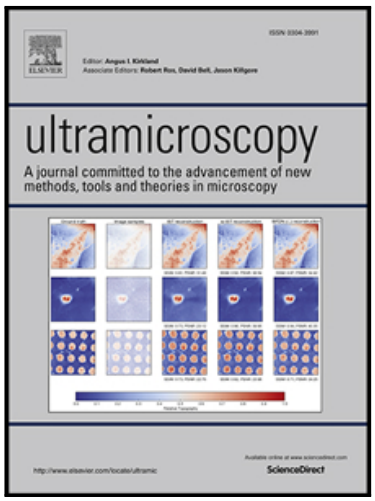

On the Role of the Second-Order Derivative Term in the Calculation of Convergent Beam Diffraction Patterns

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Highlights

- Determined the source of instability in STEM simulations using 2nd-order Schrodinger equation.
- Small amplitude oscillations present in the 2nd-order solution affect numerical efficiency.
- Differences between 1st- and 2nd-order solutions explained using Ewald surface analysis.
- Anti-aliasing of FFTs leads to reduced efficiency of numerical Dormand-Prince 4(5) solver.