t . T it ati at t a it a t t i .

I t a t t t t i t t a it i a , t a it t i t i i a a a a t i i a . T , t i i t fi t a a t a a a i a a i t a t Q a t A a Ei (QAE). A i i tai , QAE a it i a i i t a iati a i a i ia a a a t a a ti ati it a i i t t t ai t ati (i. ., La a ti i). T a i a ti ati t i t i a a i a t . Ma i t i a t a a t a a a a i t i ia , a t a a a i ati fi a I i ti a t $H(s) = \sum_i h_i s_i + \sum_{i<j} J_{ij} s_i s_j$, t i a ia s_i a t i t a −1,1 . A t ati , t ti a a t t a ati t ai i a ti ati (QUBO) i i t a ia x_i 0,1 , a it , i i $H(x) = \sum_i Q_{ii} x_i + \sum_{i<j} Q_{ij} x_i x_j$.[30] T i t it a tat i a i QUBO a i it t t t at i .

T , t i a a t i a i t t at a a i t i a t t QUBO i i t t at t it tat a ti i i . F i i it , a i t t a i t it t a i i . A a , t i i a i t a QAE t a tia it t i . H , i a i t t a i t (a , a MC- a t i i t) i i ia a i . Si t D-Wa a i a t i ti ti t a at tati ti , MC a i i t a it t a a a i (t i a a a t a i t t t).

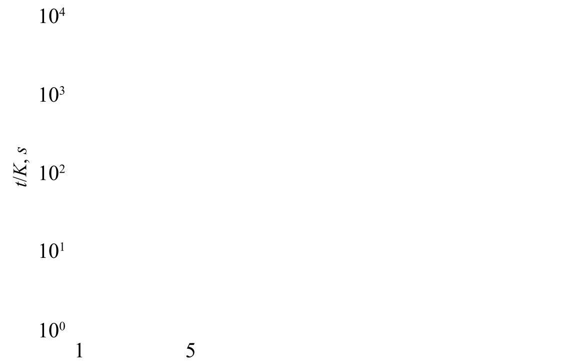
T t i t a i a : Fi t, t ti t t i i i t t i t t it tat a ati a ti i i . S , a a it t t i a i ta t i , O_2 ( ) a O_3 ( ). F t a ati , a ti i t it a i i t fit t t D- a a i . T i , t i t ti i t t ai t i t i a t i t t ti it i i t a t a a a (i. ., D-Wa a i). N i i a i t a it i i t t t t D-Wa a i . I t fi a i i ti , i i i t t a it a .

2. QUANTUM ANNEALER EIGENSOLVER ALGORITHM

2.1. Mapping of a Ground State Problem to a QUBO Problem.

T t i i i t a iati a i i . S a i t t i a tat a - i i a t a it a ti Ψ i a i a t a a i φ_α a a i ffi i t a_α: $\Psi = \sum_{\alpha=}^{B} a_\alpha \varphi_\alpha$

V(r) a a



a t t ta it t -QUBO i 47, i i 3×16 1D, $3^2 \times 6$ 2D, a $3^3 \times 2$ 3D. O t i a K a ta i (Fi 3), a t i t tia i i a it d. T a it t a i ta- ti a ti i tt i Fi 4 a a ti t

i i a it d. A t i it a i a d i fi t tia a i . A ai , t ti a K at d = 1 a K = 4 at d = 2 iat i ifi a t t ai t a a titi i i i t t t . T a a a at a d = 2 t 4 i 0.58 i i t t t ti a i t a 0.48 (B = 3). W d = 5 i i , t i a t 0.72 i i t i t t a i . T t ta it d = 5 i KB^d = 972 t 3888 K = 4 t 16 a B = 3 i t i at t ta fi ati 10^{300} t 10^{1000}. I a , Fi 3 a 4 fi t a i a $O(N_\lambda KB^d)$ t t i a a i a QUBO .

W i t ai t i t a a a t a a (D-Wa a i) a it a t a ti a t t a i a it a ti . F a , O_2 a t a a a it B = 9 a K = 1 t 7, a t ti a a t t_{dw} = 2500 . T i ti t t i a it K, a a a t at t a a a a i i . I t a t, t a i a QUBO ti t a a t t_{cl} = 30 , i i a t 2 a it a t . T ti t a a a t a a i i a i t t a a (Fi S3). I a iti , t a a i t d- i i a a i i at i a t i QUBO a titi i , i a a t a t 10 t 100 i a i t_{dw}.

3.3. Chaining in Quantum Annealer. T t ai t a i a i a a i ati t ai t it a iat a t λ. H , t i a t t ai t a at a t t ti i i a a t a a (D-Wa a i). Na , t ai t ai t a t a iat ai a t . T i a it i t a a t a a a -t -a ti it i i a i t t a it I a t, a it a i i at t (C i a a).[30] F t at , t i a t t a t a t t a a a . I t i a a , a it a a i i t -a ai . Q it it i a ai a t i a i i a it i i t t a t i a it . T a ai i t a a C i a a , a a t t ai t i a a i t t ai a t C. A it a t ai t, t a iat a t i t C it t a , a t t ai a , t a , a t t a a i i iti t t i i a T i t a a t fi a ai a t i t a i , i a i a a t λ a i . Fi 5 t at a a t i t - i i a a i t tat O_2 it a F i a i i B = 7 (m_{a} = 3) a K = 3.

A t , i t i a C t i i i
a ta a , i t ai . F a C
t i : t i a λ, i tai t i ia

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REFERENCES

(1) La , T. D.; J , F.; La a , R.; Na a a, Y.; M , C.; O'B i , J. L. Q a t t . Nature **2010** T a 11

(36) A , E.; Bai, Z.; Bi , C.; B a , S.; D a a, J.; D C , J.; G a A.; Ha a i , S.; M K , A.; S , D. LAPACK Users' guide; Sia 1999; V . 9.
(37) Ga a , I.; T i , A.; Ba i , D. T ati t tat i a t i a t i iat t tati ti a a 2. J. Chem. Phys. 2019, 150, 101104.
(38) T i , A.; Ba i , D. I t a ti t i a i ati a ia ati a j t t i APH i at tati a t i i ati a ti a i a a ti . Chem. Phys. Lett. 2014, 614, 99−103.
(39) T i , A.; Ba i , D. Vi a i ati t tia ti i a i a a a 3D t t i . J. Chem. Educ. 2015, 92, 305−309.
(40) Wa , Y.; L¨, Z.; G , F.; Ha , J.-K. A ti a it a t ai i a a ati ti i ati . International Conference on Integration of Artificial Intelligence (AI) and Operations Research (OR) Techniques in Constraint Programming; 2012; 395−408, DOI: 10.1007/978-3-642-29828-8_26.
(41) A a , T.; Ma ti -Ma , V.; H , I. T at a i a a t a a i ti i . Phys. Rev. Lett. 2017, 119, 110502.
(42) P , W.; F a , B.; T , S.; V tt i , W. Numerical Recipes: The Art of Scientific Computing; Ca i U i it P : Ca i , 1986; 364.
(43) Partitioning Optimization Problems for Hybrid Classical/Quantum Execution; D-Wa S t I .: 14-1006A-A; 2017. tt :// it . / a t / (a J 25, 2019).
(44) qOp toolset 2.5.1; D-Wa S t I .: 2018. tt :// . a . (a J 25, 2019).

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