Supplementary Material

1 ANALYSIS OF THE QUBO PROBLEM

In this section, we provide an analysis to determine the values of λ_i such that the structure of the original problem can be kept unchanged in the reformulated QUBO problem. Recall that the penalty method yields the augmented QUBO Hamiltonian:

$$H_{\mathrm{QUBO}}(\mathbf{x}) = H^*(\mathbf{x}) + \sum\nolimits_i \lambda_i P_i^2(\mathbf{x}), \quad \lambda_i \in \mathbb{R}, \tag{S1}$$

where $H^* = \sum_{i,j,k} p_k \omega_j x_{ijk}$ and with penalty terms:

$$P_1^2(\mathbf{x}) = (\sum\nolimits_j x_{ijk} - s_{1,ik})^2, \tag{S2}$$

$$P_2^2(\mathbf{x}) = (\sum_{i,j} x_{ijk} - s_{2,k})^2, \tag{S3}$$

$$P_{3,4}^2(\mathbf{x}) = (\sum\nolimits_{j,k=1}^{D_{il}} \omega_j x_{ijk} - \sum\nolimits_{k=1}^{D_{i(l+1)}} c_{ik} - s_{3,4,il} + 0.7)^2, \tag{S4}$$

$$P_5^2(\mathbf{x}) = (\sum\nolimits_{j,k\in[S_{il},D_{il}]} x_{ijk}(1 - x_{ij(k+1)}) - s_{5,il})^2. \tag{S5}$$

Following the method from Lucas (2014), a valid QUBO problem is such that:

$$\forall \mathbf{x}_1 \in \mathbb{C}, \mathbf{x}_2 \notin \mathbb{C} : H_{\mathrm{QUBO}}(\mathbf{x}_1) < H_{\mathrm{QUBO}}(\mathbf{x}_2), \tag{S6}$$

$$\forall \mathbf{x}_1, \mathbf{x}_2 \in \mathbb{C} \text{ and } H^*(\mathbf{x}_1) < H^*(\mathbf{x}_2) : H_{\mathrm{QUBO}}(\mathbf{x}_1) < H_{\mathrm{QUBO}}(\mathbf{x}_2), \tag{S7}$$

with $\mathbb{C}$ the set of all viable solutions $\mathbf{x}$. Besides, the penalty function P has the following property:

$$\forall i, \forall \mathbf{x} \in \mathbb{C} : P_i(\mathbf{x}) = 0; \ \forall \mathbf{x}' \notin \mathbb{C}, P_i(\mathbf{x}') \neq 0. \tag{S8}$$

Let $P_{i,min} := \min P_i(\mathbf{x}')$ denote the minimum value of the penalty P_i for a non-feasible $\mathbf{x}'$, and $\Delta H := \max H^* - \min H^*$. In order to satisfy condition (S6), we require $\forall i : \min_{\mathbf{x}'\notin\mathbb{C}} H^*(\mathbf{x}') + \lambda_i P_i^2(\mathbf{x}) > \max_{\mathbf{x}\in\mathbb{C}} H^*(\mathbf{x})' + \lambda_i P_i^2(\mathbf{x})$, i.e.

$$\forall i : \quad \Delta H < \lambda_i P_{i,min}^2, \tag{S9}$$

which yields

$$\max p \times \max \omega \times L_{\mathrm{time}} \times N_{\mathrm{pile}} \times N_{\mathrm{bus}} < \lambda_i P_{i,min}^2, \tag{S10}$$

where the left hand side is an upper bound of ΔH. However we can prove that we can only have P_{min} when 1 bus breaks the constraint on 1 pile. Then we can remove the term $N_{\mathrm{bus}} \times N_{\mathrm{pile}}$ out of the left terms, so the inequality (S9) does not scale with the problem size. Continuing it is easy to see that $P_{1,min} = P_{2,min} = 1$, thus:

$$\lambda_{1,2} > \max p \times \max \omega \times L_{\text{time}}. \tag{S11}$$

Note that the choice of units for the electricity price p and power ω is arbitrary. In our unit settings, we have $\lambda_{1,2} > 10$.

Penalty $P_{3,4}$ from (S4) contains continuous variables $s_{3,4,il}$. Hence, the minimum value of $P_{3,4}$ is arbitrarily small: $P_{3,4,min} = \xi$, where $\xi \to 0$. This implies:

$$\lambda_{3,4} > \frac{\max p \times \max \omega \times L_{\text{time}}}{\xi^2} \longrightarrow \infty. \tag{S12}$$

To handle this problem, we modify $P_{3,4}$ with an additional variable ε. Recall that $P_{3,4}$ is used to control the state of charge (SOC) of the bus between 0.3 and 1, and in the penalty method, we write these constraints with slack variable $s_{3,4,il} \in [0, 0.7 - \sum_{k=D_{il}}^{S_{i(l+1)}} c_{ik}]$. Modifying $P_{3,4}$ to control the SOC between $0.3 + \varepsilon$ and $1 - \varepsilon$ brings $P^2_{3,4,min} = \varepsilon^2$, from which follows the modified lower bound $\lambda'_{3,4}$:

$$\lambda'_{3,4} > \frac{\max p \times \max \omega \times L_{\text{time}}}{\varepsilon^2}. \tag{S13}$$

Similarly to $\lambda_{1,2}$ the lower bound depends on the arbitrary unit setting and choice of ε. Here, we set $\varepsilon = 0.1$, and $\lambda'_{3,4} > 1000$. Observe that controlling SOC $\in [0.3 + \varepsilon, 1 - \varepsilon]$ produces a new, reduced, viable solution space which may not include the original optimal solution. However, as long as ε remains small, this modification should have little practical impact. On the other hand, another approach consists in discretizing the consumption c_{ik}; the effect is similar to introducing ε.

Next, we discuss condition (S7). To do so, let us first revisit the binary encoding of continuous variables and the discretization error. For a continuous variable c, when using N bits, the discretization error e is $e = \frac{1}{2} \times \left(\frac{1}{2^N-1}\right) \approx \frac{1}{2^{N+1}}$. Let δH denote the minimal gap of the objective function between two valid solutions, Then condition (S7) can be satisfied by having:

$$\delta H > \lambda_i e^2, \tag{S14}$$

which gives $\lambda_{3,4} < \frac{\min \delta p \times \omega}{2^{-2N-2}}$, and does not apply to $\lambda_{1,2}$, where $\min \delta p$ is the minimal price difference between any two given times during the day (including the difference between lowest price and 0). In practice, when using $N = 8$ bit to encode the continuous variables, the upper bound is approximately 10^4.

Finally, observe that penalty P_5 (S5) is a polynomial of order 4, and is not discussed here. Mandal et al. (2020) suggest some methods to reformulate high-order terms in quadratic form. However, P_5 is to guarantee that a bus does not switch from one pile to another during one charging window, which might be neglected whenever L_{time} is small enough, i.e. each time step is long enough. Consequently, we choose first to discard this constraint in the penalty method and discuss it again in Section 4, where we break the limitation of the penalty method.

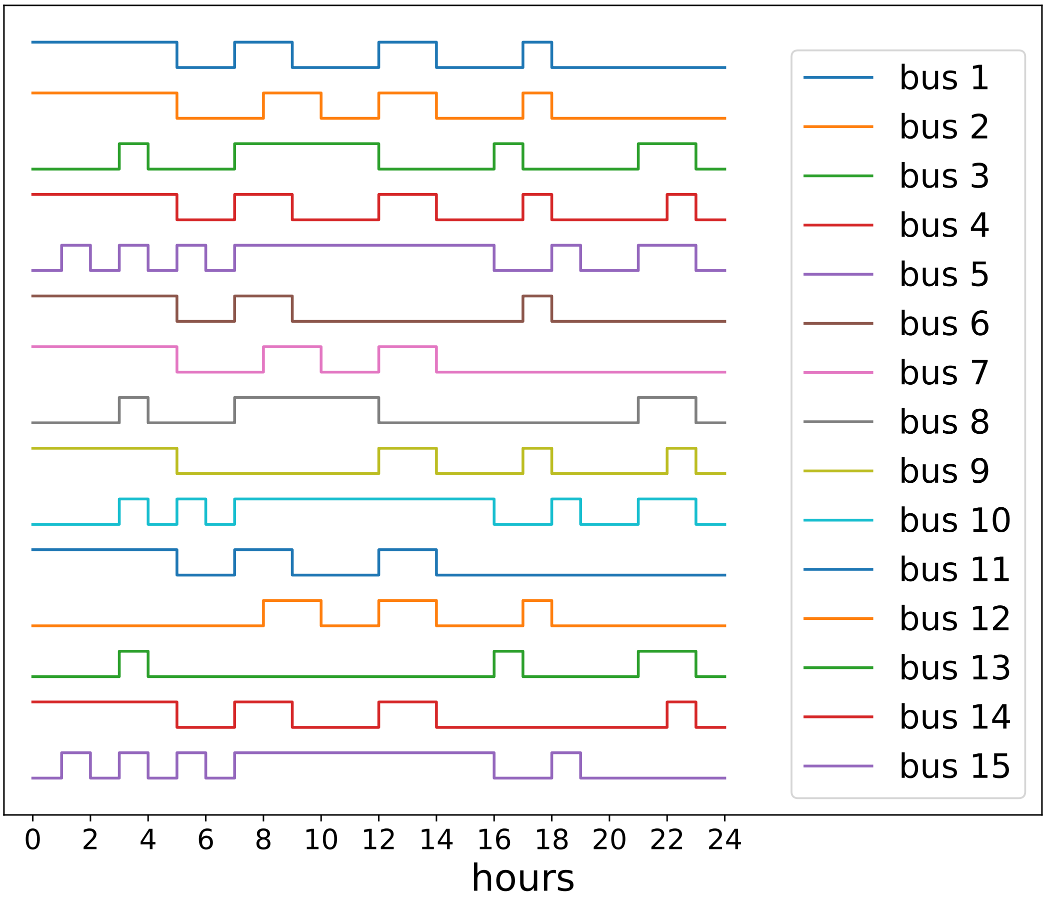

Figure S1. 15 Typical bus schedules used for random problem generation. Bump in the curve indicate when the bus is in the station and available for charging.

2 MORE EXPERIMENTAL RESULTS

2.1 Problem Generation

Figure S1 displays the 15 typical bus schedules which are used to generate different charging scheduling problems in Section 4. For each problem, we first randomly pick N_{bus} schedules. The power ratings of N_{pile} charging piles are also randomly generated, while kept in a reasonable interval so that there will be at least one possible solution.

2.2 Solving different problems with the quantum annealing sampler

Besides the results shown in Figure 2, Figure S2 displays more experiments with problems of different scales, from $N_{\text{bus}} = 1, N_{\text{pile}} = 1, L_{\text{time}} = 24$ to $N_{\text{bus}} = 2, N_{\text{pile}} = 1, L_{\text{time}} = 48$, under different penalty coefficients and different chain strengths. Similar behaviours are observed for all cases, where the optimal combinations for two parameters are found near the diagonal line. It is also observed that the ratio between the optimal penalty coefficient and the chain strength tends to grow larger as the problem size increases.

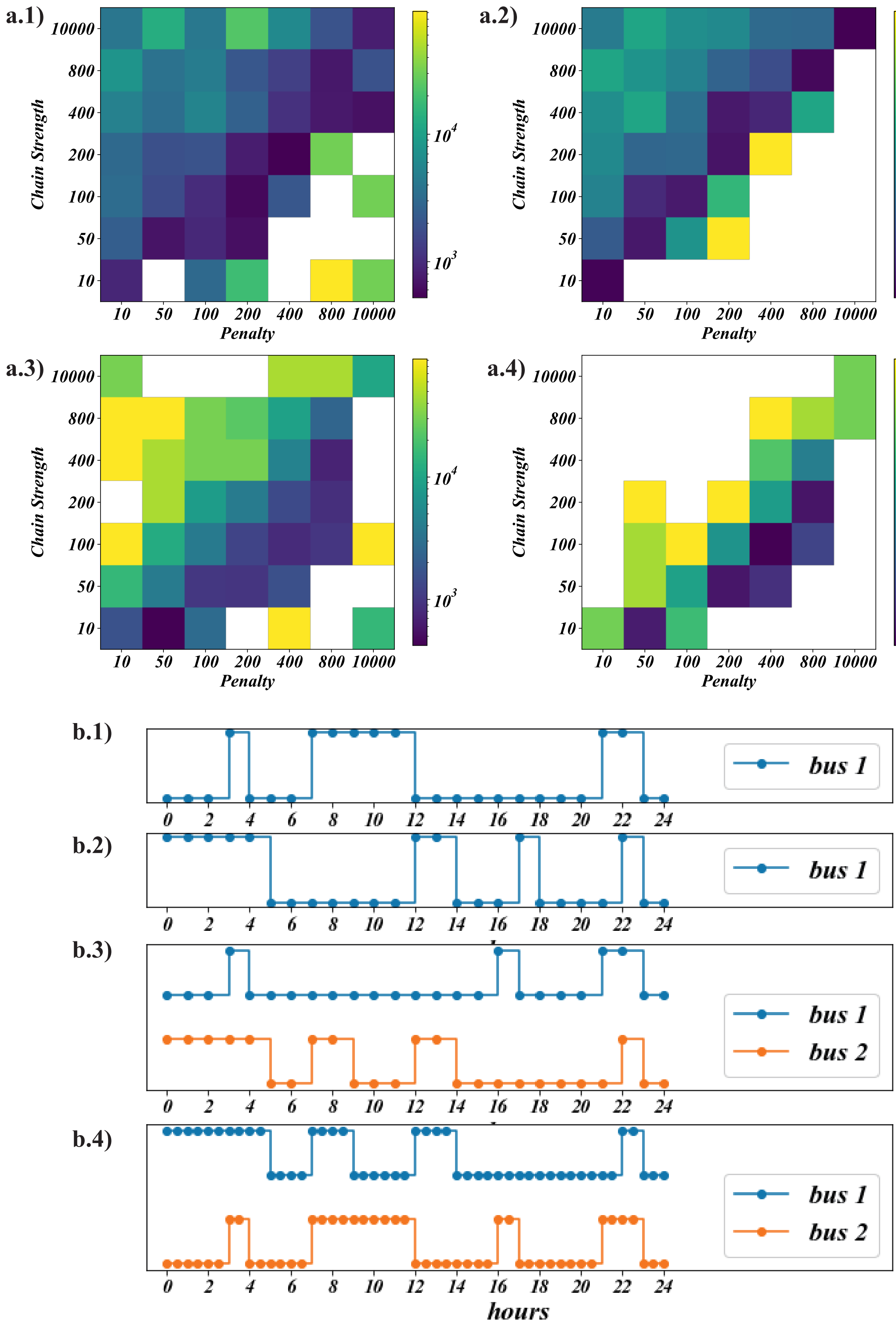

Figure S2. (a.1-4) Time to $99\%-$success in μs under different annealing parameters P, $J_{\mathrm{chain\_strength}}$ of quantum annealing, estimated from 1000 experiments for models visualized in (b.1-4), with 1 indicating that the bus is in the station and 0 otherwise. Note that in (a.4), the success is defined by obtaining a solution with cost not greater than 1.3 times the exact solution provided by Cplex solver, which differs from (a.1-3), where the success is defined by obtaining exactly the optimal solution.

2.3 Supplementary results for the Hubbard-Stratonovich transformation approach

Figure S3 shows the evolution of both the multipliers and the penalties when applying the iterative approach discussed in Section 3 and experimented in Section 4, for the same run as the one in Figure 3 (a-b). These plots illustrate the advantage of using adaptive gradient: taking P_{01}, ν_{01} as an example, there are only three times among 96 iterations when P_{01} is non-zero. However, with adaptive gradient, the multiplier ν_{01} does reach its optimal value, which is around 10. Suppose we were using a fixed learning rate to update ν, it would take much more iterations to find the same optimal value.

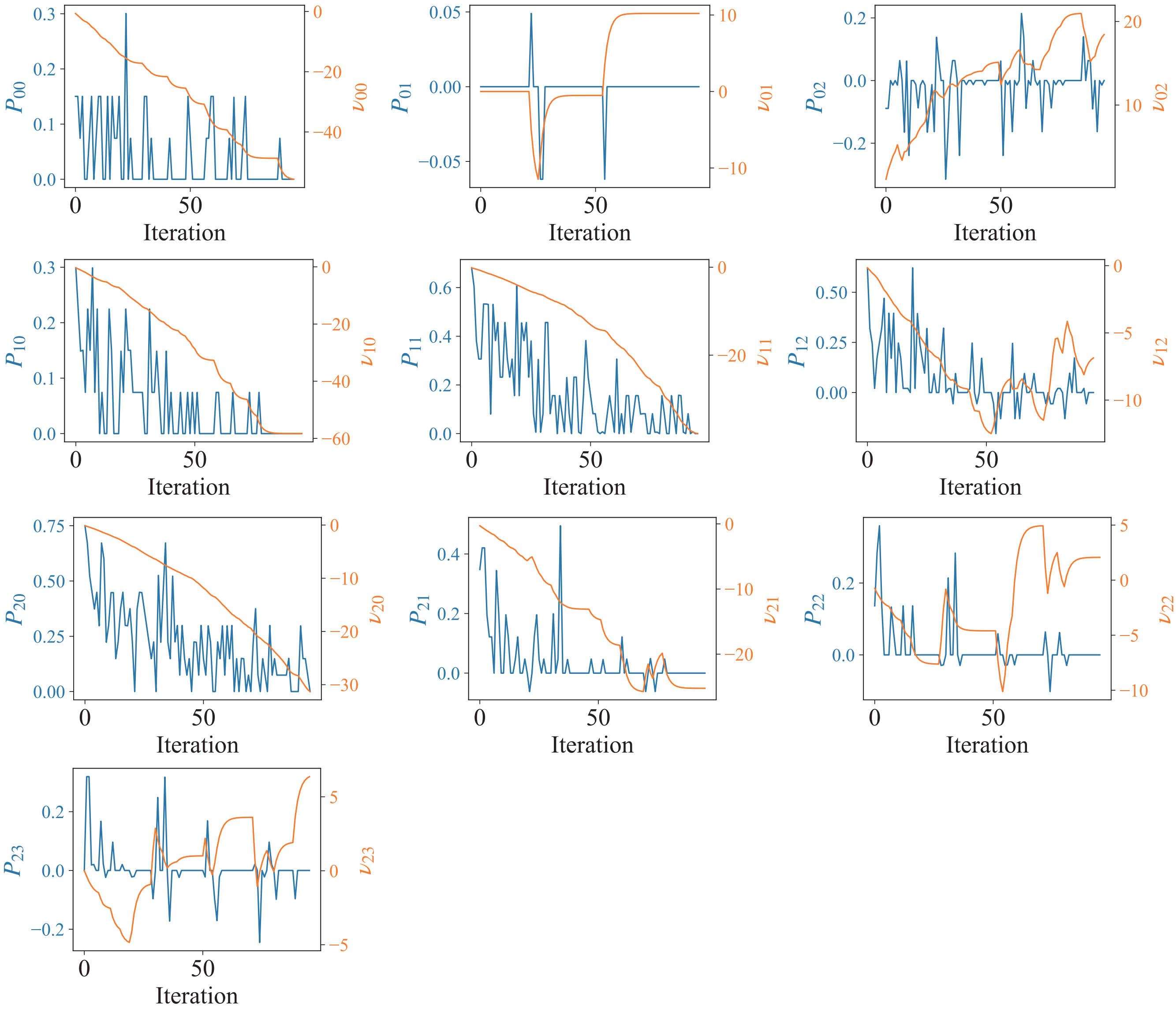

Figure S3. Multipliers ν and penalties P over iterations with the Hubbard-Stratonovich transformation.

REFERENCES

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Mandal A, Roy A, Upadhyay S, Ushijima-Mwesigwa H. Compressed quadratization of higher order binary optimization problems. *Proceedings of the 17th ACM International Conference on Computing Frontiers* (2020), 126–131. doi:url10.1145/3387902.3392627.