Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Quantum Monte-Carlo simulation of spin-one antiferromagnets with single-ion anisotropy**[1] YASUYUKI KATO, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, KEOLA WIERSCHEM, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371, YUSUKE NISHIDA, Theoretical division, T-2, Los Alamos National Laboratory, CRISTIAN BATISTA, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, PINAKI SENGUPTA, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371 — We study a spin-one Heisenberg model with uniaxial single-ion anisotropy, $D$, and Zeeman coupling to a magnetic field, B, parallel to the symmetry axis. We compute the $(D/J, B/J)$ quantum phase diagram for square and simple cubic lattices by combining analytical and Quantum Monte Carlo approaches, and find a transition between XY-antiferromagnetic and ferronematic phases that spontaneously break the U(1) symmetry of the model. In the language of bosonic gases, this is a transition between a Bose-Einstein condensate (BEC) of single bosons and a BEC of pairs. For the efficient simulation of ferronematic phase, we developed and implemented a new multi-discontinuity algorithm based on the directed-loop algorithm. The ordinary quantum Monte-Carlo methods fall into freezing problems when we apply them to this system at large $D/J$ and finite $B/J \sim 1$. The new method does not suffer from the freezing problems.

[1]This research used resources of the NERSCC (DOE Contract No. DE-AC02-05CH11231). Work at LANL was performed under the auspices of a J. Robert Oppenheimer Fellowship and the U.S. DOE contract No. DE-AC52-06NA25396 through the LDRD program.

Yasuyuki Kato
Theoretical division, T-4 and CNLS, Los Alamos National Laboratory

Date submitted: 09 Nov 2012 Electronic form version 1.4