Quantum stabilization and phase transitions in quantum anharmonic crystals

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A theory of phase transitions in quantum anharmonic crystals is presented based on the use of path integrals. In this theory, phases of thermal equilibrium of the crystal are constructed as probability measures on spaces of continuous paths whereas the crystal itself is an infinite system of interacting anharmonic oscillators attached to the vertices of the d-dimensional simple cubic lattice. Correspondingly, a phase transition is understood as the existence of multiple phases at the same values of the external parameters, such as temperature etc. The relevant model parameters are: particle's mass m; interaction intensity J; rigidity R characterizing the spectrum of the Hamiltonian of a single oscillator. For a harmonic oscillator, R is merely Hook's law constant. Sufficient conditions are obtained and analyzed for the phase transition to occur at some temperature, respectively, not to occur at all temperatures. The latter effect – quantum stabilization, holds if $R > dJ$, which in the harmonic case is just the condition for the crystal to be stable. That is why, R is called effective quantum rigidity. It is shown that, in the case of double-well anharmonic potentials, R can be made as big as one wants by making m small (isotopic effect) or by applying sufficiently large external pressure.