eSTA approach to Josephson Junction

1 Josephson Junction from the ground-up

Here I will summarize the paper [GO07] where the Josephson Junction is derived. We are considering N particles in a double well potential, the form of which is

$$V_{dw} = \frac{1}{2}m\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) + \frac{V_0}{2}\left(1 + \cos\frac{2\pi}{d_{sw}}x\right). \tag{1}$$

Usually this problem is really hard to solve at involves many body particles etc. However the single particle spectrum of the double well is almost degenerate for the first two levels, while there is a wide gap between the second and third eigentates of the double well Hamiltonian. This allows us to introduce the *two mode approximation* in which only the first two eigentates are considered. It has been shown how with this assumption the Hamiltonian of the system can be written as

$$H = \hat{H}_0 + \hat{H}_{int} \tag{2}$$

$$\hat{H}_0 = \int \mathrm{d}\mathbf{r}\left(-\frac{\hbar^2}{2m}\hat{\Psi}^\dagger\nabla^2\hat{\Psi} + \hat{\Psi}^\dagger V_{dw}\hat{\Psi}\right), \tag{3}$$

$$\hat{H}_{int} = \frac{g}{2}\int \mathrm{d}\mathbf{r}\hat{\Psi}^\dagger\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi} \tag{4}$$

with $\hat{\Psi}$ field operator that (loosely speaking) creates / annihilates a particle in the position $\mathbf{r}$ and g is the coupling constant. Now we take into account only the mean-field ground and excited states (which I assume they are $\Phi_g = |N,0\rangle$ and $\Phi_e = |0,N\rangle$) so we can rewrite the general wavefunction $\hat{\Psi}$ as

$$\hat{\Psi} = \hat{c}_g\Phi_g + \hat{c}_e\Phi_e \tag{5}$$

with $\hat{c}_g^\dagger$ and $\hat{c}_e^\dagger$ the creation operator for the ground and excited states respectively. A more convenient choice in this case is usually to choose the left and right operators

$$\hat{c}_l^\dagger = \frac{1}{\sqrt{2}}\left(\hat{c}_g^\dagger + \hat{c}_e^\dagger\right) \qquad \hat{c}_r^\dagger = \frac{1}{\sqrt{2}}\left(\hat{c}_g^\dagger - \hat{c}_e^\dagger\right). \tag{6}$$

With this choice, we can now rewrite $\hat{\Psi}$

$$\hat{\Psi} = \frac{1}{\sqrt{2}}\left(\hat{c}_l(\Phi_g + \Phi_e) + \hat{c}_r(\Phi_g - \Phi_e)\right). \tag{7}$$

We are now in the position to insert eq. (7) into eq. (2) and by doing some calculations, we obtain the two-mode Hamiltonian

$$\hat{H}_{2M} = \frac{E_c}{8}\left(\hat{c}_r^\dagger\hat{c}_r - \hat{c}_l^\dagger\hat{c}_l\right)^2 - \frac{E_j}{N}\left(\hat{c}_l^\dagger\hat{c}_r - \hat{c}_r^\dagger\hat{c}_l\right) + \frac{\delta E}{4}\left(\hat{c}_l^\dagger\hat{c}_r - \hat{c}_r^\dagger\hat{c}_l\right)^2 \tag{8}$$

where

- E_j describes the tunneling rate from one well to the other.
- E_c corresponds to the local interaction within the two wells.
- δE takes into account additional two-particles processes.

In many discussions, the last term δE is often neglected and thus the Hamiltonian eq. (8) can be further simplified and becomes

$$\hat{H}_{2M} = \frac{E_c}{2}\hat{n}^2 - \frac{2E_j}{N}\hat{\alpha} \tag{9}$$

with $\hat{n}^2$ the population imbalance and $\hat{\alpha}$ the tunneling operator. Their form is

$$\hat{n} = \frac{\hat{c}_r^\dagger \hat{c}_r - \hat{c}_l^\dagger \hat{c}_l}{2}, \qquad \hat{\alpha} = \frac{\hat{c}_l^\dagger \hat{c}_r + \hat{c}_r^\dagger \hat{c}_l}{2} \tag{10}$$

and we will see that these two operators are basically the same thing as the ones in [JDTM+12]

- Write down the calculations that allow us to get from the textbook example to the two JJ Hamiltonians (the one with the angular momentum and the one with number operators)
- Explain where they got STA from
- Explain what we did with eSTA up to now
- Explain how we can improve on that with the full calculation

2 Josephson Junction Approximation

2.1 JJ in angular momentum formalism

In this section we will outline the calculations that allow STA to be applied in these Josephson Junction settings. Starting from eq. (9) it can be shown that the operators $\hat{n}$ and $\hat{\alpha}$ behave as pseudoangular momentum operators if we set

$$\hat{J}_z = \frac{\hat{c}_r^\dagger \hat{c}_r - \hat{c}_l^\dagger \hat{c}_l}{2} = \hat{n}, \qquad \hat{J}_x = \frac{\hat{c}_r^\dagger \hat{c}_l - \hat{c}_l^\dagger \hat{c}_r}{2} = \hat{\alpha}, \qquad \hat{J}_y = \frac{\hat{c}_r^\dagger \hat{c}_l - \hat{c}_l^\dagger \hat{c}_r}{2i} \tag{11}$$

and we obtain the Bose Hubbard Hamiltonian

$$H_{BH} = U\hat{J}_z^2 - 2J\hat{J}_x \tag{12}$$

if the value U and J are chosen accordingly. It can also be shown that the operators defined in eq. (11) follow in fact the angular momentum relations.
By using the pseudoangular momentum approach, a system of N particles can be described as a single particle with spin $N/2$ and the basis set is of the form $\{|m\rangle\}$ with $m = -N/2, ..., N/2$ eigenstates of the $\hat{J}_z$ operator.
The Hamiltonian of the system is then defined via eq. (12) and the general state $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \sum_{m=-N/2}^{N/2} c_m |m\rangle . \tag{13}$$

The Schrödinger equation is then written as

$$i\partial_t |\Psi\rangle = H_{BH} |\Psi\rangle \tag{14}$$

If we want to apply STA to eq. (14), we need to perform some approximations. In the following I will try to perform the same approximation they used in [JDMP10] in order to move from the discrete to the continuous variable. I will follow the calculations I found in [JDMP10] as they give a better idea on what is the Hamiltonian of the system and what are the steps and approximations we need to make in order to obtain an idealised version of the Hamiltonian where we can apply STA. My plan is to obtain the idealised version of the Hamiltonian they used in [JDTM+12]. The first thing to do is to define a new dimensionless Hamiltonian $H_S = \frac{H_{BH}}{NJ}$ that reads

$$H_S = -\frac{2}{N}\hat{J}_x + \frac{U}{NJ}\hat{J}_z^2 = -\frac{2}{N}\hat{J} + \frac{2\Lambda}{N^2}\hat{J}_z^2 \tag{15}$$

where we defined $\Lambda = NU/(2J)$. The corresponding Schrödinger equation then becomes $\frac{i}{NJ}\partial_t |\Psi\rangle = H_S |\Psi\rangle$ and if we introduce the dimensionless time $\tau = t/J$, it simplifies even more, becoming

$$\frac{i}{N}\partial_\tau |\Psi\rangle = \left(-\frac{2}{N}\hat{J}_x + \frac{2\Lambda}{N^2}\hat{J}_z^2\right)|\Psi\rangle \tag{16}$$

2.2 JJ Hamiltonian in continous variables

We now want to find a differential equation for the coefficients c_m of eq. (13). In order to do that, we are going to project eq. (16) onto $\langle m|$. Moreover, we are going to use the fact that $\hat{J}_x = \frac{1}{2}\left(\hat{J}_+ + \hat{J}_-\right)$. If we are to project onto $\langle m|$ we should remember how the ladder operators $\hat{J}_\pm$ act. In particular, we can see we are only interested in those states $|k\rangle$ such that $\hat{J}_\pm |k\rangle = \beta_k |m\rangle$ with β_k some coefficient depending on the quantum number k. We are interested in such states as they are the ones which the projection on $\langle m|$ is non zero and we can see that for a fixed m only the states $|m \pm 1\rangle$ meet the requirements. Take for example $|m+1\rangle$ then

$$\langle m|\hat{J}_-|m+1\rangle = \sqrt{\left(\frac{N}{2}+m+1\right)\left(\frac{N}{2}-m\right)}\,\langle m|m\rangle = \beta_m \tag{17}$$

where we set $\beta_m = \sqrt{\left(\frac{N}{2}+m+1\right)\left(\frac{N}{2}-m\right)}$.

By putting everything back together, we obtain

$$\langle m|\frac{i}{N}\partial_t|\Psi\rangle = \langle m|\tilde{H}_S|\Psi\rangle \tag{18}$$

$$\frac{i}{N}\frac{d}{dt}c_m(t) = -\frac{2}{N}\left(b_m c_{m+1}(t) + b_{m-1}c_{m-1}(t)\right) + \frac{2\Lambda}{N^2}m^2 c_m(t) \tag{19}$$

where in this case we set $b_m = \beta_m/N$. The result in eq. (19) gives us a Schrödinger equation for the coefficients c_m which is discrete. We now need to move from a discrete formualtion to a continuous one and we are going to do that by performing a change of variable. If we look at the definition of b_m, we see that we can collect the $N/2$ term as shown in the following

$$b_m = \frac{1}{N}\sqrt{\left(\frac{N}{2}+m+1\right)\left(\frac{N}{2}-m\right)} = \frac{1}{N}\sqrt{\frac{N^2}{4}\left(1+\frac{m}{N/2}+\frac{1}{N/2}\right)\left(1-\frac{m}{N/2}\right)} \tag{20}$$

and if we define the continuous variable $z = \frac{m}{N/2}$ and $h = \frac{1}{N/2}$, we obtain

$$\frac{1}{2}\sqrt{(1+z+h)\,(1-z)} := b_h(z) \tag{21}$$

where we can see that $b_h(z-h) = \sqrt{(1+z)\,(1-z-h)}$ which can be mapped back to b_{m-1}. Additionaly, if we define $\sqrt{N/2}c_m = \psi(z)$ we see that $\psi(z \pm h)$ can be mapped to $c_{m\pm1}$. Finally, by recalling that for a function $f(x)$ we have $f(x \pm \epsilon) = e^{\pm\epsilon\partial_x}f(x)$ we can rewrite eq. (19) as

$$\cancel{\frac{1}{2}}ih\partial_t\psi(z) = -\cancel{\frac{1}{2}}[e^{-i\hat{p}}b_h(z) + b_h(z)e^{i\hat{p}}]\psi(z) + \cancel{\frac{1}{2}}\Lambda z^2\psi(z) \tag{22}$$

where $\hat{p} = -ih\partial_z$.

2.3 Approximation to Harmonic Oscillator

If we want to mimic the calculations made in [JDTM+12] we need to perform a Taylor expansion of both the $e^{\pm i\hat{p}}$ part and the $b_h(z)$ function up to the second order in h such as

$$e^{-i\hat{p}} \simeq 1 \pm h\partial_z - \frac{1}{2}h^2\partial_z^2 \tag{23}$$

$$b_h(z) \simeq 1 + h\partial_h b_h(z)|_{h=0} + \frac{1}{2}h^2\partial_h^2 b_h(z)|_{h=0}. \tag{24}$$

By carrying out the calculations,we obtain the following Schrödinger equation

$$ih\partial_t\psi(z) = -h^2\partial_z\left(b_0(z)\partial_z\psi(z)\right) + \left[\Lambda z^2 - 2b_0(z)\right]\psi(z) \tag{25}$$

where $b_0(z) = \sqrt{1-z^2}$. We can retrieve equation (7) in [JDTM+12] by setting a new $\tilde{h} \equiv h/2 = 1/N$. In the following we will stick to definition of $h = 1/N/2$ instead of using the other definition.

The last approximation we need to perform in order to obtain an oscillator-like Schrödinger equation for this system is given by neglecting the z dependence of the effective mass term and expanding the $\sqrt{1-z^2}$ term into $1 - z^2/2$ in the external potential term. We can finally write down the Schrödinger equation

$$i h \partial_t \psi(z) = H_{ho} \psi(z) \tag{26}$$

where the Hamiltonian of the system is given by

$$H_{ho} = -h^2 \partial_z^2 + (1+\Lambda) z^2 = -h^2 \partial_z^2 + \frac{1}{4}\omega^2 z^2 \tag{27}$$

if we set $\omega^2 \equiv 4(1+\Lambda)$.

3 eSTA Calculations

3.1 Introduction

Now that we managed to approximate the Hamiltonian of the system to eq. (27) where we can apply an STA protocol, we are in a position to calculate the eSTA corrections as well. In the eSTA formalism, we need two Hamiltonians:

- the Hamiltonian $\mathcal{H}_S$ of the real system
- the Hamiltonian $\mathcal{H}_0$ of the idealised version of the system, where STA can be applied

and referring to the previous section, we can see that

$$\mathcal{H}_0 \to H_{ho} \qquad\qquad \mathcal{H}_s \to H_N. \tag{28}$$

We now need the STA wavefunctions for this system and we are going to do that by making some modifications to the ones obtained in [CRS+10] which are wavefunctions for the harmonic oscillator and are thus defined as

$$|\eta_n(z,t)\rangle = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n! b}} e^{\left\{-i\left(n+\frac{1}{2}\right)\int_0^t dt\ \omega_0/b^2\right\}} e^{\left\{i\frac{m}{2\hbar}\left(\frac{\dot{b}}{b}+i\frac{\omega_0}{b^2}\right)z^2\right\}} H_n\left[\left(\sqrt{\frac{m\omega_0}{\hbar}}\frac{z}{b}\right)\right]. \tag{29}$$

with ω_0 the initial frequency for time $t = 0$ and $b = b(t)$ a polynomial function that is connected to the control parameter $\omega(t)$ via the Ermakov equation

$$\omega^2(t) b(t) + \dot{b}(t) = \omega_0 / \dot{b}^3(t). \tag{30}$$

Finally $H_n(x)$ is the Hermite polynomial of order n. We can adapt the wavefunction in eq. (29) to the Bose Hubbard Hamiltonian by making the substitution

$$\hbar \to h \qquad\qquad m \to \frac{1}{2} \tag{31}$$

And obtain the wavefunctions $\chi_n(z,t)$ that are STA solutions for eq. (27)

$$|\chi_n(z,t)\rangle = \left(\frac{\omega_0}{2\pi h}\right)^{1/4} \frac{1}{\sqrt{2^n! b}} e^{\left\{-i\left(n+\frac{1}{2}\right)\int_0^t dt\ \omega_0/b^2\right\}} e^{\left\{\frac{i}{4h}\left(\frac{\dot{b}}{b}+i\frac{\omega_0}{b^2}\right)z^2\right\}} H_n\left[\left(\sqrt{\frac{\omega_0}{2h}}\frac{z}{b}\right)\right]. \tag{32}$$

3.2 eSTA formulations

The wavefunctions eq. (32) and the two Hamiltonians are the starting points to evaluate the eSTA corrections. These corrections are calculated by making approximation about the value of the fidelity landscape and we need to define some variables conveniently. We will start by defining the variables G_n and K_n that will later be used to calculate the corrections. If we call χ_n the nth STA wavefunctions, we can evaluate G_n with the following formula

$$G_n = \int_0^{t_f} dt \, \langle \chi_m | \Delta H | \chi_0 \rangle \tag{33}$$

where ΔH is the difference between the original Hamiltonian H_0 and the approximated one H_{ho}. Similarly we can calculate the numbers K_n with

$$K_n = \int_0^{t_f} dt \, \langle \chi_m | \vec{\nabla} H | \chi_0 \rangle \tag{34}$$

where $\vec{\nabla} H$ is the gradient of the Hamiltonian with respect to the control parameter. To summarize and to put everything in perspective, we have

- G_n as a complex number
- K_n is a vector of complex numbers.

In the first formulation of the eSTA protocol, there was an assumptions by virtue of which the optimal fidelity of the protocol has been set to 1. In this case, the corrections were calculated via:

$$-\frac{\left(\sum_{n=1}^{\mathcal{N}} |G_n|^2\right) \left[\sum_{n=1}^{\mathcal{N}} \mathrm{Re}(G_n^* \vec{K}_n)\right]}{\left|\sum_{n=1}^{\mathcal{N}} \mathrm{Re}(G_n^* \vec{K}_n)\right|^2} \tag{35}$$

where $\mathcal{N}$ is the number of STA wavefunctions we take into account. The assumption of the fidelity being 1 has been deemed to optimistic, and recently a new formalism has been proposed. In this case, the only assumption is that exists a point where the fidelity hits a local maximum. If we follow this prescription, the corrections can be calculated via

$$\frac{\vec{v} \|v\|^3}{\vec{v}^T \mathrm{H} \vec{v}} \tag{36}$$

where

$$\vec{v} = \sum_{n=1}^{\mathcal{N}} \mathrm{Re}(G_n^* \vec{K}_n) \tag{37}$$

and H is the Hessian matrix approximation given by

$$\mathrm{H}_{l,k} = \sum_{n=1}^{\mathrm{N}} \left[G_n (W_n)_{l,k} - \left(\vec{K}_n^*\right)_k \left(\vec{K}_n\right)_l \right] \tag{38}$$

where we W_n is a matrix evaluated by taking the second derivative with respect of the control parameter.

3.3 Gn in Josephson Junction

In order to calculate the eSTA corrections, we need to evalute the difference between the two Hamiltonians

$$\Delta H = H_N - H_{ho} = -e^{-i\hat{p}} b_h(z) - b_h(z) e^{i\hat{p}} + h^2 \partial_z^2 - z^2 \tag{39}$$

where we can see that the control parameter ω is cancelled out.
The correction numbers G_n are found according to eq. (33) and since we are only interested in the effects of ΔH when applied to the ground state of the STA wavefunctions $|\chi_0\rangle$, we can expand the exponential parts in eq. (39) and obtain

$$\Delta H \chi_0(z,t) = -b_h(z-h)\chi_0(z-h,t) - b_h(z)\chi_0(z+h,t) + h^2\partial_z^2\chi_0(z,t) - z^2\chi_0(z,t). \tag{40}$$

We can exploit some symmetries of the system in order to avoid calculating some integrals. In particular due to the parity of the STA wavefunctions eq. (32) we can show that both G_{2n+1} and $\vec{K}_{2n+1}$ are identically 0 for $n \in \mathbb{N}$ thus saving us a lot of time and effort. Moreover, it can be shown that $\langle \chi_{2m}|\partial_z^2|\chi_0\rangle = \langle \chi_{2m}|z^2|\chi_0\rangle = 0$ for $m \neq 1$. In addition, we can numerically see that

$$\int_0^{t_f} \langle \chi_{2m}(z,t)|b_h(z-h)\chi_0(z-h,t)\rangle = \int_0^{t_f} \langle \chi_{2m}(z,t)|b_h(z)\chi_0(z+h,t)\rangle \tag{41}$$

for each $m \in \mathbb{N}$.

3.4 Kn in Josephson Junction

The quantity $\vec{K}_n$ can be evaluated using the following formula of eq. (34) where $\nabla H_N(\vec{\lambda}_0, t)$ is the gradient of the Hamiltonian of the system with respect to the control parameters.
The idea here is to start with the control parameter Λ that works for the STA protocol and add another polynomial $P_{\vec{\lambda}}(t)$ that would take some values $\vec{\lambda} = (\lambda_1, ..., \lambda_n)$ in the interval for some $t \in [t_1, t_n]$ with $\lambda_1 = \lambda_n = 0$, and $t_1 = t_0, t_n = t_f$. We can consider values $(\lambda_1, ..., \lambda_n)$ as variables and then define a new $\tilde{\Lambda}(t) = \Lambda(t) + P_{\vec{\lambda}}(t)$ where $\nabla H_N(\vec{\lambda}_0, t)$ means $(\partial_{\lambda_1} H_N, ..., \partial_{\lambda_n} H_N)$. Since we want to interpolate just for a limited number of points, it is helpful to use the Lagrange interpolation that would take the form

$$P_{\vec{\lambda}}(t) = \sum_{j=1}^{n} \lambda_j \prod_{\substack{k=1 \\ k\neq j}}^{n} \frac{t-t_k}{t_j-t_k}. \tag{42}$$

It can be simplified even further by recalling that $\lambda_1 = \lambda_n = 0$

$$P_{\vec{\lambda}}(t) = \sum_{j=2}^{n-1} \lambda_j \prod_{\substack{k=2 \\ k\neq j}}^{n-1} \frac{t-t_k}{t_j-t_k}. \tag{43}$$

Recalling the form of H_N from eq. (22) we can see that the only part dependent from λ_i is the z^2 term. Now taking the gradient of H_N with respect to the control parameters in this case only amounts to perform the following derivatives

$$\partial_{\lambda_i} H_N = \partial_{\lambda_i} \tilde{\Lambda}(t) z = \partial_{\lambda_i}\left(\Lambda z^2 + P_{\vec{\lambda}}(t) z^2\right) = z^2 \prod_{\substack{k=2 \\ k\neq i}}^{n-1} \frac{t-t_k}{t_i-t_k} \tag{44}$$

We are now in a position to calculate the following quantity

$$\langle \chi_m|\partial_{\lambda_i} H_N|\chi_0\rangle = \prod_{\substack{k=2 \\ k\neq i}}^{n-1} \frac{t-t_k}{t_i-t_k} \langle \chi_m|z^2|\chi_0\rangle \tag{45}$$

and we can recall that this integral is non-zero only for $m = 2$.

3.5 Final formulation of the corrections in Josephson Junction

If we apply the results we obtained in the previous section, we can see that the only non zero values are $\vec{K}_2$ and G_2. In such a way that eq. (37) eq. (38) simplify significantly, and we can write

$$\vec{v} = \mathrm{Re}(G_2^* \vec{K}_2) \tag{46}$$

$$\mathrm{H}_{l,k} = \left(\vec{K}_2^*\right)_k \left(\vec{K}_2\right)_l \tag{47}$$

3.6 Useful Integrals

For the sake of the argument here we will write down the solution to two of the integrals we need to calculate and which are analytically solvable.

$$\langle \chi_2 | z^2 | \chi_0 \rangle = \int_{\mathbb{R}} dz \chi_2^*(z,t) z^2 \chi_0(z,t) = e^{2i \int_0^t dt\, \omega_0 / b^2} \frac{\sqrt{2} hb}{\omega_0} \tag{48}$$

$$\langle \chi_2 | \partial_z^2 | \chi_0 \rangle = \int_{\mathbb{R}} dz \chi_2^*(z,t) \partial_z^2 \chi_0(z,t) = e^{2i \int_0^t dt\, \omega_0 / b^2} \frac{\left(\omega_0 - ib\dot{b}\right)^2}{\sqrt{8} h \omega_0 b^2} \tag{49}$$

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