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Nuclear quantum effects at metal-insulator transition of (Ga,Mn)As HANNES RAEBIGER, SOUNGMIN BAE, Yokohama National University — $Ga_{1-x}Mn_xAs$ exhibits a Mott transition at the Mn concentration of $x_{\mathrm{crit}} \approx 1\%$. We carry out self-interaction corrected density-functional calculations for this concentration regime, and in the find an insulator ground state I for $x < 0.5\%$, and a metal ground state M for $x > 1\%$. At $x = 0.93\%$, however, I and M appear on a double well adiabatic potential energy curve, being separated only by a small energy barrier. Solving the Schrödinger eq. for nuclear motion along this adiabatic potential shows that, this energy barrier is smaller than the zero-point nuclear oscillations, i.e., the ground state must be described by the non-adiabatic superposition wavefunction $\Phi = c_M(Q;x)\phi^M + c_I(Q;x)\phi^I$, where ϕ^M and ϕ^I are the metallic and insulator states, respectively, and the expansion coefficients depend both on nuclear co-ordinates Q and Mn concentration x. This implies that the Mott transition occurs continuously via a series of *excitonic phases*, as suggested by Kohn,[1] but with the exception that the excitonic phase superposition states (charge density waves) can only be described after inclusion of nuclear quantum effects.

[1]Kohn, Phys. Rev. Lett. **19**, 789 (1968).

Hannes Raebiger
Yokohama National University

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