Calculation of ground state energy of a "4 $\times$ 4" flux qubit Josephson junction array using diffusion quantum Monte Carlo Method

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Paper Presented at
PERFIK 2012, Bukit Tinggi, Pahang, Malaysia

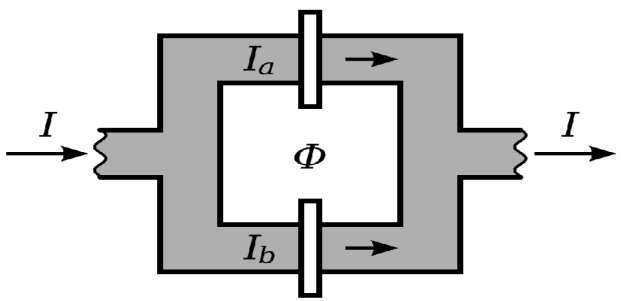
21 Nov 2012

ABSTRACT

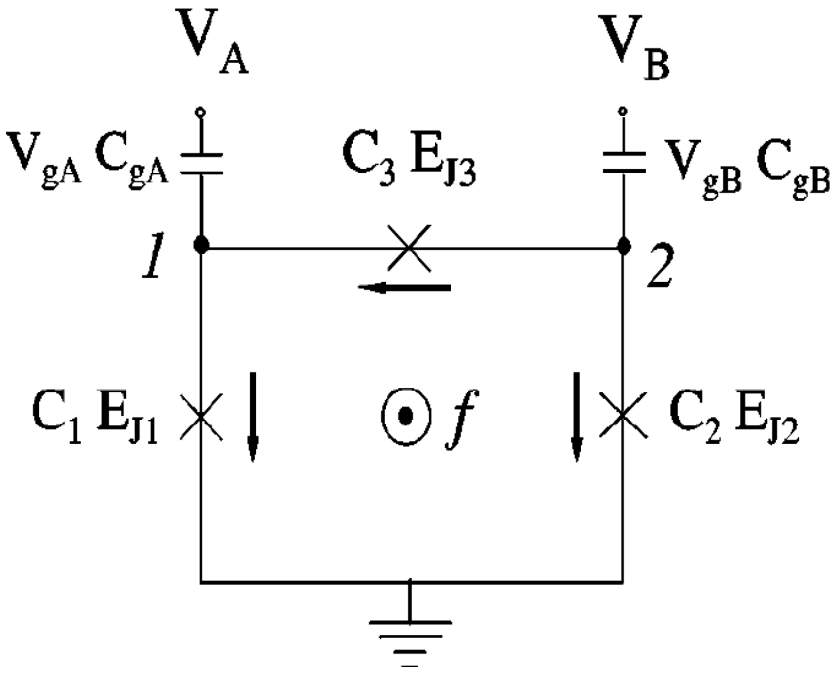
Under the right parametric conditions a Josephson Junction (JJ) can act as a qubit as it reduces to a two-state quantum system, which is the very basic required feature for any system to act as a qubit. In this paper we shall investigate the ground state energy of a new Josephson junction array (JJA) 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.

SQUID

- Superconducting Quantum Interference Device as qubit - a two-state quantum system
- A feasible qubit - addressed, controled, measured, coupled to its neighbors, and decoupled from the environment.

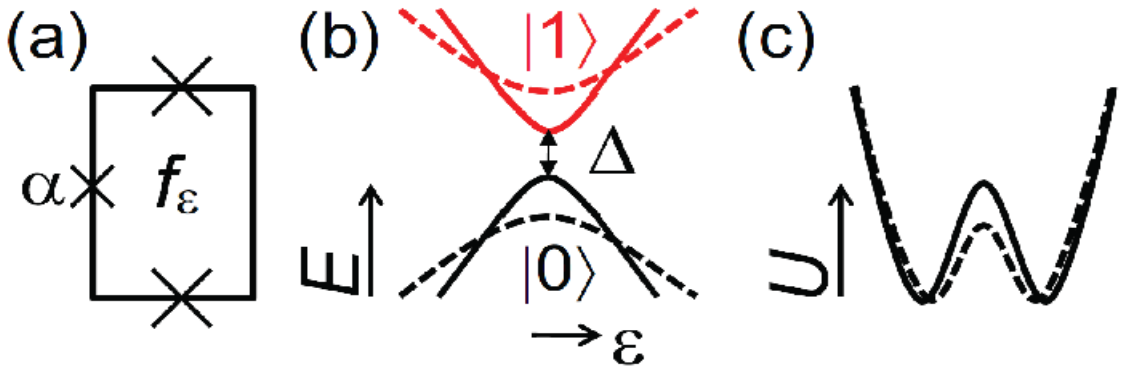


Josephson Persisten-Current Qubit (Flux qubit)



- J. E. Mooij *et. al.*, Josephson Persistent-Current Qubit, Science **285** (1999) 1036.
- T. P. Orlando *at al.*, Superconducting persistent-current qubit. Phys. Rev. B 60 (1999) 15398.
- The qubit consists of a micrometer-sized loop with three or four Josephson junctions.

Flux Qubit Hamiltonian



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

$$\mathcal{H}_q = -1/2(\epsilon\sigma_z + \Delta\sigma_x).$$

- ϵ - Magnetic energy bias
- Energy gap Δ - coupling constant controlling the mixing between the two persistent current state - tunable via f_ϵ, the magnetic flux threading the closed loop.
- $\Delta \ll \epsilon$ - maximal mixing; $\Delta \gg \epsilon$ - total decopling between

Main objective of this work

- The main aim of this work is to calculate the gap between the lowest two energy levels of a "4 $\times$ 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

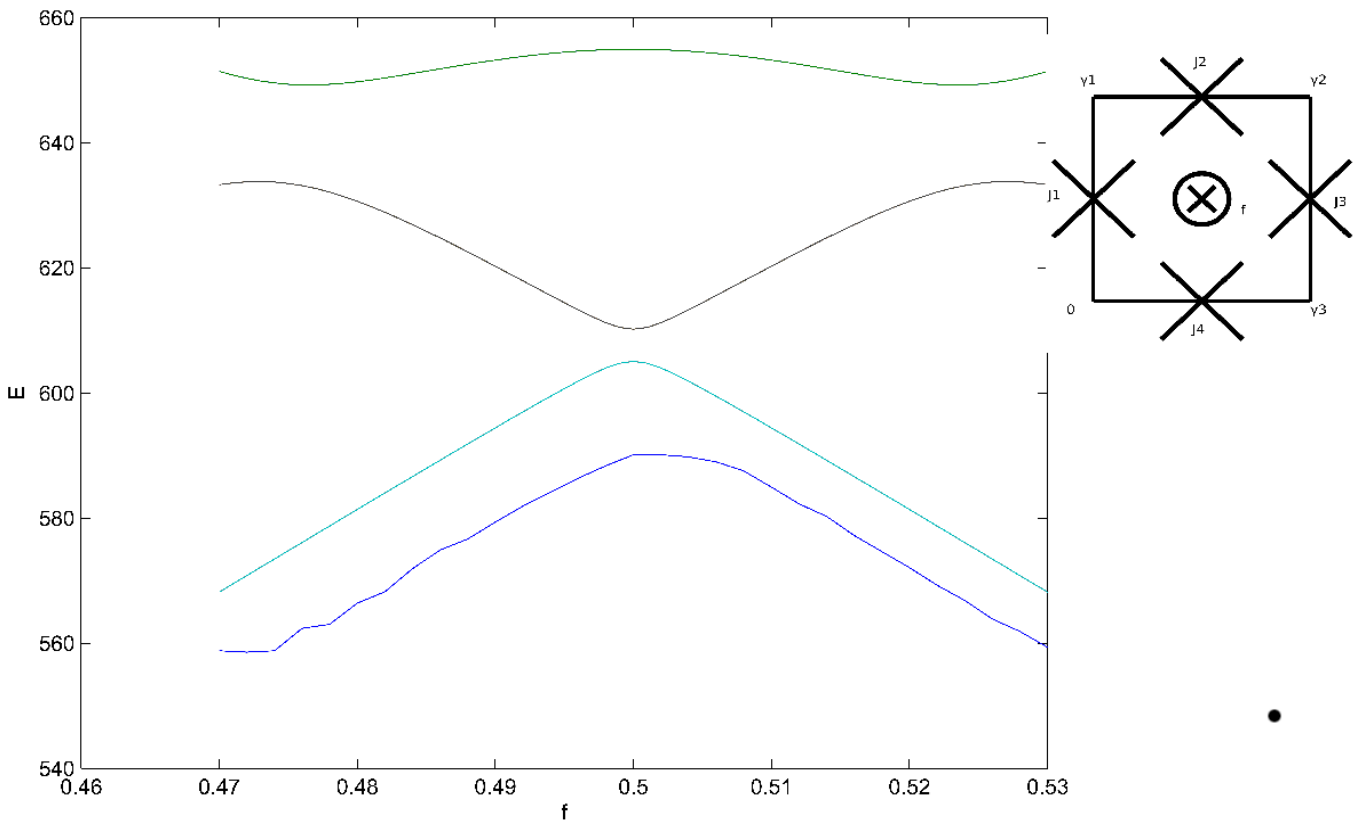
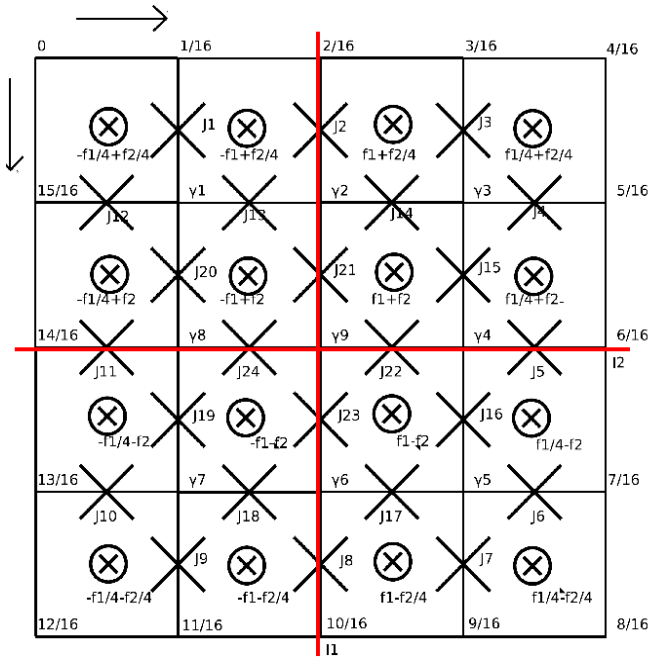


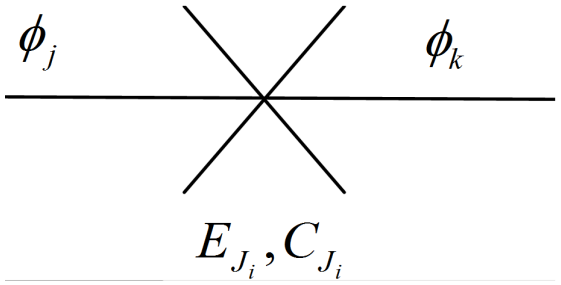
Figure 5.6: Ground state calculated with DMC (bottom line) superimposed on the results from Lanczos (top three lines) with $N_{\max} = 8$. Params for the DMC are: $N_{\text{walkers}} = 8000$, $N_{\text{iters}} = 800$, $\alpha = 0.3$ and $\tau = 0.002$

“4 × 4” Josephson Junction Array (JJA)



- Originally proposed by J. E. Mooij, from TU Delft.
- Martijn and Thijssen (Master thesis (2009), TU Delft, The Netherlands, unpulished) attempted to calculate the energy spectrum (ground state and first few excited states) of the 4×4 JJA.
- This work is a follow-up of their numerical work.

Lagrangian of a Josephson Junction (JJ)



- 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 Lagragian of an uncoupled JJ (indexed by J_i)

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

where

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

Lagrangian of N_0 independent JJ

- $$\begin{aligned} \mathcal{L}_{N_0} &= \sum_{Ji=1}^{N_0} \frac{1}{2} m_{Ji} (\Delta \dot{\phi}_{Ji})^2 - E_{Ji}(1 - \cos \Delta \phi_{Ji}) \\ &\equiv T - V. \end{aligned} \tag{1}$$
- Kinetic energy equivalent made up of the charging energy of the JJA:

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

- 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 4×4 JJA, but not all d.o.f. ϕ_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 ϕ_i)

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

- 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

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

- ϕ a dimension-N vector containing all independent phases ϕ_i.
- The "mass matrix" $\mathbf{M}$ and $V(\phi)$ determine the dynamics of the JJA.

Hamiltonian

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

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

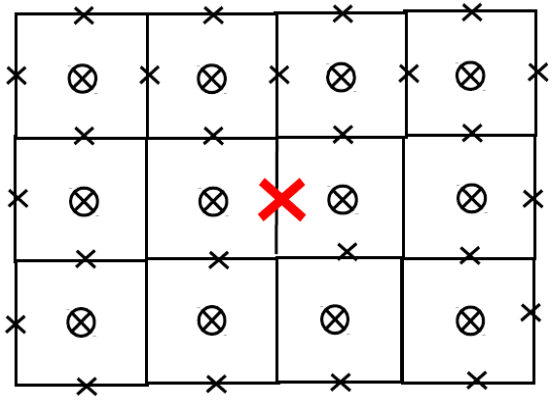
$$\mathcal{H}(\mathbf{p}, \phi) = \mathbf{p}^{\mathsf{T}}\dot{\phi} - \mathcal{L} = \frac{1}{2}\mathbf{p}^{\mathsf{T}}\mathbf{M}^{-1}\mathbf{p} + V(\phi)$$

- $\mathbf{p} = \{p_1, p_2, \cdots, p_N\}$;$\phi = \{\phi_1, \phi_2, \cdots, \phi_N\}$ 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 $\mathbf{M}$ 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 $\mathbf{M}$ are made up of the charging energies of each JJ, which are expressed in terms of "capacitances" C_{Ji}, $J_i \in \{1, 2, 3, \cdots, N\}$.
- $V(\phi)$ 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 Δ_1 and Δ_2.

$$\mathbf{M} = m \begin{pmatrix} 4 & -1 & 0 & -1 & 0 & 0 \\ -1 & 3+q & -1 & 0 & -q & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 \\ -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & -q & 0 & -1 & 3+q & -1 \\ 0 & 0 & -1 & 0 & -1 & 4 \end{pmatrix}.$$

Potential Energy for a JJA with 6 d.o.f

$$
\begin{aligned}
& V(\phi_1, \phi_2, \cdots, \phi_6)/E_J \\
= \; & 16 + q - \cos(\phi_1 - \frac{\pi}{7} + \Delta_2) - \cos(\phi_1 + \frac{\pi}{7}) - \cos(\phi_4 - \phi_1 + \Delta_2) \\
- \; & \cos(\phi_4 + \frac{2\pi}{7}) - \cos(\phi_4 + \frac{4\pi}{7} - \Delta_2) - \cos(\phi_2 - \phi_1) \\
- \; & \cos(\phi_2 - \frac{2\pi}{7} + \Delta_1) - \cos(\phi_3 - \frac{3\pi}{7} + \Delta_2) - \cos(\phi_6 + \frac{6\pi}{7} - \Delta_2) \\
- \; & \cos(\phi_3 - \frac{5\pi}{7}) - \cos(\phi_6 + \phi_3 + \Delta_2) - \cos(\phi_3 + \phi_2) \\
- \; & \cos(\phi_5 - \phi_4) - q\cos(\phi_5 - \phi_2 + \Delta_1) - \cos(\phi_6 - \frac{6\pi}{7}) \\
- \; & \cos(\phi_6 - \phi_5) - \cos(\phi_5 + \frac{5\pi}{7} - \Delta_1). \qquad (2)
\end{aligned}
$$

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

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.

Diffusion Quantum Monte Carlo

- The strategic method of choice to abstract solutions from a multi-dimensional quantum Hamiltonian.
- Based on Green's function for the imaginary-time Schroedinger 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
        $P(\eta) = \frac{1}{\sqrt{4\pi\eta}} \mathrm{e}^{-\eta^2/4\gamma}$
   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

$$E_T = E_0 + \alpha ln\left(\tilde{N}/N\right)$$

Tranforming $\mathbf{M}$ 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:

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

- The conjugate momenta and phases transform according to

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

$$\phi \to \phi' = \mathbf{D}^{\frac{1}{2}}\mathbf{U}^{\mathrm{T}}\phi$$

...

- In the basis $\{\mathbf{p}', \phi'\}$, the Hamiltonian now looks

$$\mathcal{H}(\mathbf{p}', \phi') = \sum_{i}^{N} -\frac{1}{2}\frac{\partial^2}{\partial \phi_i'^2} + V'(\phi')$$

- $p_i' = i\frac{\partial}{\partial \phi_i'}$
- 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

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

$$\phi \rightarrow \phi' = \mathbf{D}^{\frac{1}{2}}\mathbf{U}^{\mathsf{T}}\phi$$

Results for JJA with 6 d.o.f

- 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 Δ_2, Δ_1, and q. Δ_2 is not independent from Δ_1, and we relate them via the parameter α_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 ($\Delta_2 = \Delta_1 \cdot \alpha_J$)

No.	$\Delta_1/(2\pi)$	α_J	q	GS Energy by DMC	GS Energy by Lanczos
1	0.5	0.2	1.3	9.12304	9.12690
2	0.5	0.2	1.5	9.13582	9.13440
3	-0.5	0.2	5.0	9.18559	9.18613
4	10.5	0.2	5.0	9.18109	9.18613
5	10.5	0.9	5.0	7.86102	7.86450

Lanczos vs. DQMC

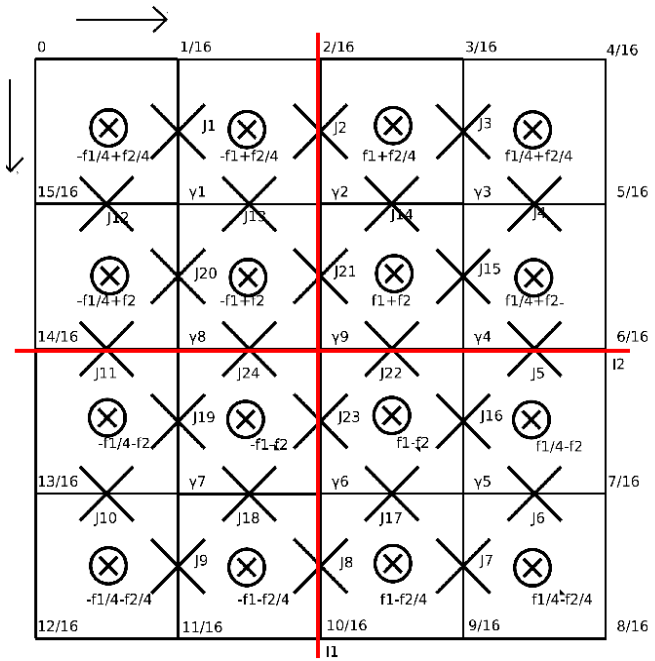
- The 4 by 4 JJA has 9 d.o.f.
- Lanczos method scale badly with computational cost.
- Lanczos can still handle 6 d.o.f but not 9 d.o.f
- Hence it must be solved using DMC.

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:

$$C_{21} = C_{22} = C23 = C24 = qC$$

$$EJ21 = EJ22 = EJ23 = EJ24 = qE_J$$



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

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

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

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

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

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

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

$$- \cos(\phi_9 - \phi_6 + \Delta_2) - \cos(\phi_3 - \phi_2 - \Delta_4) - \cos(\phi_3$$

$$- \phi_6 - \Delta_2) - \cos(\phi_7 - \phi_4 + \Delta_2) - \cos(\phi_7 - \phi_8 + \Delta_4)$$

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

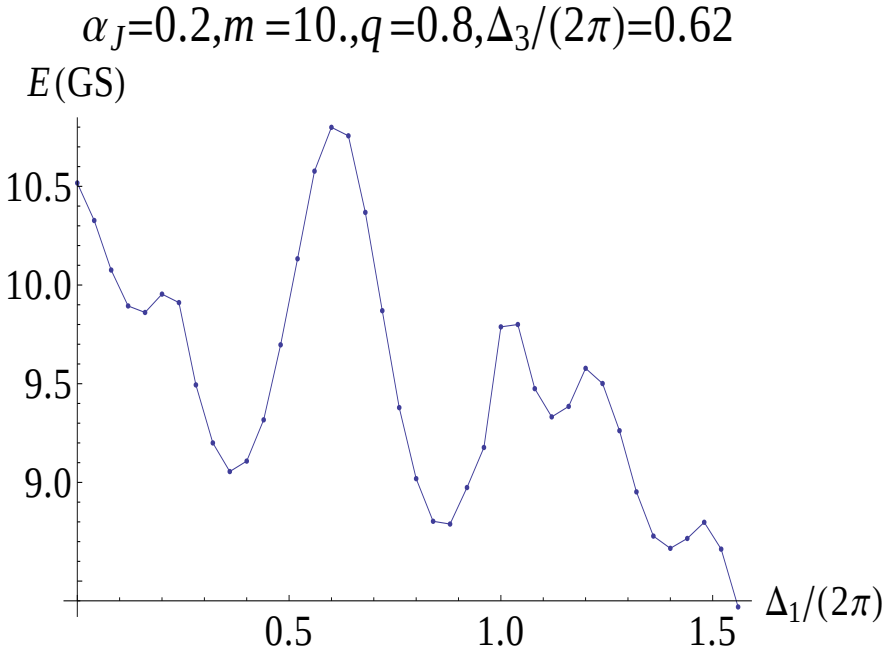
$$- q[\cos(\phi_5 - \phi_2 + \Delta_1) + \cos(\phi_5 - \phi_8 - \Delta_1)]$$

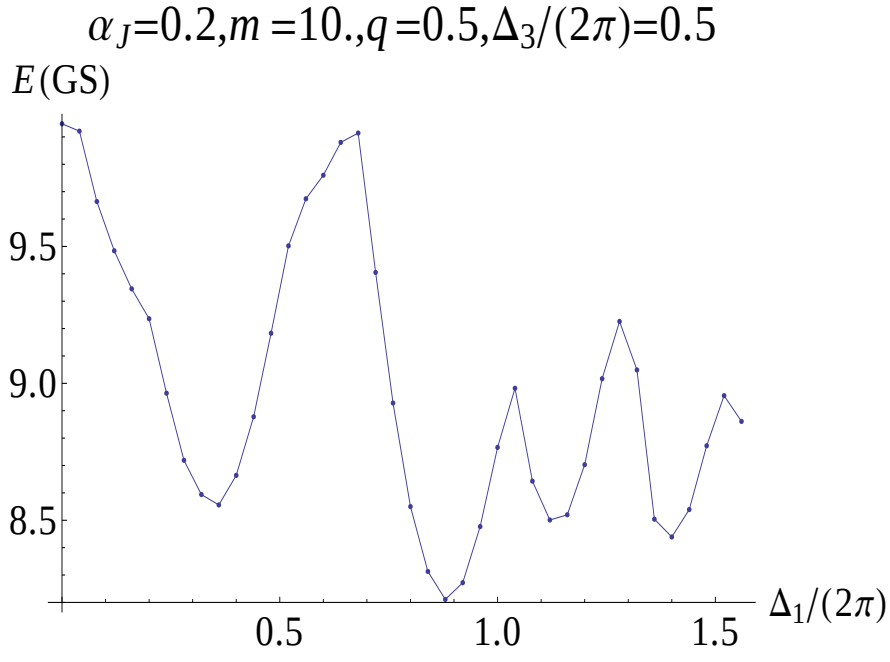
Numerical Parameters

- The 4 by 4 JJA admits four magnetic frustration Δ_1,Δ_2,Δ_3,Δ_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, Δ_1, Δ_3 and α_J as independent parameters.
- We will fix q, Δ_3, α_J and find $E(\mathrm{GS})$ as a function of Δ_1 so that we can tell how the GS energy is controlled by changing the external magnetic field Δ_1.

GS as a function of frustration Δ_3 for the 4 by 4 JJA calculated using DMC

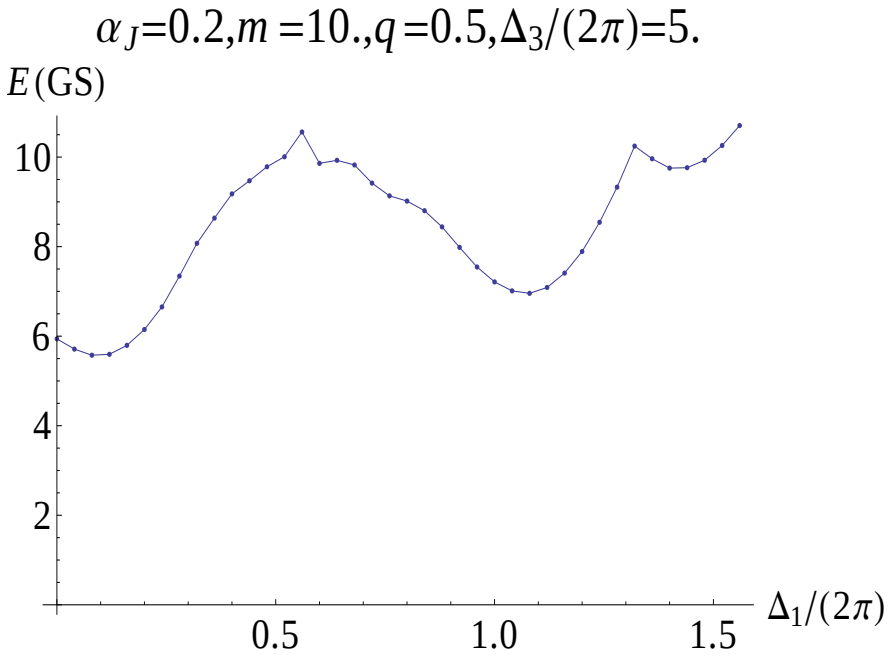
Table: Examples of GS energies at selected parameters

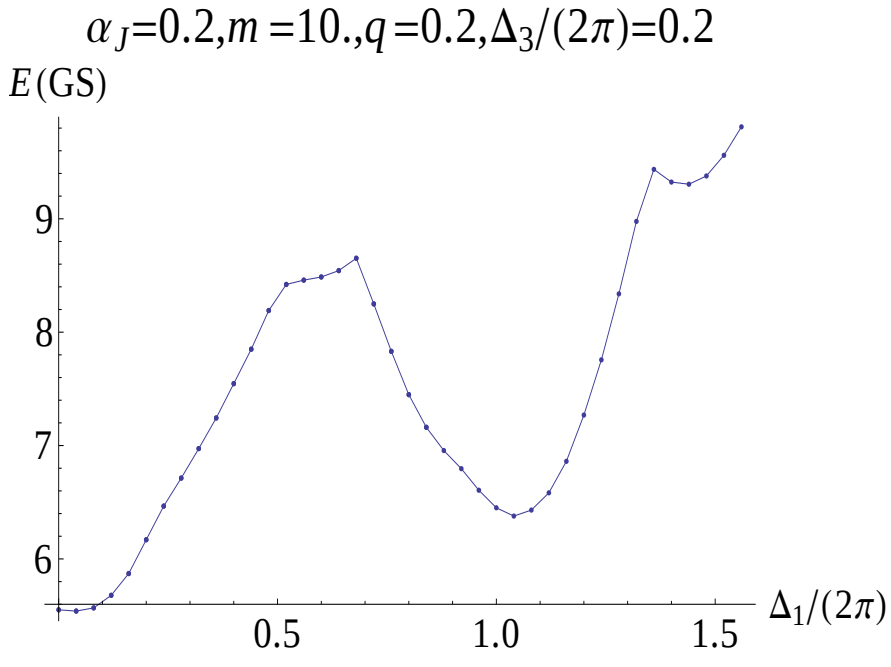




GS as a function of frustration Δ_3 for the 4 by 4 JJA calculated using DMC (cont.)

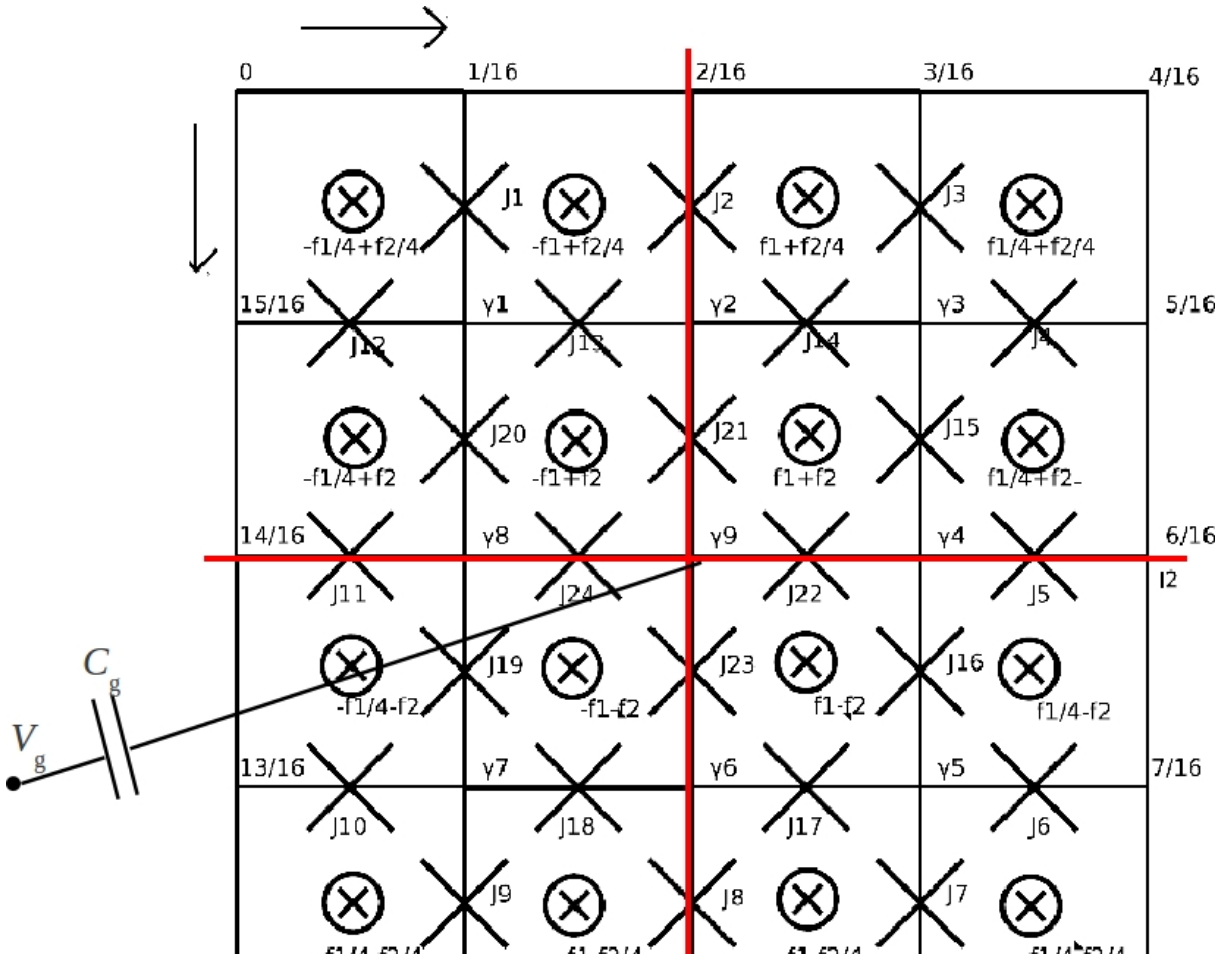
Table: Examples of GS energies at selected parameters





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

- γ' the superconducting island with absolute phase $\phi_{\gamma'}$, biased by V_g capacitively coupled controlled gate voltage via a gate capacitor $C_g = \gamma C$.
- $$T(\dot{\phi}) = \frac{1}{2}\dot{\phi}^{\mathrm{T}}\mathbf{M}\dot{\phi} + \frac{1}{2}\left(\dot{\phi}_{\gamma'} m_g \dot{\phi}_{\gamma'}\right) - \left(\frac{\Phi_0}{2\pi} Q_g \dot{\phi}_{\gamma'}\right)$$
- $Q_g = V_g C_g$, $m_g = \frac{C_g}{C} m = \gamma m$.

Hamiltonian in the presence of the voltage bias

$$\mathcal{H} = \frac{1}{2}\left(\mathbf{p} + \frac{\Phi_0}{2\pi} Q_g \mathbf{v}_{\gamma'}\right)^{\mathrm{T}} \mathbf{M}_s^{-1} \left(\mathbf{p} + \frac{\Phi_0}{2\pi} Q_g \mathbf{v}_{\gamma'}\right) + V(\phi)$$

$$\mathbf{M}_s = \mathbf{M} + \gamma m \mathbf{v}_{\gamma'} \mathbf{v}_{\gamma'}^{\mathrm{T}},$$

- $\mathbf{v}_{\gamma'}$ a column vector of dimension N with all entries zero except that corresponding to the γ' dof, which has entry 1.
- Momentum is "shifted", i.e., $\mathbf{p} \rightarrow \mathbf{p} + \frac{\Phi_0}{2\pi} Q_g \mathbf{v}_{\gamma'}$

Fokker-Planck 'force' term

- 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.

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

- 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)

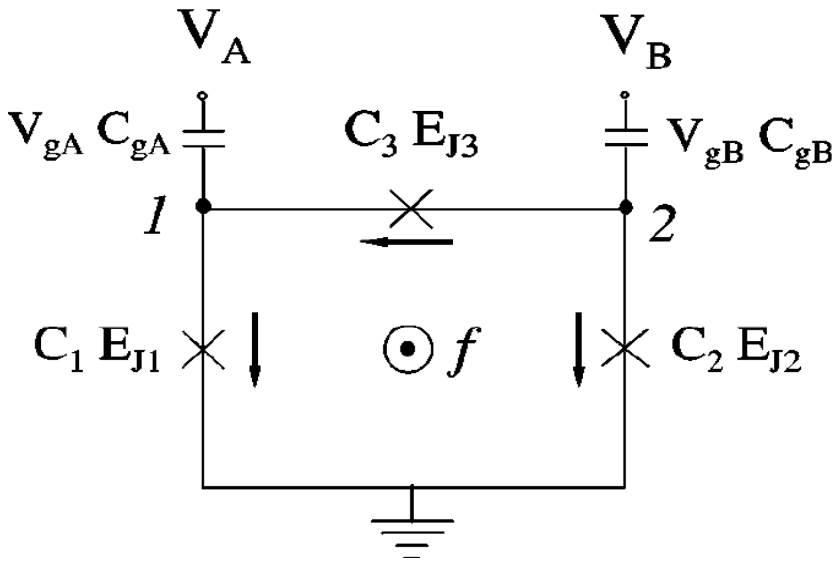


Figure: The three-junction qubit. Josephson junctions 1 and 2 both have Josephson energies E_J and capacitance C and Josephson junction 3 has a Josephson energy and capacitance q times larger. The nodes 1 and 2 represent the superconducting islands (nodes) that are coupled by gate capacitors $C_g = \gamma C$ to gate voltages V_A and V_B.

Calculated eigen energies from Orlando et al (PRB 1999)

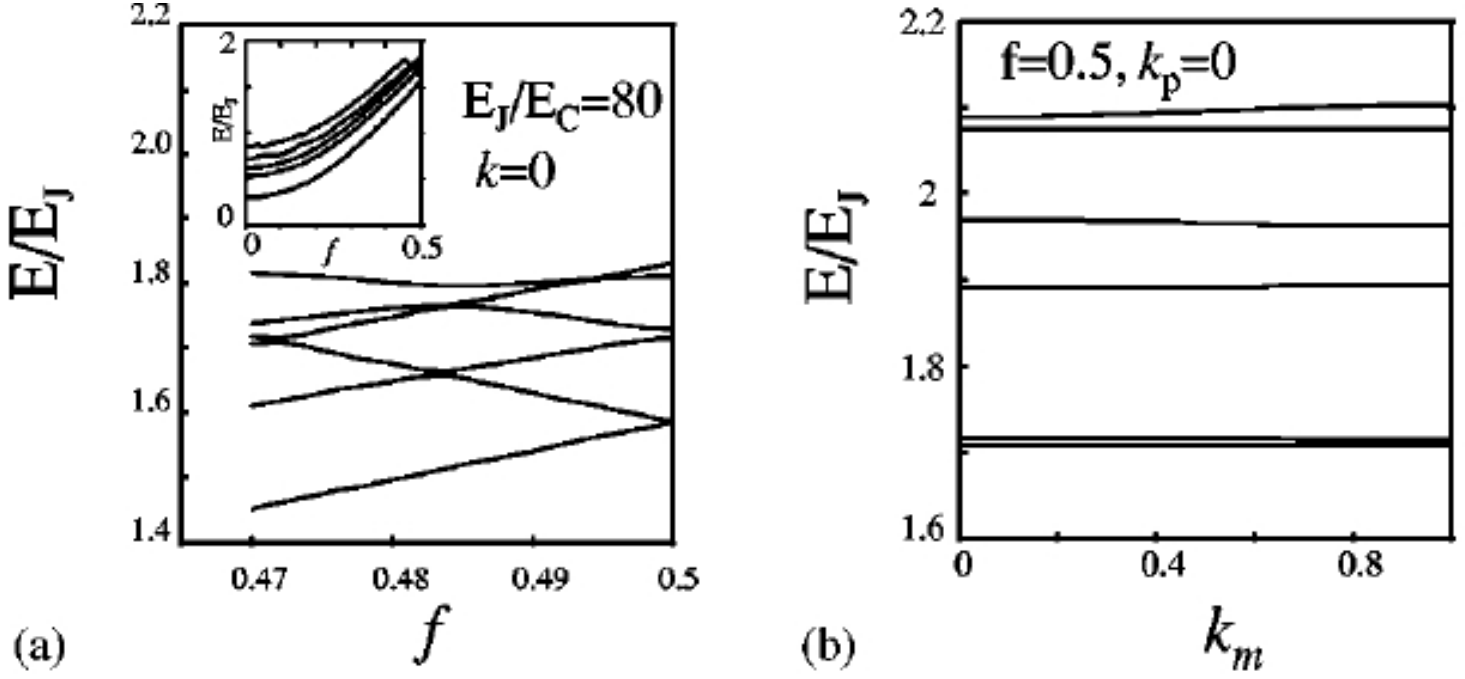
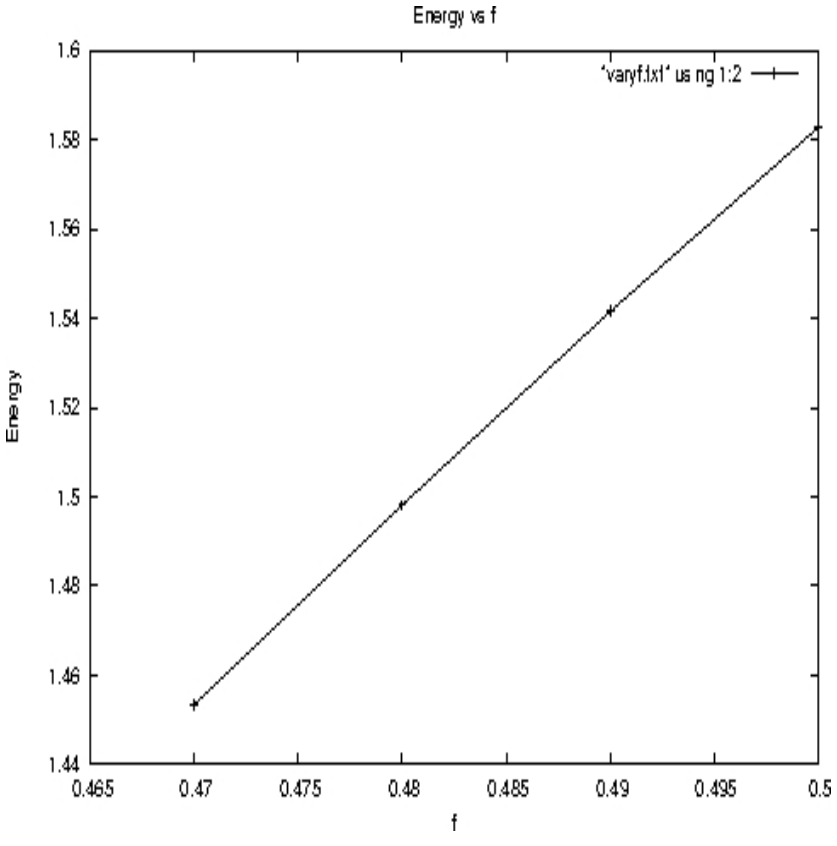
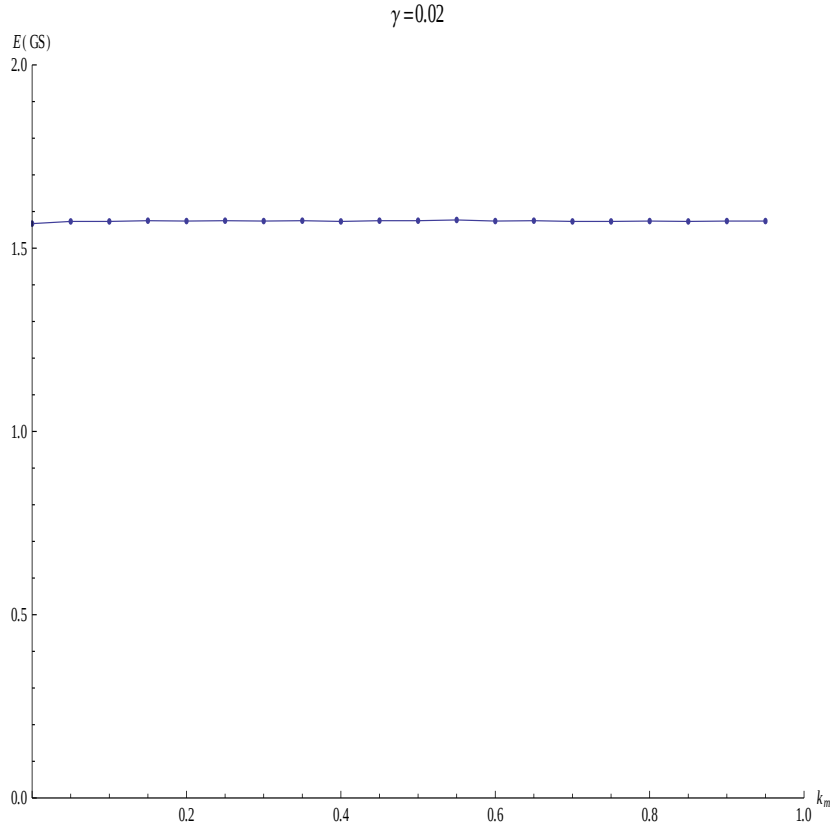


FIG. 4. The energy levels E vs frustration and gate voltage for $E_J/E_c = 80$, $\alpha = 0.8$, and $\gamma = 0.02$. The gate voltage is related to the **k** values by $[k_p, k_m] = (\gamma C/2e)[V_A + V_B, V_A - V_B]$, (a) E/E_J vs f_b near $f_b = 1/2$ for $[k_p, k_m] = [0,0]$, and (b) E/E_J vs k_m for $k_p = 0$.

GS energy vs f and GS energy vs k_m from DQMC



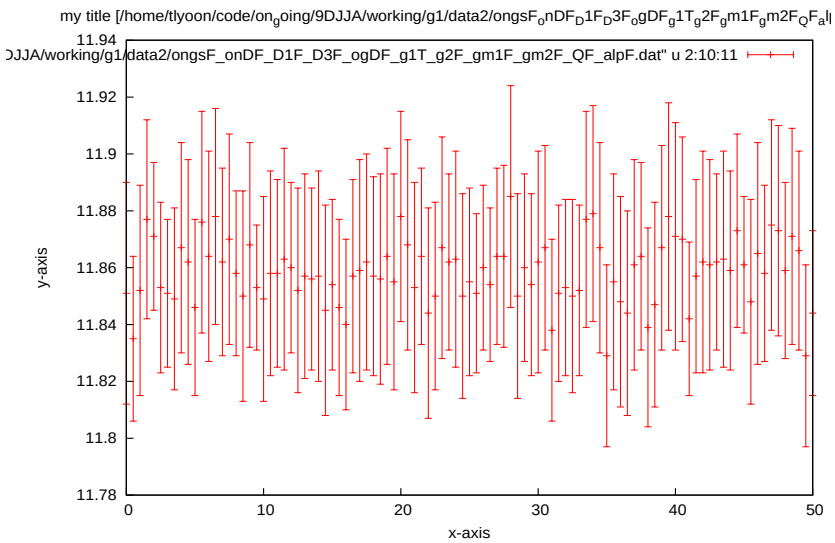


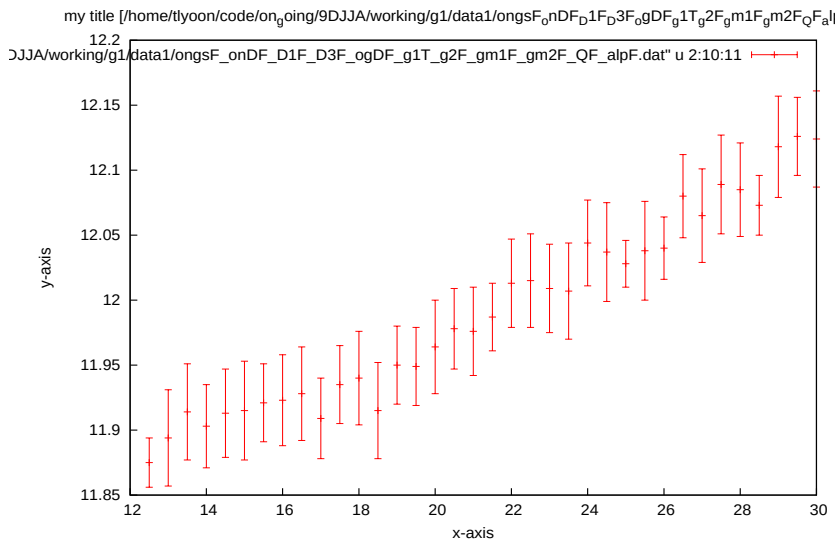
Comparison between the DQMC result against the Orlando PRB 99 paper

- 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.

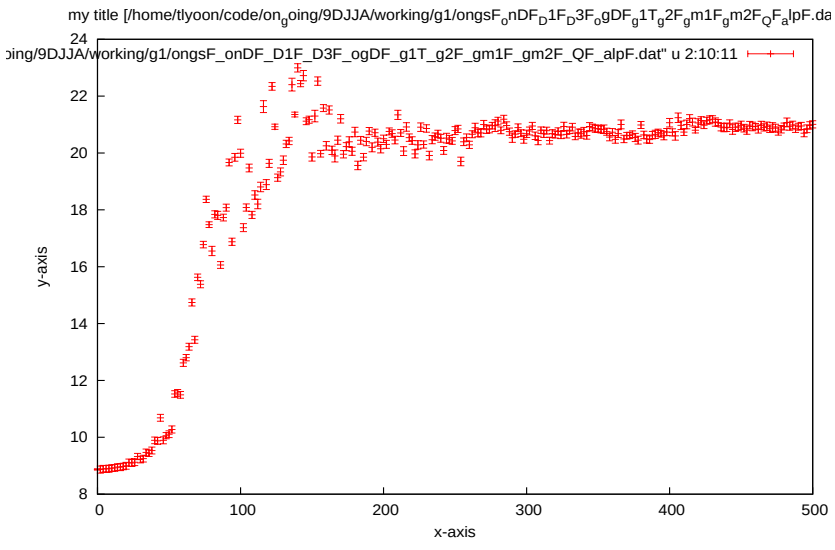
GS energy vs V_1 from DQMC for the 4 by 4 JJA

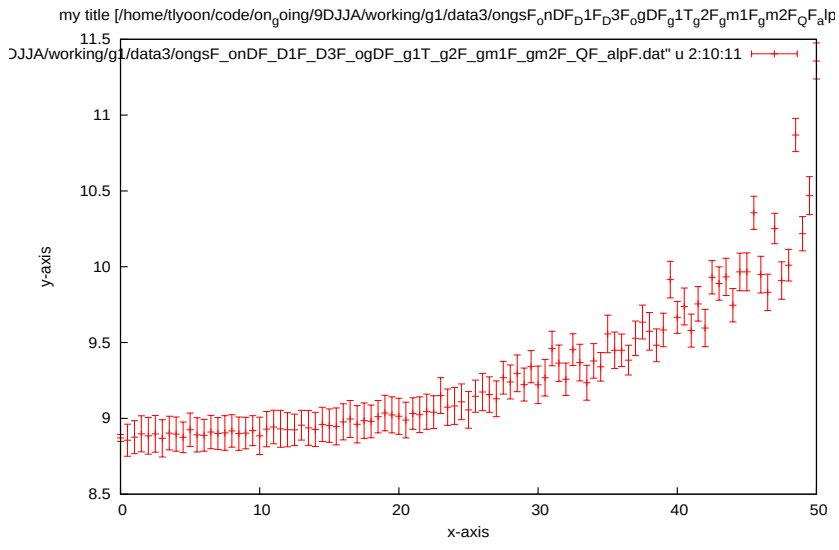
- The variation of the GS energy as the function of external voltage coupled to any selected superconducting island in the 4 by 4 JJA can now be calculated using the DQMC.
- Samples of some GS profile as a function of the external bias using some selected set of parameters are shown:





GS energy V_1 from DQMC for the 4 by 4 JJA





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.
- D. M. Ceperley and B. Bernu, The calculation of excited state properties with quantum Monte Carlo, J. Chem. Phys. **89** (1988) (6316)
- B. Bernu, D. M. Ceperley, W. A. Lester, Jr., The calculation of excited states with quantum Monte Carlo. II Vibrational excited states, J. Chem. Phys. **93** (1990) (552)
- Work still in progress.

Conclusion

- 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.

Acknowledgement

- We acknowledge that it was Jos M. Thijssen who provided the original suggestion to this QMC calculation.
- We also acknowledge that the "4 $\times$ 4" JJA is the original idea of Prof. J. E. Mooij from TU Delft.
- YTL wishes to acknowledge the support of FRGS grant by the Malaysian Ministry of Higher Education, Phase 2/2010, 203/PFIZIK/6711169.