Calculation of ground state energy of a “4 × 4” flux qubit Josephson junction array using diffusion quantum Monte Carlo Method

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Under the right parametric conditions a Josephson Junction (JJ) can act as a qubit as it reduces to a two-state quantum system, which is the very basic required feature for any system to act as a qubit. In this paper we shall investigate the ground state energy of a new Josephson junction array (JJA) design, dubbed “4 × 4” flux qubit, using Diffusion Monte Carlo (DMC) method. Technical details of the DMC calculation of the ground state energy shall be presented. The ground state energy calculated with the DMC code is shown to be consistent with known results calculated using Lanczos method by other authors for similar JJA with a smaller d.o.f.
- Superconducting Quantum Interference Device as qubit - a two-state quantum system
- A feasible qubit - addressed, controlled, measured, coupled to its neighbors, and decoupled from the environment.
The qubit consists of a micrometer-sized loop with three or four Josephson junctions.

The energy eigenstates are linear combinations of clockwise and counterclockwise persistent-current states.

Qubit Hamiltonian:

\[ \mathcal{H}_q = -\frac{1}{2}(\epsilon \sigma_z + \Delta \sigma_x) \]

- \( \epsilon \) - Magnetic energy bias
- Energy gap \( \Delta \) - coupling constant controlling the mixing between the two persistent current state - tunable via \( f_\epsilon \), the magnetic flux threading the closed loop.
- \( \Delta \ll \epsilon \) - maximal mixing; \( \Delta \gg \epsilon \) - total decoupling between
The main aim of this work is to calculate the gap between the lowest two energy levels of a “4 × 4” Josephson Junction Array (JJA). We wish to see how the size of the gap can be externally controlled to open or close up. The code shall provide a theoretical guidance to engineer a multi-qubit system on a single JJA. Method used: Diffusion Quantum Monte Carlo method.
Example of two-level energy system (Figure adopted from Martijn and Thijssen, Master thesis (2009), TU Delft, The Netherlands, unpublished

**Figure 5.6:** Ground state calculated with DMC (bottom line) superimposed on the results from Lanczos (top three lines) with $N_{\text{max}} = 8$. Params for the DMC arc: $N_{\text{walkers}} = 8000$, $N_{\text{iters}} = 800$, $\alpha = 0.3$ and $\tau = 0.002$
Originally proposed by J. E. Mooij, from TU Delft.
Martijn and Thijssen (Master thesis (2009), TU Delft, The Netherlands, unpublished) attempted to calculate the energy spectrum (ground state and first few excited states) of the $4 \times 4$ JJA.
This work is a follow-up of their numerical work.
Consider a JJA comprised of uncoupled $N_0$ Josephson junctions.

Each JJ is characterised by the Josephson energy $E_{J_i}$ and charging energy $E_{C_{J_i}} = e^2/2C_{J_i}$.

Phase difference across the JJ is $\Delta \phi_{J_i} = \phi_j - \phi_k$.

The Lagrangian of an uncoupled JJ (indexed by $J_i$)

$$\mathcal{L}_{J_i}(\Delta \phi_{J_i}, \Delta \dot{\phi}_{J_i}) = T_{J_i}(\Delta \dot{\phi}_{J_i}) - V_{J_i}(\Delta \phi_{J_i}),$$

where

$$T_{J_i}(\Delta \dot{\phi}_{J_i}) \equiv \frac{1}{2} m_{J_i}(\Delta \dot{\phi}_{J_i})^2, \quad V_{J_i}(\Delta \phi_{J_i}) \equiv E_{J_i}(1 - \cos \Delta \phi_{J_i}),$$

$$m_{J_i} \equiv C_{J_i} \left(\frac{\Phi_0}{2\pi}\right)^2.$$
Lagrangian of \( N_0 \) independent JJ

\[
\mathcal{L}_{N_0} = \sum_{J_i=1}^{N_0} \frac{1}{2} m_{J_i} (\Delta \dot{\phi}_{J_i})^2 - E_{J_i} (1 - \cos \Delta \phi_{J_i})
\]
\[
\equiv T - V. \tag{1}
\]

Kinetic energy equivalent made up of the charging energy of the JJA:

\[
T \equiv \sum_{J_i=1}^{J_i=N_0} \frac{1}{2} C_{J_i} V_{J_i}^2 = \sum_{J_i=1}^{J_i=N_0} \frac{1}{2} m_{J_i} (\dot{\phi}_j - \dot{\phi}_k)^2.
\]

Potential energy equivalent is

\[
V = \sum_{J_i=1}^{J_i=N_0} E_{J_i} (1 - \cos(\Delta \phi_{J_i}))
\]
Constraints on the phases and effective degrees of freedom (d.o.f)

- $N_0 = 24$ in the $4 \times 4$ JJA, but not all d.o.f. $\phi_i$ are independent.
- Flux quantisation in a closed loop causes couplings among the phases, rendering the effective number of d.o.f of the system to reduce to $N = 9$ (i.e., 9 independent phases $\phi_i$)

$$\left( \sum_{Ji} \Delta \phi_{Ji} \right) + 2\pi f = 0,$$

- $f$ net magnetic frustration threading the loops, a variable experimentally controllable.
The Lagrangian

In the presence of the boundary conditions from quantisation of magnetic flux, the “net” Lagrangian is

\[ \mathcal{L}(\phi, \dot{\phi}) = T(\dot{\phi}) - V(\phi), \]

- Total charging energy taking the form

\[ T(\dot{\phi}) = \frac{1}{2} \phi^T \mathbf{M} \dot{\phi}. \]

- \( \phi \) a dimension-\( N \) vector containing all independent phases \( \phi_i \).
- The “mass matrix” \( \mathbf{M} \) and \( V(\phi) \) determine the dynamics of the JJA.
The Hamiltonian can be obtained via Legendre transformation of $\mathcal{L}$

$$\mathcal{H} = \sum_i \dot{\phi}_i \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} - \mathcal{L}$$

The conjugate momentum is

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} = m_{ij} \dot{\phi}_j \Rightarrow p = M \dot{\phi}.$$ 

$$\mathcal{H}(p, \phi) = p^T \dot{\phi} - \mathcal{L} = \frac{1}{2} p^T M^{-1} p + V(\phi)$$

- $p = \{p_1, p_2, \cdots, p_N\}; \phi = \{\phi_1, \phi_2, \cdots, \phi_N\}$ are the d.o.f. of the Hamiltonian.
- $[p_i, \phi_j] = i\hbar \delta_{ij}$
How the mass matrix and potential energy were derived

The explicit expressions of $M$ and $V(\phi)$ can be determined by a two major factors:

1. How the JJs are coupled (via the geometrical design of the JJA)
2. How the magnetic frustration is distributed among the JJs, subjected to the constraints of magnetic quantisation condition.

Entries in $M$ are made up of the charging energies of each JJ, which are expressed in terms of “capacitances” $C_{J_i}$, $J_i \in \{1, 2, 3, \cdots, N\}$.

$V(\phi)$ determined by how the magnetic frustration is distributed among the loops in the JJA, and on $E_{J_i}$. 
Mass matrix for a JJA with 6 d.o.f, 3 by 4 squares

Assume:
- $C$ and $E_J$ for all JJ except the one right at the middle of the JJA, which is $q$ times larger. Let $m = C \left( \frac{\Phi_0}{2\pi} \right)^2$ (the “mass”)
- Threaded by external frustrations $\Delta_1$ and $\Delta_2$.

\[
M = m \begin{pmatrix}
4 & -1 & 0 & -1 & 0 & 0 \\
-1 & 3 + q & -1 & 0 & -q & 0 \\
0 & -1 & 4 & 0 & 0 & -1 \\
-1 & 0 & 0 & 4 & -1 & 0 \\
0 & -q & 0 & -1 & 3 + q & -1 \\
0 & 0 & -1 & 0 & -1 & 4
\end{pmatrix}
\]
Potential Energy for a JJA with 6 d.o.f

\[ V(\phi_1, \phi_2, \cdots, \phi_6)/E_J = 16 + q - \cos(\phi_1 - \frac{\pi}{7} + \Delta_2) - \cos(\phi_1 + \frac{\pi}{7}) - \cos(\phi_4 - \phi_1 + \Delta_2) \]
\[ - \cos(\phi_4 + \frac{2\pi}{7}) - \cos(\phi_4 + \frac{4\pi}{7} - \Delta_2) - \cos(\phi_2 - \phi_1) \]
\[ - \cos(\phi_2 - \frac{2\pi}{7} + \Delta_1) - \cos(\phi_3 - \frac{3\pi}{7} + \Delta_2) - \cos(\phi_6 + \frac{6\pi}{7} - \Delta_2) \]
\[ - \cos(\phi_3 - \frac{5\pi}{7}) - \cos(\phi_6 + \phi_3 + \Delta_2) - \cos(\phi_3 + \phi_2) \]
\[ - \cos(\phi_5 - \phi_4) - q \cos(\phi_5 - \phi_2 + \Delta_1) - \cos(\phi_6 - \frac{6\pi}{7}) \]
\[ - \cos(\phi_6 - \phi_5) - \cos(\phi_5 + \frac{5\pi}{7} - \Delta_1). \]

(2)

The 6 d.o.f case was first calculated by Martijn using Lanczos algorithm for the first few excited states (M.Sc. thesis, 2009, TU Delft, unpublished).
What we want to know?

Given the knowledge of $\mathbf{M}$ and $V(\phi)$, we wish to calculate the ground state energy as a function of $E_C$, $E_J$, and the external magnetic flux $f$.

- We want to know the GS energy (the first eigen value).
- We also wish to calculate the next few excited energy levels, but it can only be done using Excited State QMC.
- In the present work only the DQMC result on the GS is to be discussed. The excited state result will be presented elsewhere soon.
The strategic method of choice to abstract solutions from a multi-dimensional quantum Hamiltonian.

Based on Green’s function for the imaginary-time Schrödinger equation

Lanczos method is only suitable for low dimensional Hamiltonian.

For details of the method, see J. M. Thijjsen, Computational Physics, 2nd edition, Cambridge University Press.
DMC algorithm for a Hamiltonian with a unit mass matrix

Put the walkers at random positions in configurational space;
REPEAT
  FOR all walkers DO
    Select a walker at random;
    Shift that walker from its position $R$ to a new position $R'$
    according to the Gaussian transition probability with a variance
    1 according to $\phi_i(t + \Delta t) = \phi_i(t) + \eta\sqrt{\Delta t}$, where
    $P(\eta) = \frac{1}{\sqrt{4\pi\eta}}e^{-\eta^2/4\gamma}$
    Evaluate $q = \exp(-\Delta\tau[V(R') - E_T])$
    Eliminate the walker or create new ones at $R'$,
    depending on $s = q + r$, where $r$ is random, uniform between
    0 and 1;
  END FOR;
  Update $E_T$ according to
  $E_T = E_0 + \alpha \ln\left(\tilde{N}/N\right)$
Transforming $\mathbf{M}$ into a diagonal form

- DMC described in previous slide works in the basis where the mass matrix is a unit matrix.
- In general, the mass matrix $\mathbf{M}$ is non-diagonal, real, symmetric, and has non-zero eigenvalues.
- It needs to be transformed into a diagonal form via unitary diagonalisation:

$$\mathbf{U}^T \mathbf{M} \mathbf{U} = \mathbf{D} = (\mathbf{D}^{\frac{1}{2}})^2$$

- The conjugate momenta and phases transform according to

$$\mathbf{p} \rightarrow \mathbf{p}' = \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T \mathbf{p}$$

$$\phi \rightarrow \phi' = \mathbf{D}^{\frac{1}{2}} \mathbf{U}^T \phi$$
In the basis \( \{p', \phi'\} \), the Hamiltonian now looks

\[
H(p', \phi') = \sum_{i}^{N} -\frac{1}{2} \frac{\partial^2}{\partial \phi'^2_i} + V'(\phi')
\]

- \( p'_i = i \frac{\partial}{\partial \phi'_i} \)
- The information of the entries in the original mass matrix has now been absorbed into the potential energy via the transformed d.o.f as in

\[
p \rightarrow p' = D^{-\frac{1}{2}} U^T p
\]

\[
\phi \rightarrow \phi' = D^{\frac{1}{2}} U^T \phi
\]
Referring to the mass matrix and potential energy of the $3 \times 4$ JJA, the ground state energy (GS) is a function of the magnetic frustration $\Delta_2, \Delta_1$, and $q$. $\Delta_2$ is not independent from $\Delta_1$, and we relate them via the parameter $\alpha_J$, defined via $\Delta_2 = \alpha_J \Delta_1$.

We compare the GS calculated using Lanczos method (code provided by J.M. Thijjsen with our DMC code) to find that the agreement is excellent.
Comparison between DMC and Lanczos results

Table: GS energy for the JJA with 6 d.o.f \((\Delta_2 = \Delta_1 \cdot \alpha_J)\)

<table>
<thead>
<tr>
<th>No.</th>
<th>(\Delta_1/(2\pi))</th>
<th>(\alpha_J)</th>
<th>(q)</th>
<th>GS Energy by DMC</th>
<th>GS Energy by Lanczos</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>0.2</td>
<td>1.3</td>
<td>9.12304</td>
<td>9.12690</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
<td>0.2</td>
<td>1.5</td>
<td>9.13582</td>
<td>9.13440</td>
</tr>
<tr>
<td>3</td>
<td>-0.5</td>
<td>0.2</td>
<td>5.0</td>
<td>9.18559</td>
<td>9.18613</td>
</tr>
<tr>
<td>4</td>
<td>10.5</td>
<td>0.2</td>
<td>5.0</td>
<td>9.18109</td>
<td>9.18613</td>
</tr>
<tr>
<td>5</td>
<td>10.5</td>
<td>0.9</td>
<td>5.0</td>
<td>7.86102</td>
<td>7.86450</td>
</tr>
</tbody>
</table>
• The 4 by 4 JJA has 9 d.o.f.
• Lanczos method scale badly with computational cost.
• Lanczos can still handle 6 d.o.f but not 9 d.o.f
• Hence it must be solved using DMC.
Design of the 4 by 4 JJA

Assume the charging and Josephson energies of the four JJs about the center of the JJA obey the relation:

\[ C_{21} = C_{22} = C_{23} = C_{24} = qC \]

\[ EJ21 = EJ22 = EJ23 = EJ24 = qE_J \]
Mass Matrix for the 4 by 4 JJA

\[ \mathbf{M} = m \begin{pmatrix}
4 & -1 & 0 & -1 & 0 & 0 \\
-1 & 3 + q & -1 & 0 & -q & 0 \\
0 & -1 & 4 & 0 & 0 & -1 \\
-1 & 0 & 0 & 4 & -1 & 0 \\
0 & -q & 0 & -1 & 3 + q & -1 \\
0 & 0 & -1 & 0 & -1 & 4
\end{pmatrix}. \]
Potential Energy for the 4 by 4 JJA

\[ V(\phi_1, \phi_2, \cdots, \phi_9) = 20 + 4q \]

\[ - \cos(\phi_1 - \frac{\pi}{8} + \Delta_2) - \cos(\phi_1 + \frac{\pi}{8} - \Delta_4) - \cos(\phi_2 - \frac{\pi}{4} + \Delta_1) \]

\[ - \cos(\phi_3 - 3\frac{\pi}{8} + \Delta_2) - \cos(\phi_3 - 5\frac{\pi}{8} + \Delta_4) - \cos(\phi_4 + \frac{\pi}{4} - \Delta_3) \]

\[ - \cos(\phi_6 - 3\frac{\pi}{4} + \Delta_3) - \cos(\phi_7 + 3\frac{\pi}{8} - \Delta_4) - \cos(\phi_7 - \Delta_2 + 5\frac{\pi}{8}) \]

\[ - \cos(\phi_8 + 3\frac{\pi}{4} - \Delta_1) - \cos(\phi_9 + 7\frac{\pi}{8} - \Delta_2) - \cos(\phi_9 - 7\frac{\pi}{8} + \Delta_4) \]

\[ - \cos(\phi_1 - \phi_2 + \Delta_4) - \cos(\phi_9 - \phi_8 - \Delta_4) - \cos(\phi_1 - \phi_4 - \Delta_2) \]

\[ - \cos(\phi_9 - \phi_6 + \Delta_2) - \cos(\phi_3 - \phi_2 - \Delta_4) - \cos(\phi_3 \phi_6 - \Delta_2) - \cos(\phi_7 - \phi_4 + \Delta_2) - \cos(\phi_7 - \phi_8 + \Delta_4) \]

\[ - q[\cos(\phi_5 - \phi_4 - \Delta_3) + \cos(\phi_5 - \phi_6 + \Delta_3)] \]

\[ - q[\cos(\phi_5 - \phi_2 + \Delta_1) + \cos(\phi_5 - \phi_8 - \Delta_1)] \]
The 4 by 4 JJA admits four magnetic frustration \(\Delta_1, \Delta_2, \Delta_3, \Delta_4\) which are not all independent, and a parameter \(q\).

\[
\Delta_2 = \Delta_1 \cdot \alpha_J \\
\Delta_4 = \Delta_3 \cdot \alpha_J
\]

We will take \(q, \Delta_1, \Delta_3\) and \(\alpha_J\) as independent parameters.

We will fix \(q, \Delta_3, \alpha_J\) and find \(E(\text{GS})\) as a function of \(\Delta_1\) so that we can tell how the GS energy is controlled by changing the external magnetic field \(\Delta_1\).
**Table:** Examples of GS energies at selected parameters

<table>
<thead>
<tr>
<th>$D_3$</th>
<th>$H_2 P$</th>
<th>$L$</th>
<th>$E_{HGS}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>1.0</td>
<td>1.5</td>
<td>9.0</td>
</tr>
<tr>
<td>9.0</td>
<td>9.5</td>
<td>10.0</td>
<td>10.5</td>
</tr>
</tbody>
</table>

$\alpha_J = 0.2, m = 10, q = 0.8, \Delta_3/(2\pi) = 0.62$

$\alpha_J = 0.2, m = 10, q = 0.5, \Delta_3/(2\pi) = 0.5$
GS as a function of frustration $\Delta_3$ for the 4 by 4 JJA calculated using DMC (cont.)

**Table:** Examples of GS energies at selected parameters

\[
\begin{array}{cccc}
D1 & H2pL & 2 & 4 & 6 & 8 & 10 \\
\hline
0.5 & 1.0 & 1.5
\end{array}
\]

\[
\begin{array}{cccc}
E(H) & GS & L & aJ = 0.2, m = 10., q = 0.5, D3 \rightarrow H2pL = 5. \\
\hline
0.5 & 1.0 & 1.5
\end{array}
\]

\[
\begin{array}{cccc}
E(GS) & 0.5 & 1.0 & 1.5 \\
\hline
0.5 & 1.0 & 1.5
\end{array}
\]

\[
\alpha_J = 0.2, m = 10., q = 0.5, \Delta_3/(2\pi) = 5.
\]

\[
\alpha_J = 0.2, m = 10., q = 0.2, \Delta_3/(2\pi) = 0.2
\]
JJA with external voltage bias

Experimentally, it is easier to control the GS profile using voltage bias coupled capacitively to the island at the center of a JJA than using magnetic frustration.
Modification to kinetic energy part of the Hamiltonian by external voltage bias

- $\gamma'$ the superconducting island with absolute phase $\phi_{\gamma'}$, biased by $V_g$ capacitively coupled controlled gate voltage via a gate capacitor $C_g = \gamma C$.

- 

$$T(\dot{\phi}) = \frac{1}{2} \dot{\phi}^T M \dot{\phi} + \frac{1}{2} \left( \dot{\phi}_{\gamma'} m_g \dot{\phi}_{\gamma'} \right) - \left( \frac{\Phi_0}{2\pi} Q_g \dot{\phi}_{\gamma'} \right)$$

- $Q_g = V_g C_g$, $m_g = \frac{C_g}{C} m = \gamma m$. 
Hamiltonian in the presence of the voltage bias

\[ \mathcal{H} = \frac{1}{2} \left( p + \frac{\Phi_0}{2\pi} Q_g v_{\gamma'} \right)^T M_s^{-1} \left( p + \frac{\Phi_0}{2\pi} Q_g v_{\gamma'} \right) + V(\phi) \]

\[ M_s = M + \gamma m v_{\gamma'} v_{\gamma'}^T, \]

- \( v_{\gamma'} \) a column vector of dimension \( N \) with all entries zero except that corresponding to the \( \gamma' \) dof, which has entry 1.
- Momentum is “shifted”, i.e., \( p \to p + \frac{\Phi_0}{2\pi} Q_g v_{\gamma'} \)
The shift in the conjugate momentum can be handled by the Fokker-Plank (FP) equation which admits a force term $F$ to the corresponding Green’s function for the imaginary-time Schroedinger equation.

$$F[\phi_i(t)] \equiv -\frac{\Phi_0}{2\pi}Qg\delta_{i,\gamma'}$$

To implement the FP term in DMC: Displace the random walker with the rule

$$\phi_i(t + \Delta t) = \phi_i(t) + \frac{\Delta t}{2}F[\phi_i(t)] + \eta\sqrt{\Delta t}$$
Deploying the DMC code with a FP term to reproduce the JJA with 2 dof as discussed by Orlando et al (PRB 1999)

**Figure:** The three-junction qubit. Josephson junctions 1 and 2 both have Josephson energies $E_J$ and capacitance $C$ and Josephson junction 3 has a Josephson energy and capacitance $q$ times larger. The nodes 1 and 2 represent the superconducting islands (nodes) that are coupled by gate capacitors $C_g = \gamma C$ to gate voltages $V_A$ and $V_B$. 
FIG. 4. The energy levels $E$ vs frustration and gate voltage for $E_J/E_C = 80$, $\alpha = 0.8$, and $\gamma = 0.02$. The gate voltage is related to the $k$ values by $[k_p, k_m] = (\gamma C/2e)[V_A + V_B, V_A - V_B]$, (a) $E/E_J$ vs $f_b$ near $f_b = 1/2$ for $[k_p, k_m] = [0,0]$, and (b) $E/E_J$ vs $k_m$ for $k_p = 0$. 

Calculated eigen energies from Orlando et al (PRB 1999)
GS energy vs $f$ and GS energy vs $k_m$ from DQMC
Comparison between the DQMC result against the Orlando PRB 99 paper

- Our DMC code correctly reproduces the ground state energy as presented in Fig. 4(a) of Orlando PRB99, $E/E_J = 1.58$ around $f = 0.5$.
- When the external voltages are switched on with $k_p = 0, k_m = [0.0, 1.0]$, $E/E_J$ is found to centered around 1.58, and is very insensitive to the gate voltages.
- This agreement confirm the correctness of our code in the case of the JJA with 2 d.o.f with external bias.
The variation of the GS energy as the function of external voltage coupled to any selected superconducting island in the 4 by 4 JJA can now be calculated using the DQMC.

Samples of some GS profile as a function of the external bias using some selected set of parameters are shown:
GS energy $V_1$ from DQMC for the 4 by 4 JJA

![Graph 1](/home/tlyoon/code/on_going/9DJJA/working/g1/ongsF_onDF_D1F_D3F_ogDF_g1T_g2F_gm1F_gm2F_QF_alpF.dat u 2:10:11)

![Graph 2](/home/tlyoon/code/on_going/9DJJA/working/g1/data3/ongsF_onDF_D1F_D3F_ogDF_g1T_g2F_gm1F_gm2F_QF_alpF.dat u 2:10:11)
What’s next?

- We still need to calculate the excited state eigen values for the JJA, which can not be obtained using DQMC.
- Need Excited state quantum Monte Carlo method.
- Work still in progress.
A DQMC code was developed to calculate the GS energy of the 4 by 4 JJA design containing 9 d.o.f.

It tells us how the GS eigenvalue can be controlled by external voltage and magnetic flux.

The code is successfully developed and reproduces some known results for similar flux qubit JJA but with smaller d.o.f.

So now we have an efficient numerical code that can tell us how the GS of the 4 by 4 JJA varies as a function of external voltage bias and magnetic frustration.
We acknowledge that it was Jos M. Thijssen who provided the original suggestion to this QMC calculation.

We also acknowledge that the “4 × 4” JJA is the original idea of Prof. J. E. Mooij from TU Delft.

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