

Eigenvalues of nanoscale molecular magnets

— ナノスケール分子磁性体のエネルギー固有値 —

Institute of Industrial Science, The University of Tokyo Manabu Machida ¹

準位統計を調べるためには、系の高エネルギーの状態を知る必要がある。ところが、分子磁性体はしばしば直接対角化できないほど大きなハミルトニアンを持つ。分子磁性体の物性を準位統計の観点から研究するための基礎として、 V_{15} と呼ばれる分子磁性体を例にとり、そのエネルギー固有値を求めた。我々は、以前光武らによって開発された数値手法が、分子磁性体の固有値を求める際にも有用であることを確認した。

Recently, nanoscale molecular magnets have been studied intensively. We often need to obtain energy levels of nanomagnets whose Hilbert space are too large to diagonalize directly. Especially, if we are interested in the spectral statistics, we need levels in high energy region. [1]

In this paper, we make use of the arbitrary range anomaly quantum dynamics (ARAQD) devised by Mitsutake, Iitaka, and Okamoto[3] to draw the necessary number of levels in high energy region. We calculate energy levels in a desired range in the spectrum by using the ARAQD and the subspace iteration method (SIM) [2]. We also confirm that our numerical method works by comparing the obtained levels with energy levels obtained by direct diagonalization.

We illustrate the numerical method using nanomagnet V_{15} . [4, 5] Although V_{15} itself has a large Hilbert space ($2^{15} = 32768$), an irreducible space of V_{15} is not too large ($\simeq 5000$).

The Hamiltonian of V_{15} in the magnetic field is given by[6]

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{\langle i,j \rangle} \vec{D}_{ij} \cdot [\vec{S}_i \times \vec{S}_j] - H_S \sum_i S_i^z. \quad (1)$$

We adopt the same values of the parameters in $\mathcal{H}$ as used in Ref. 7.

Let us assume that we want to obtain $k_{\max}$ energy levels in the range $(\mu, \mu + \varepsilon)$. According to Ref. 3, starting from random states $|\Psi_k^{(0)}\rangle$ and $|\Psi_k^{(1)}\rangle$, we obtain approximated states $|\Psi_k^{(n_{\max})}\rangle$ ($k = 1, \dots, k_{\max}$) by the recursion relation

$$|\Psi_k^{(n+1)}\rangle = \left[2 - 4 \frac{(\mathcal{H} - \mu)(\mathcal{H} - \mu - \varepsilon)}{E_C(E_C - \varepsilon)} \right] |\Psi_k^{(n)}\rangle - |\Psi_k^{(n-1)}\rangle. \quad (2)$$

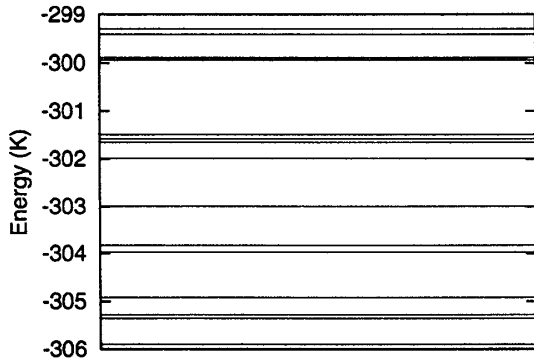
¹E-mail: machida@iis.u-tokyo.ac.jp

Here, the condition $E_C > \max_{\lambda} \left\{ |E_{\lambda} - \mu| \mid E_{\lambda} \text{ are eigenvalues of } \mathcal{H} \right\}$ must be satisfied. Using $\left\{ \left| \Psi_k^{(n_{\max})} \right\rangle \right\}$ for sufficiently large $n_{\max}$, we obtain a $k_{\max} \times k_{\max}$ small Hamiltonian as[2]

$$\tilde{H}_{jk} = \left\langle \Psi_j^{(n_{\max})} \right| \mathcal{H} \left| \Psi_k^{(n_{\max})} \right\rangle. \quad (3)$$

Finally, we obtain $k_{\max}$ energy levels in the energy range $(\mu, \mu + \varepsilon)$ by diagonalizing $\tilde{H}$.

We take the irreducible space which contains 4821 levels.[1] The energy spectrum ranges from $-3649.59(\text{K})$ to $2918.67(\text{K})$. By setting $\mu = -580(\text{K})$, $\varepsilon = 550(\text{K})$, $E_C = 5000(\text{K})$, and $k_{\max} = 512$, we obtain 512 levels. We find that 376 energy levels in the range from $-401.05(\text{K})$ to $-192.23(\text{K})$ are consistent with levels obtained by direct diagonalization up to ten digits. Fig. 1 shows energy levels around $-300(\text{K})$ obtained by the present method. Thus, we confirm the combination of the ARAQD and the SIM is useful to obtain energy levels of huge Hamiltonians in high energy region.



The author would like to thank Dr. T. Iitaka for valuable discussions. The author also would like to thank Prof. S. Miyashita and Prof. N. Hatano. The simulation was partially carried out by using the computational facilities of the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo.

Figure 1: Energy levels of V_{15} obtained by the combination of the ARAQD and SIM.

References

- [1] M. Machida and S. Miyashita, submitted to Physica E.
- [2] F. Chatelin, *Valeurs propres de matrices* (Eigenvalues of matrices) (Masson, Paris, 1988) [in French].
- [3] A. Mitsutake, T. Iitaka, and Y. Okamoto, Comp. Phys. Comm. **96** (1996), 217.
- [4] A. Müller and J. Döring, Angew. Chem. Int. Ed. Engl. **27** (1988), 1721.
- [5] D. Gatteschi, L. Pardi, A. L. Barra, A. Müller, and J. Döring, Nature **354** (1991), 465.
- [6] H. De Raedt, S. Miyashita, K. Michielsen, and M. Machida, Phys. Rev. B **70** (2004) 064401.
- [7] M. Machida, T. Iitaka, and S. Miyashita, submitted to J. Phys. Soc. Jpn. Suppl.