROCHA DOS SANTOS, RUBEM MONDAINI, Universidade Federal do Rio de Janeiro, KARIM BOUADIM, Ohio State University, THEREZA PAIVA, Universidade Federal do Rio de Janeiro — We have examined the behavior of the compressibility, of the dc-conductivity, and of the Drude weight as probes of the density-driven metal-insulator transition in the Hubbard model on a square lattice. These quantities have been obtained through determinantal quantum Monte Carlo simulations at finite temperatures on lattices up to 16×16 sites. While the compressibility and the dc-conductivity are known to suffer from 'closed-shell' effects due to the presence of artificial gaps in the spectrum (caused by the finiteness of the lattices), we have established that the former tracks the average sign of the fermionic determinant, and that a shortcut often used to calculate the conductivity may neglect important corrections. We have also performed systematic studies of the dependence of our data with the imaginary-time interval. Our analyses also show that, by contrast, the Drude weight is not too sensitive to finite-size effects, being much more reliable as a probe to the insulating state.

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