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Monte Carlo Simulations for 2D Materials: Parallelization Strategy and Degeneracy in MoS_2

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ABSTRACT

We employ an in-house developed ensemble Monte Carlo (EMC) carrier transport simulations [1, 2] to analyze the effects of degeneracy in MoS_2. Therefore, the Pauli exclusion principle and the effects of dielectric screening are taken into account. The static dielectric function is computed through the temperature-dependent and carrier density-dependent polarizability [3,4]. Then, the matrix elements associated with the electron-phonon coupling are renormalized [5] by this dielectric function. Carrier mobility and high-field drift velocity for various carrier densities and temperatures are extracted and discussed.

In order to expand our EMC simulator and to lighten the large computational burden linked to these simulations, we have developed a parallelization strategy of the code. The parallelization is not a trivial task as the motion of the particle ensemble depends on their prior motion and cannot be performed independently [6]. The Message Passage Interface (MPI) is used to parallelize the EMC simulator. The improvement in the CPU times in the simulation of 2D materials and the interdependence of the number of cores and the total quantity of simulated particles are discussed.

EMC MODEL AND SCREENING

- Ensemble simulation of:
  - n-type MoS_2: K, K' and $Q_{1\text{-}6}$ conduction band valleys [7].
  - p-type MoS_2: Γ, K, and K' valence band valleys [7].
- **Considered phonon modes [7]:**
  - Intravalley acoustic phonons.
  - Intervalley acoustic phonons.
  - Optical phonons.
- Aggregated phonon modes to account for:
  - TA and LA.
  - TO(E'), LO(E') and A1 (homopolar).

- In degenerate conditions scattering probabilities are calculated by renormalizing the matrix elements with the dielectric function.
- The dielectric function is computed using the Temperature and Fermi level-dependent polarizability given by the Madalgue approximation [8]:

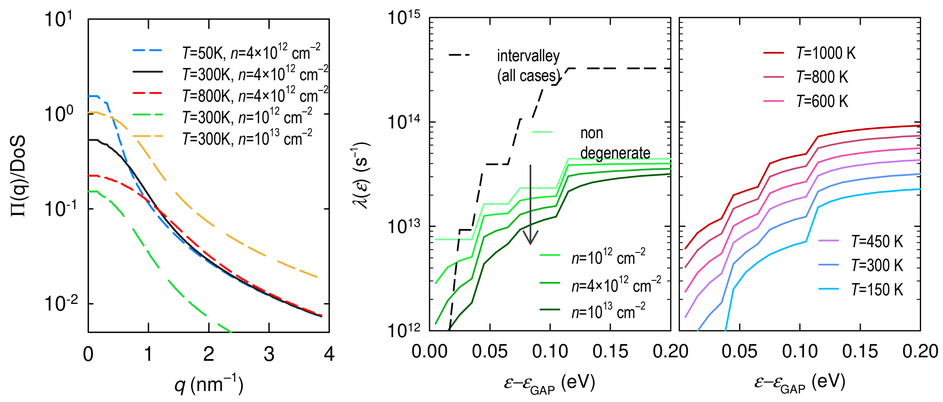
$$|\mathcal{H}_{\mathrm{scr}}|^2 \rightarrow \left|\frac{\mathcal{H}}{\epsilon(q,T,\mu)}\right|^2 \Rightarrow \begin{cases} \lambda^{\mathrm{qel}}_{\mathrm{scr}}(\varepsilon) = \dfrac{D_1^2 m^* k_B T}{2\pi\hbar^3 v_s^2}\displaystyle\int_0^{2\pi}\frac{d\vartheta}{\epsilon(q,T,\mu)^2} \\ \lambda^{\mathrm{qel}}_{\mathrm{scr}}(\varepsilon) = \dfrac{D_0^2 m^*}{4\pi\rho\hbar\omega}\left(n+\frac{1}{2}\pm\frac{1}{2}\right)\displaystyle\int_0^{2\pi}\frac{d\vartheta}{\epsilon(q,T,\mu)^2} \end{cases}$$

$$\epsilon(q,T,\mu) = 1 + \frac{e^2}{\kappa q}\Pi(q,T,\mu),$$

with

$$\Pi(q,T,\mu) = \int_0^{\infty}\frac{g m^*\left[1-\Theta(q-2k_F)\sqrt{1-(2k_F-q)^2}\right]}{8\pi\hbar^2 k_B T\cosh^2\left(\frac{\mu-\xi}{2k_B T}\right)}d\xi$$

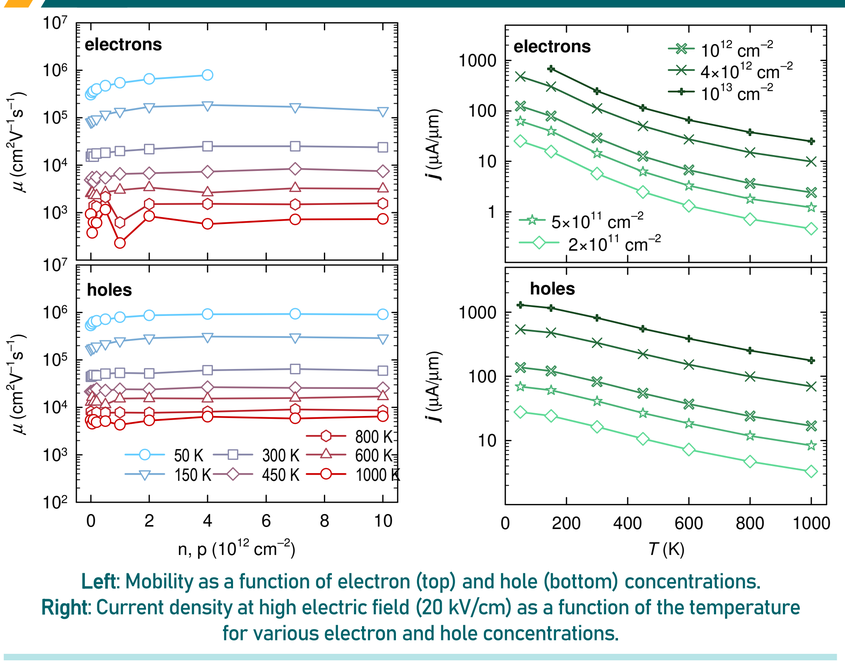
and $k_F = \sqrt{2m^*\mu}/\hbar$



Left: Polarizability as a function of wavevector **q** for various temperatures and electron densities. **Center**: Scattering probability as a function of electron energy at T=300K for intravalley and intervalley transitions. **Right**: Intravalley scattering probabilites with $n = 10^{13}$ cm^{-2}.

- This screening model only affects carrier interactions involving intravalley transitions.
- Reductions of intravalley scattering at low energies can be of an order of magnitude.
- Drop in polarizability with increasing temperature increases carrier-phonon scattering activity.

ELECTRON AND HOLE MOBILITY



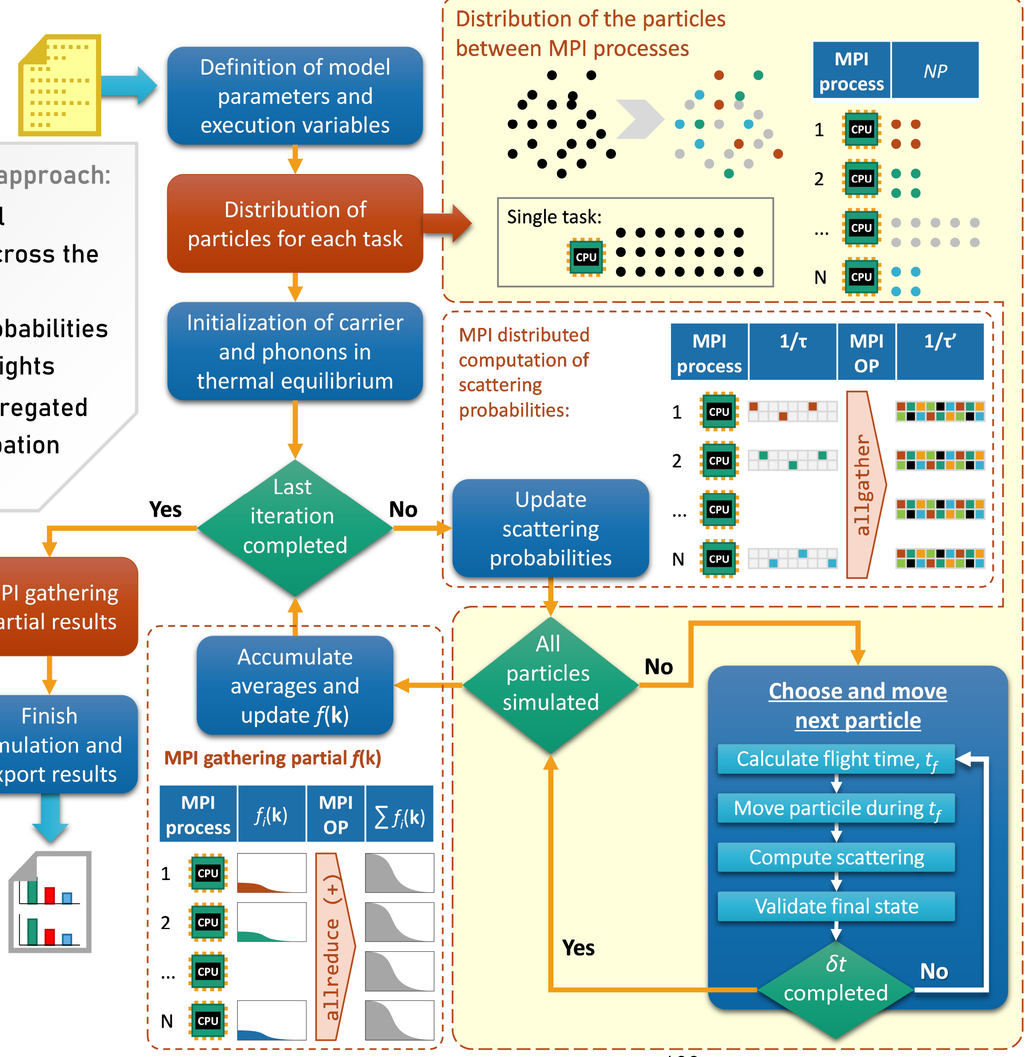
Left: Mobility as a function of electron (top) and hole (bottom) concentrations. **Right**: Current density at high electric field (20 kV/cm) as a function of the temperature for various electron and hole concentrations.

- Mobility shows weak dependence with carrier density, with a trend to increase when degeneracy is increased at low carrier concentrations.
- Mobility at high T and low n shows non-monotonous behavior due to the occupancy of the Q-valley.
- High-electric field current scales almost linearly with carrier concentration: carrier density has a little effect on the high-field drift velocity.

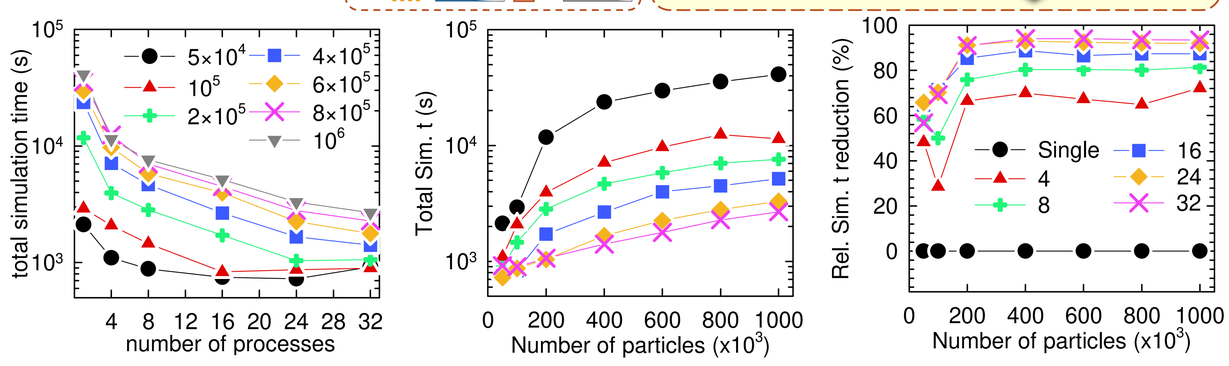
PARALLELIZATION STRATEGY: MPI-EMC

Message Passing Interface (MPI):
- First message-passing interface standard
- Standardization: source-code portability
- Allows efficient implementation

EMC-MPI parallelized flow chart:



Implementation approach:
- Computational distribution across the cluster cores: Scattering probabilities and particle flights
- Gathering aggregated results (occupation functions)



- At 50.000 simulated particles, the optimum number of CPUs is between 8 and 16. Simulations with large number of particles decrease the computational burden associated to intercommunication overhead: the best parallelization candidates.
- Greater reduction in simulation time when passing from a 1 CPU to 4 CPUs, communication between them may interfere causing a relative simulation time reduction of 60% when the number of particles is larger than 200.000 for 4 CPUs and of 95% for 32 CPUs.

CONCLUSIONS

- The consideration of carrier-phonon screening is mandatory for an adequate description of intravalley interactions.
- Screening decreases dramatically as temperature increases: a very small effect at high electric field (hot carrier temperatures).
- Polarizability around M, Q, and K energy bandstructure points should be studied.
- The calculation of polarizability will allow a study of other interactions such as charged impurities and dielectric surface polar phonons (SPPs).
- Both carrier mobility and high-field drift velocity show a very little dependence on the electron and hole densities.
- The diffusive transport in intrinsic MoS_2 is strongly dependent on the increase in phonon scattering mediated by temperature.
- Parallelization strategy under Message Passage Interface (MPI) in our sequential MC simulator has been implemented: a heavy computational burden for simulations with a large particle number is relieved by an optimal number of 8 CPUs.

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