Accurate Determination of Relativistic Effects in Atoms by Quantum Annealing

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We implement the relativistic version (with the Dirac-Coulomb-Breit Hamiltonian) of the recently proposed quantum-classical hybrid Quantum Annealing Eigensolver (QAE) algorithm and couple it with an improved workflow to accurately predict on D-Wave Advantage hardware the fine structure splittings of isoelectronic highly-charged Boron-like ions. We found that our improved workflow led to better convergence and increased precision with little overhead. We show that our method results in a difference of at most 1.9 percent with respect to experiment.

I. INTRODUCTION

Quantum annealing (QA) has been steadily gaining importance as the most promising alternative to the traditional gate-based quantum computing.¹² The advances made on the hardware front, especially the D-Wave machines, have led to a surge in the number of interesting works in the field.¹³ In particular, there has been recent interest in using QA for the electronic structure problem of atoms and molecules.¹⁴,¹⁵ Xia et al.¹⁶ proposed an approach to convert the electronic structure Hamiltonian to the Ising Hamiltonian, thereby making the computation amenable to D-Wave hardware, and allowing for the computation of ground state energies of atoms and molecules. Another interesting direction is the progress made in the recently proposed Quantum Annealing Eigensolver (QAE) algorithm to the computation of molecular vibrational spectra,¹⁷ ground state,¹⁸ and excited state energies,¹⁹ of atoms and molecules.

Relativistic effects are very important, and play a crucial role in several atomic and molecular phenomena. For example, the color of gold is attributed to relativity.¹⁴ Relativistic calculations of atomic and molecular systems are also necessary ingredients in probing fundamental physics in the field of low-energy non-accelerator particle physics. In spite of this, the treatment of relativistic effects in quantum many-body theoretic calculations has received limited attention in quantum computing,²¹ save for a handful of works using the variational quantum eigensolver algorithm.²²,²³ In this work, we intend to begin addressing this gap by choosing an appropriate property, the purely relativistic fine structure splitting, in the framework of QA. In particular, we work with the QAE algorithm, but extend its scope by including relativistic effects.

The fine structure splitting arises due to the coupling between the orbital angular momentum (L) and the spin angular momentum (S) in an atom. Although the property originates due to relativity, it is influenced by electron correlation.²⁵,²⁶ Thus, to be able to capture correlation effects effectively for obtaining accurate results, not only does one need to employ a suitable quantum algorithm such as QAE, but also aim to go beyond implementing a relativistic version of the algorithm to modify the workflow. To that end, we have incorporated changes keeping in mind practical considerations such as qubit connectivity and noise-prone outputs on the D-Wave Advantage machine, including but not limited to improved optimization of the Lagrange multiplier leading to faster convergence, priority listing of configuration interaction (CI) coefficients on the basis of first order many-body perturbation theory that improves convergence, and tuning chain strengths.

We now briefly comment on choice of systems for our work. Since fine structure splitting is a relativistic property, we choose moderately heavy systems, where relativistic effects are noticeable. However, as mentioned earlier, the fine structure splitting can be affected by correlation effects, and hence we choose the well-studied highly-charged ions from the Boron isoelectronic sequence for which experimental data is available,²⁷,²⁸ since correlation effects decrease in importance as we go to heavier ions in this family.

The organization of this manuscript is as follows: Section I provides the relevant theoretical background to the QAE algorithm with its desired modification in order to compute the fine structure splitting accurately, followed by details of hybrid quantum annealing framework. We compare our results obtained from simulation and D-Wave annealer, with respect to experiment, along with description of problem setting in Section III. We conclude in section IV.

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II. THEORY AND METHODOLOGY

We present our method to perform fine structure splitting calculations on atomic systems using a quantum annealer. While an extension of this method can be applied to estimate the splitting of any spectral line, in this work, we have restricted ourselves to compute the splitting between the $^2P_{1/2}$ state and the $^2P_{3/2}$ state in the Boron Isolelectronic sequence. The first step involves computing the Dirac-Coulomb-Breit Hamiltonians of specific angular momenta ($J=\frac{3}{2}$ and $J=\frac{5}{2}$) through an appropriate program on a traditional computer (GRASP2) [31], as described in section A. Section A also explains the procedure to calculate the fine structure splitting on a classical computer, and whose results we would compare our QAE values with. Then, we compute the energies of the $^2P_{1/2}$ and $^2P_{3/2}$ states using the QAE algorithm with our own hybrid quantum annealing scheme. Finally, taking their difference gives us the fine structure splitting.

A. Calculation of fine structure splitting on traditional computers

The Dirac-Coulomb Hamiltonian is diagonalized using configuration state function (CSF)-based relativistic CI, with the procedure being carried out twice to get the energies for the $^2P_{1/2}$ as well as the $^2P_{3/2}$ states. We then take the difference between the two energies to obtain the fine structure splitting with the Dirac-Coulomb Hamiltonian. Note that the CSFs are built out of single particle orbitals, which are evaluated using an average level calculation (state-averaged calculation) within the multi-configuration Dirac-Fock procedure [25].

The Breit interaction is the leading order relativistic correction to the Coulomb interaction between two electrons. We treat it as a perturbation to the Dirac-Coulomb Hamiltonian, and evaluate the first order shift in energy due to the Breit interaction, once for the $^2P_{1/2}$ state, and then for the $^2P_{3/2}$ state. In each case, the energy correction is added to the energy obtained from diagonalizing the Dirac-Coulomb Hamiltonian.

B. Calculation of fine structure splitting using QAE

The QAE algorithm computes the eigenvalues of a given Hamiltonian by implicitly applying the variational principle, by starting with an energy functional and then minimizing it. The method becomes an iterative procedure if higher excited states are needed, by imposing the orthogonality constraint with the lower states [13]. The energy functional, $\epsilon$, to be minimized is given by

$$\epsilon = \langle \Psi | H | \Psi \rangle - \lambda (\langle \Psi | \Psi \rangle - 1),$$

where $H$ and $|\Psi\rangle$ are the Hamiltonian and the wave function of the system, respectively. $\lambda$ refers to the Lagrange multiplier, with the accompanying term denoting the normalization condition for the wave function. The wave function can be expressed as $|\Psi\rangle = \sum_{\alpha} a_{\alpha} |\Phi_{\alpha}\rangle$, where $a_{\alpha}$ refer to the expansion coefficients corresponding to a basis $\{\Phi_{\alpha}\}$. Upon minimizing the energy functional with respect to the expansion coefficients, we can obtain the ground state energy. It is worth noting that the optimization of the expansion coefficients takes place while treating $\lambda$ as a constant. The optimization of $\lambda$ is done using a classical routine, and is discussed in section III. Upon expressing $|\Psi\rangle$ as a linear combination of an appropriate basis, Eq. (1) becomes

$$\epsilon = \sum_{\alpha,\beta} a_{\alpha} a_{\beta} H_{\alpha\beta} - \lambda \sum_{\alpha} a_{\alpha}^2$$

where $H_{\alpha\beta} = \langle \Phi_{\alpha} | H | \Phi_{\beta} \rangle$. To convert the expression in its quadratic unconstrained binary optimization (QUBO) form in order to make it compliant with the D-Wave hardware, we represent $a_{\alpha}$ in the $i^{th}$ iteration, denoted by $a^{(i)}_{\alpha}$, in binary using $K$ bits through a novel qubit encoding scheme given by

$$a^{(i)}_{\alpha} = m_{\alpha} + s_{\alpha} \sum_{k=0}^{K-1} f_k 2^{-k} q_i^k;$$

where,

$$m_{\alpha} = a^{(i-1)}_{\alpha}$$

$$s_{\alpha} = 2^{-(i+1)/2} \forall \alpha$$

where $f_k = -1$ if $k = 0$ or 1 otherwise, and $q_i$ are binary variables. $m_{\alpha}$ and $s_{\alpha}$ are updated in each iteration; $m_{\alpha}$ for a given iteration is chosen to be the expansion coefficient from the previous iteration, while the second term in Eq (3) serves as the correction to the first, owing to the negative of the iteration number occurring on the exponent. $a_{\alpha}$ are initialized to zeroes.

The mapping scheme discussed above increases the Hamiltonian size from $B \times B$ to $BK \times BK$. The explicit form of the QUBO Hamiltonian after the above conversion is given as

$$F_Q = \sum_{\alpha,\beta=1}^{B} \left( \sum_{n,m=0}^{K-1} f_n Q_{nm}^{\alpha\beta} f_m + C_{\alpha\beta} \right),$$

where

$$Q_{nm}^{\alpha\beta} = (s^2 f_n f_m 2^{-(n+m)} + \delta_{nm} \delta_{\alpha\beta} m_{\alpha}s_{\alpha} 2^{-n+1}) H'_{\alpha\beta},$$

$$C_{\alpha\beta} = m_{\alpha} m_{\beta} H_{\alpha\beta},$$

and

$$H'_{\alpha\beta} = (H_{\alpha\beta} - \lambda \delta_{\alpha\beta}).$$

The first and second term of $Q_{nm}^{\alpha\beta}$ maps to the quadratic biases (couplings), and linear biases of the
FIG. 1. Illustration of our relativistic QAE workflow for the computation of fine structure splitting. The Lagrange multiplier, $\lambda^{(0)}$, is initialized to $\langle \Phi_0 | H | \Phi_0 \rangle$. $\{a_\alpha\}$ denotes the list of expansion coefficients from the CI expansion of the wave function. $E_f$ and $|\Psi_f\rangle$ refer to the final ground-state energy and its corresponding wavefunction obtained using the presented workflow, respectively. Floating Qubit Encoding is abbreviated as FQE in the figure.

qubits, respectively. $C_{\alpha,\beta}$ is a constant addition in the entire QUBO. The matrix $Q$ is symmetric, and so we supply its upper triangle with off-diagonal terms multiplied by two. After providing $F_Q$ to the annealer, we obtain the qubit state configuration that achieves the minimum energy.

C. Workflow improvements

In this subsection, we discuss the strategies that we employed to improve convergence as well as the desired precision in our fine structure splitting results. Towards the end of the subsection, we briefly discuss our results from a hybrid sampler.

When the connectivity of a problem is higher than the number of couplers available per qubit, the embedder creates chains of hardware qubits which map to the same logical qubit, thereby increasing the total number of qubits required. Our simulations revealed that increasing the size of a dense hamiltonian dramatically increases the number of chained qubits employed and degrades the annealer’s ability to obtain optimal solutions. To solve these issues, decomposition strategies divide a QUBO into subproblems to reduce the number of hardware qubits. The subproblem is then solved on the QPU and the result is merged with the original problem’s solution. These methods however, come at the cost that they make the optimization procedure iterative, where each time a small subset of the variables are optimized. To obtain optimal solutions in least iterations, appropriate strategies for partitioning the problem into sub-problems will play a crucial role.

a. Decomposition We implement a physics-inspired method where all qubits associated to a subset of the expansion coefficients are optimized together. This can be thought of as a successive increase of the configuration space, where configurations are added based on their decreasing contribution to the $1^{st}$ order perturbed wavefunction corresponding to the ground state of the system. This assumption doesn’t hold well as $j$ increases or as $\phi_j$ becomes less significant. For the ground state however, the assumption correctly predicts the perturbation order of coefficients which account for 99.99% contribution to the energy.

b. $\lambda$ optimization Figure 2 shows the variation of ground state energy with $\lambda$ by minimizing eq. 1 with numpy. In previous implementations of QAE, the optimal normalization penalty $\lambda_{\text{opt}}$ over an appropriate range of $\lambda$ is found classically by either scanning [11] or through bisection [12]. In this work, we use a new strategy that is motivated from the configuration interaction theory. We know that in eq. 1, the wavefunction normalization condition for $\Psi$ requires $\lambda$ to be equal to the eigenvalues of the Hamiltonian. So we initialize $\lambda$ to the Dirac-Fock energy of the Hamiltonian ($\langle \Phi_0 | H | \Phi_0 \rangle$), and update it to the new energy obtained while solving the QUBO iteratively. When $\lambda$ goes beyond $\lambda_{\text{opt}}$ (producing trivial wavefunction solutions), we switch to the method of bisection.

c. Embedding We focused on optimizing the chain strengths such that chained qubits remain strongly coupled during annealing, but also at the same time do not dominate the QUBO model’s energy. After testing different strategies in simulations, we found that using the RMS of the sub-problem’s quadratic biases times a factor gives the best results.

d. Post-processing Since the normalization condition is not strictly imposed but rather with the addition of a penalty, we use the available extra degree
of freedom to scale the coefficients after every iteration such that their maximum becomes -1. This allows the smaller coefficients to be captured with lesser values of $K$.

The process of updating $\lambda$ and choosing the next sub-configuration space to optimize was integrated together to further decrease the total iterations required for the entire optimization procedure.

Fig. 1 illustrates the code execution, including the hybrid workflow. The initialization step consists of setting all qubits to zero and $\lambda$ to the Dirac-Fock energy, and then generating the QUBO problem and priority list. We then proceed to the hybrid workflow by pre-deciding the number of coefficients ($\Gamma$) to optimise in each iteration. The hybrid scheme then starts out by optimizing the first $\Gamma$ dominant configurations, and then keeps expanding the wavefunction space by adding the next $\Gamma$ lower-order configurations successively. When all $a_\alpha$ are computed, we start again and subsequent iterations optimize $a_\alpha$ further by estimating the correction to it. Implementing the method in code was done in python using D-Wave’s Ocean [32] and hybrid [33] software development kits.

III. RESULTS AND DISCUSSIONS

The number of coefficients to be optimized in an anneal ($\Gamma$) was chosen such that the problem decomposes into as less subproblems as possible, while also ensuring that the results do not suffer too much. The relevant information is provided in table III. For our present encoding, we took $K = 10$.

We employ two different basis for all calculations. The first basis consists of 7 relativistic configurations (RC7) $(1s_{1/2})^2(2s_{1/2})^2(2p_{1/2})^1$, $(1s_{1/2})^2(2s_{1/2})^2(2p_{3/2})^1$, $(1s_{1/2})^2(2p_{1/2})(2p_{3/2})^2$, $(1s_{1/2})^2(2p_{1/2})^2(2p_{3/2})$, and $(1s_{1/2})^2(2p_{3/2})^3$ which are derived from the two most dominant non-relativistic configurations $(1s^22s^22p^3$ and $1s^22p^5)$. The second basis consists of 33 relativistic configurations (RC33) by considering the non-relativistic complete active space. In each basis, the size of $2P_{1/2}$ and $2P_{3/2}$ Hamiltonians are further reduced to configurations with parity consistent with the required state. Thus, the number of configurations for $2P_{1/2}$ and $2P_{3/2}$ states are 2 and 4, respectively in RC7; while in RC33 there are 9 and 16 configurations, respectively.

After the $2P_{1/2}$ and $2P_{3/2}$ states have been computed using QAE, we take the energy difference to compute the splitting, which reported in Table I for Ca$^{15+}$, Fe$^{21+}$, Kr$^{31+}$, and Mo$^{37+}$. Here we use results from GRASP to serve as the reference calculation. The QAE algorithm was executed through simulated annealing and the D-Wave Advantage 5000Q machines available on amazon braket. We point towards two different methods of performing simulated annealing: Hardware independent and Hardware specific calculations. In the former, we directly sample the QUBO obtained from eq. (4), while the latter performs simulations after reducing the all-to-all connectivity of original QUBO to the topology of the D-Wave machines. Hence, the former gives insights on best results possible with any quantum annealer while the latter gives more practical estimates. A comparison between both versions has been reported in table I. Henceforth, simulations in short would refer to results from simulator with Advantage 5000Q hardware specific topology.

The deviation between simulations and hardware for all systems is less than $1.5 \times 10^{-4}$Ha. Meanwhile, the difference between hardware and GRASP are all less than $10^{-3}$ Ha and hence the desired chemical accuracy in literature has been obtained using purely quantum sampling procedures.

We now show that the results can be further improved by using a classical optimization method, specifically, the discrete analogue of gradient descent, called Steepest descent. The motivation comes from the fact that quantum annealers are optimal for searching regions of global
TABLE I. Fine structure splitting for the two choices for the number of configurations, RC7 and RC33, which are explained in Section III. In the Table, ‘relCI’ refers to the results obtained from relativistic configuration interaction (in Ha) method explained in Section IIA, ‘Simulation’ gives our mean relativistic QAE results from a traditional computer (over ten repetitions), but with hardware aspects such as connectivity taken into account, while the column ‘Hardware’ gives the mean QAE results on the D-Wave Advantage machine (over five repetitions). The quantities in parentheses are $\Delta_s = \frac{\text{relCI} - E_{\text{Simulation}}}{\text{relCI}} \times 100$ and $\Delta_h = \frac{\text{relCI} - E_{\text{Hardware}}}{\text{relCI}} \times 100$. ‘Expt’ stands for the experimental value (in Ha).

| System  | relCI | Simulation ($\Delta_s$ %) | Hardware ($\Delta_h$ %) | RelCI | Simulation ($\Delta_s$ %) | Hardware ($\Delta_h$ %) | Expt   |
|---------|-------|---------------------------|------------------------|-------|---------------------------|------------------------|--------|
| Ca$^{15+}$ | 0.166339 (0.19) | 0.166336 (0.19) | 0.1663446 | 0.166336 (0.19) | 0.163446 | 0.163596 (-9.22) | 0.163673 (-13.93) | 0.166831 |
| Fe$^{21+}$ | 0.537410 (0.05) | 0.537413 (0.06) | 0.532338 | 0.537413 (0.05) | 0.532508 (-3.20) | 0.532572 (-4.40) | 0.538863 |
| Kr$^{31+}$ | 2.239037 (0.22) | 2.238988 (0.23) | 2.228510 | 2.238984 (0.23) | 2.228510 (-1.11) | 2.228881 (-1.67) | 2.244283 |
| Mo$^{37+}$ | 4.383275 (0.06) | 4.383249 (0.05) | 4.368093 | 4.383253 (0.05) | 4.368603 (-1.27) | 4.368535 (-1.01) | 4.393963 |

FIG. 4. Energy error wrt relCI at every iteration of the workflow for $^2P_{3/2}$ of B-like Kr (RC33) using (a) D-Wave Advantage6 QPU and (b) D-Wave Advantage6 QPU with Steepest Descent. The solid lines present the results at every iteration, while dotted lines present the error of the global sample.

The best estimate on any expansion coefficient through previous qubit encoding strategies was limited by the number of qubits (K) used to represent it. Increasing K beyond 10 doesn’t improve the results either, because errors due to chaining start dominating, and so capturing coefficients below $10^{-3}$ becomes infeasible with the fixed point encoding scheme proposed originally [12]. With the new representation, we were able to capture the coefficients with the precision of $10^{-5}$, and one can go well beyond it based on their requirements. From Full CI (FCI) theory, we know that $\lambda_{\text{opt}}$ should be equal to $E_{\text{FCI}}$. Since the initial guess of $\lambda$ (the Dirac-Fock energy) is already near $E_{\text{FCI}}$, optimizing it by feeding in the results from previous iterations requires lesser iterations than the previously proposed scanning [11] and bisection [12] methods.

The major source of discrepancy with experiment is the limited number of excited configurations considered in the QAE calculation. The ironic increase in error with configurations is not known, and could be due to inadequate optimization of the relativistic atomic basis.

On the QAE side, the major bottleneck currently is due to the limited connectivity of the D-Wave annealers. Increasing the connectivity would allow lesser chains for embedding larger QUBO problems, improving the quality of results and convergence over iterations. For the present problem using our hybrid workflow, the $P_{16}$ pegasus graph [35]) Advantage6 machines allow...
TABLE II. 16 × 16 B-like Kr Hamiltonian results through Rel. CI calculations from GRASP, exact diagonalization from numpy, all-to-all connected QA simulator, D-Wave Advantage 6.1 structured QA simulator, D-Wave Advantage6 QPU, and hybrid D-wave Advantage6 QPU with Steepest Descent optimizer. ∆% denotes percentage fractional difference with respect to exact diagonalization.

| J    | relCI (Ha) | Exact (Ha) | Ideal Simulation (Δ% × 10^{-9}) | HD Simulation (Δ% × 10^{-5}) | Hardware (Δ% × 10^{-5}) | Hybrid Sampler (Δ% × 10^{-8}) |
|------|------------|------------|----------------------------------|-------------------------------|--------------------------|-------------------------------|
| 1/2  | -1730.364641 -1730.364613 | 5.91       | 0.37                             | 0.53                          | 3.22                     |                                |
| 3/2  | -1728.136131 -1728.136140 | 5.54       | 2.01                             | 2.90                          | 6.38                     |                                |

Basis State Problem sub-Problem Total size size iterations

| Basis | State | Problem size | sub-Problem size | Total iterations |
|-------|-------|--------------|------------------|------------------|
| RC7   | 2P_{1/2} | 20         | 10               | 10               |
|       | 2P_{3/2} | 40         | 10               | 20               |
| RC33  | 4P_{1/2} | 90         | 30               | 30               |
|       | 2P_{3/2} | 160        | 40               | 45               |

TABLE III. Workflow parameters for QAE runs.

IV. CONCLUSIONS

We have developed the relativistic variant of the QAE algorithm to calculate fine structure splittings of Boron-like highly charged atomic ions, \( Ca^{15+} \), \( Fe^{21+} \), \( Kr^{31+} \), and \( Mo^{37+} \). Further, we improved the workflow of the resulting algorithm, including an improved optimization strategy for the Lagrange multiplier occurring in the energy functional, priority listing of the CI coefficients based on considerations from many-body perturbation theory, floating qubit encoding method, and tuning the chain strength. We carried out our relativistic QAE calculations with the above mentioned improvements on both a traditional computer but having accounted for hardware considerations such as connectivity (simulation) as well as on D-Wave device (hardware).

We benchmark our results with relativistic CI calculations carried out on a traditional computer. We carry out two sets of all the above mentioned computations, one with the most dominant configurations for the systems chosen and the second with thirty three configurations. We find that for RC7, our simulation results differ at most by 0.22 percent with respect to the results obtained from relativistic CI, which translates to \( \sim \mu Ha \) precision for the lighter \( Ca^{15+} \) and \( Fe^{21+} \) ions, and \( \sim mHa \) and \( \sim 10 \mu Ha \) precision for \( Kr^{31+} \) and \( Mo^{37+} \).

Our hardware results display the same trend as those from simulation. For the case of RC33, there is an expected slight reduction in precision on account of a much larger system size, but results from both simulation and hardware is well within the desired ‘chemical accuracy’ of \( \sim 1 \) mHa with respect to relativistic CI results. It is important to note that our hardware results from both RC7 and RC33 differ with experiment for all of the considered systems by at most 0.25 percent and 1.7 percent, respectively.

Since the QAE algorithm can be used to perform diagonalization of any electronic structure matrix, the accurate results obtained from this work could serve as a stepping stone to future relativistic atomic and molecular applications, including those that involve probing new physics beyond the Standard Model of elementary particles.
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