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Numerically solving the Schrödinger Equation for SQUID rings

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ABSTRACT

Here we present some mathematical and computational tools for the numerical analysis of SQUID rings. Much of this text is taken from my own thesis based on work done by many others and as such this does not comprise original research (although this collated form of the information has not, to the best of our knowledge, been published in this form elsewhere). Instead this paper is intended as a quick start guide for those interested in numerical modelling of SQUID ring based systems.

INTRODUCTION

The (flux mode) Hamiltonian for the SQUID ring in an external magnetic field Φ_x, is given by

$$H = \frac{Q^2}{2C} + \frac{(\Phi - \Phi_x)^2}{2\Lambda} - \frac{\hbar I_c}{2e}\cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \qquad (1)$$

where the magnetic flux threading the ring, Φ, and the total charge across the weak link Q take on the roles of conjugate variables for the system with the imposed commutation relation $[\Phi, Q] = i\hbar$. Here Φ_x is the external applied magnetic flux and incorporates the drive term for the ring. Here C, I_c, and L are, respectively, the external flux bias, capacitance and critical current of the weak link and the inductance of the ring. We will define $\hbar\nu = \frac{\hbar I_c}{2e}$. Finally, $\Phi_0 = h/2e$ is the flux quantum. We have assumed here that the microwave field that is introduced to the system can be modeled in the way that it couples to the external flux as a purely classical field. For later connivance we separate this into two components according to $\Phi_x(t) = \Phi_{x_{\text{stat}}} + \Phi_{\text{dynamic}}(t)$ where $\Phi_{x_{\text{stat}}}$ is the static magnetic flux bias and the time dependent microwave field is given by $\Phi_{\text{dynamic}}(t)$. It is immediately evident that while the first two terms of this Hamiltonian present no problems for numerical analysis -- being the driven simple harmonic oscillator -- the cosine term is somewhat harder to work with. It is in dealing with this term that this paper is focused. As this paper is approached very much a tutorial style references will not be given throughout instead the reader is refereed to two key works in this field (and references therein), namely (Bossche, Brouers, Spiller, Clark, Prance, and Diggins,1995; Diggins, Ralph, Everitt, Prance, Prance, Whiteman, Widom, and Srivastava,1998).

DISCUSSION

Here we discuss the method that we use to computationally solve the time independent Schrdinger equation (TISE) and time dependent Schrdinger equation (TDSE) for the SQUID. This comprises of several stages, firstly we outline the method used to solve the TISE for the SQUID as the instantaneous eigenvectors for the Hamiltonian (1) orm an ideal basis for expanding the solutions to the TDSE, we then proceed to express the TDSE as a set of first order coupled ordinary differential equations, so that standard methods (such as Runge Kutta) for initial value problems can be applied. Finally we discuss the computation of the expectation values of the observables for energy and screening current.

A. THE TISE

If we consider the Hamiltonian (1) we notice that if we translate the co-ordinate Φ by Φ_x, the external flux term would appear in the Josephson current term, so that we are left with a Hamiltonian that consists of a simple harmonic oscillator term and a non-trivial perturbation due to the Josephson junction. The unitary transform needed to do this is given by

$$V(t) = \exp\left(-i\,\frac{\Phi_x(t)Q}{\hbar}\right) \qquad (2)$$

Then the translation is performed on the Hamiltonian in the usual way to obtain

$$V^{?}(t)H(t)V(t) = \frac{Q^2}{2C} + \frac{\Phi^2}{2\Lambda} - \hbar\nu\cos\left(\frac{2\pi(\Phi+\Phi_x(t))}{\Phi_0}\right) \qquad (3)$$

Solving the eigenvalue problem for a Hamiltonian of this form is achieved by using the simple harmonic oscillator sates (denoted here by $|n\rangle$ and $|m\rangle$) as a basis for expanding the eigenfunctions and computing the Heisenberg matrix representation of the Hamiltonian in this basis. Eigenvectors and eigenvalues may then simply be found using standard numerical techniques. In order to compute these matrix elements we first note:

$$\left\langle n\left|\frac{Q^2}{2C}+\frac{\Phi^2}{2\Lambda}-\hbar\nu\cos\left(\frac{2\pi(\Phi+\Phi_x(t))}{\Phi_0}\right)\right|m\right\rangle = \left\langle n\left|\frac{Q^2}{2C}+\frac{\Phi^2}{2\Lambda}\right|m\right\rangle - \hbar\nu\left\langle n\left|\cos\left(\frac{2\pi(\Phi+\Phi_x(t))}{\Phi_0}\right)\right|m\right\rangle \quad (4).$$

We then expand the cosine term to obtain:

$$\left\langle n\left|\cos\left(\frac{2\pi(\Phi+\Phi_x(t))}{\Phi_0}\right)\right|m\right\rangle = \cos\left(\frac{2\pi\Phi_x(t)}{\Phi_0}\right)\left\langle n\left|\cos\left(\frac{2\pi\Phi}{\Phi_0}\right)\right|m\right\rangle - \sin\left(\frac{2\pi\Phi_x(t)}{\Phi_0}\right)\left\langle n\left|\sin\left(\frac{2\pi\Phi}{\Phi_0}\right)\right|m\right\rangle \quad (5).$$

The problem now reduces to computing $\left\langle n\left|\cos\left(\frac{2\pi\Phi}{\Phi_0}\right)\right|m\right\rangle$ and $\left\langle n\left|\sin\left(\frac{2\pi\Phi}{\Phi_0}\right)\right|m\right\rangle$. While this may seem initially complicated the solution is found simply by using the power series expansion of $\sin$ and $\cos$. For finite values of n and m these matrix elements are quite straight forward to compute. Below we show and example Java method for computing $\left\langle n\left|\cos\left(\frac{2\pi\Phi}{\Phi_0}\right)\right|m\right\rangle$ (we leave the other term for the reader to derive). This method takes in a scaling factor (allowing the use of different, natural, units) and an array of $\ln(\Gamma(n))$ and results are placed in the object NCM.

```
private void ncm(double f,double GammLn[])
        double sum, temp1, temp2;
        int    n, nmax, i, j, row, column;
        for(row=0;row<dimension;row++) {
            for(column=0;column<dimension;column++) {
                sum=0.0;
                nmax=((row<column)?row:column);
                for (n=0;n<=nmax;++n) {
                    i=row+column-2*n;
                    if(((i>>1<<1) == i) || i==0) {
                        j=i/2;
                        temp1=Math.pow(f,i)*2.0;
                        temp1 =Math.exp(0.5*GammLn[row]+0.5*GammLn[
                        column]
                                    -GammLn[n]-GammLn[row-n]-GammLn[
                                    column-n]);
                        temp2=(((j>>1<<1)==j)?1.0:-1.0); // -1^j
                        sum+=temp1*temp2/2.0;
                    }
                }
                NCM.set(row,column,sum*Math.exp(-f*f/2.0));
            }
        }
    }
```

Hence, computing the matrix element of the ring Hamiltonian is readily broken down into relatively straightforward tasks. We note that the eigenvectors of the Hamiltonian form a very efficient basis for solving the TDSE. However, when we consider the TDSE in that has been translated in this way we obtain and extra term in the Hamiltonian. Hence the effective Hamiltonian is given by

$$\mathbf{H} = V^{?}(t)H(t)V(t) - i\hbar V^{\dagger}(t)\frac{\partial}{\partial t}V(t) \qquad (6)$$

which yields a time dependent Hamiltonian effective of the form.

$$\mathbf{H} = \frac{Q^2}{2C} + \frac{\Phi^2}{2\Lambda} - \hbar\nu\cos\left(\frac{2\pi(\Phi+\Phi_x(t))}{\Phi_0}\right) - Q\frac{\partial}{\partial t}\Phi_x(t). \qquad (7)$$

B. The TDSE

The choice of a basis with which to find the solutions of the time dependent Schrödinger equation is of great importance -- an inefficient choice of basis would increase computational time dramatically. In the time independent case we chose the eigenstates of the simple harmonic oscillator basis, as this is very effective for small values of $\hbar\nu$ because the Josephson current acts as a perturbation on what is essentially a simple harmonic oscillator Hamiltonian. When the external field is time dependent however it becomes sensible to use a time dependent co-moving

basis, i.e. solutions of the Schrödinger equation at that point in time can be represented using relatively few basis sates that are the instantaneous eigenvectors of equation (3).
As this operator (3) is Hermitian we know that it's eigenvalues are real and moreover if the eigenvalues are non-degenerate (which they are) the eigenvectors of this operator form a complete orthogonal basis set. Moreover we are freely allowed to normalise these eigenvectors to obtain a orthonormal basis that spans the whole function space. we will represent these states by $|\kappa\rangle$
We wish to solve the equation

$$\mathrm{H}\left|\psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle \qquad (8)$$

We do this by representing $|\psi\rangle$ as a series expansion of the instantaneous eigenstates of (3). That is we will reduce the complexity of finding solutions to the time dependent Schrödinger equation by representing them in terms of an efficient basis set. we already know how to construct this basis as it is an identical problem to the eigen problem of the time independent Schrödinger equation. Consequently is is simple to reduce to a a set of first order differential equations for the coefficients of the basis sates that can be found computationally using standard methods such as Runge Kutta integration. Representing $|\psi(t)\rangle$ as a linear combination of the states $|\kappa(t)\rangle$ yields

$$\left|\psi(t)\right\rangle = \sum_{\kappa=0}^{\infty} b_{\kappa}(t)\left|\kappa(t)\right\rangle \qquad (9)$$

where the $b_{\kappa}(t)$ are unknown. By direct substitution from 7 we get an equation of the form

$$\sum_{k=0}^{\infty}\left\{V^{\dagger}(t)H(t)V(t) - Q\frac{\partial}{\partial t}\Phi_x(t)\right\}b_k\left|\kappa(t)\right\rangle = i\hbar\sum_{k=0}^{\infty}\frac{\partial}{\partial t}\left\{b_{\kappa}(t)\left|\kappa(t)\right\rangle\right\} \qquad (10)$$

now we use the fact that we are using eigenstates of the operator VHV as basis states and we project on the left by another eigenstate of $V^{\dagger}HV$ and use the orthonormality of these eigenstates to obtain

$$b_{\lambda}E_{\lambda} - \frac{\partial}{\partial t}\Phi_x(t)\sum_{k=0}^{\infty}\left\langle\lambda(t)\right|Q\left|\kappa(t)\right\rangle = i\hbar\left\{\frac{\partial}{\partial t}b_{\lambda}(t) + \sum_{k=0}^{\infty}b_{\kappa}(t)\left\langle\lambda(t)\left|\overrightarrow{\frac{\partial}{\partial t}}\right|\kappa(t)\right\rangle\right\} \qquad (11)$$

where $E_{\kappa}(t)$ is the eigenvalue corresponding to the eigenvector $|\kappa(t)\rangle$ of the operator $V^{\dagger}HV$ at time t and the arrow is used to denote upon which state the time derivative operator acts. Now recall that we get the states $|\kappa(t)\rangle$ from solving the eigenvalue equation for $V^{\dagger}HV$ using an expansion in terms of eigenvectors $|n\rangle$ of the simple harmonic oscillator, that is

$$\left|\kappa(t)\right\rangle = \sum_{n=0}^{\infty}v_{\kappa,n}\left|n\right\rangle \qquad (12)$$

note that the coefficients $v_{\kappa,n}$ are purely real. The charge operator Q (in analogy to the momentum operator) has the following expectation value with the simple harmonic oscillator states $|n\rangle$

$$\left\langle m\left|Q\right|n\right\rangle = i\sqrt{\frac{\hbar\omega_0 C}{2}}\left(\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}\right) \qquad (13)$$

where $\omega = 1/\sqrt{C\Lambda}$. Now we can consider the $\langle\lambda(t)|Q|\kappa(t)\rangle$ term in equation (11) using this

relation and the eigenstate expansion given in equation (12)

$$\left\langle \lambda(t)\left|Q\right|\kappa(t)\right\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} v_{\kappa,m} v_{\lambda,n} \left\langle m\left|Q\right|n\right\rangle = i\sqrt{\frac{\hbar\omega_0 C}{2}} \sum_{m=0}^{\infty} v_{\kappa,m} v_{\kappa,m+1}\sqrt{m+1} - v_{\kappa,m-1} v_{\kappa,m}\sqrt{m} \quad (14)$$

In order to get all the terms in this equation in a form we can handle we expand the last term in equation (11) in terms of simple harmonic oscillator states.

$$\left\langle \lambda(t)\left|\frac{\overrightarrow{\partial}}{\partial t}\right|\kappa(t)\right\rangle = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} v_{\kappa,m}\frac{\partial}{\partial t} v_{\kappa,n}\left\langle m\left|n\right.\right\rangle = \sum_{m=0}^{\infty} v_{\lambda,m}\frac{\partial}{\partial t} v_{\kappa,m} = \frac{\partial\Phi_x}{\partial t}\sum_{m=0}^{\infty} v_{\kappa,m}\frac{\partial v_{\kappa,m}}{\partial\Phi_x} \quad (15)$$

In the last part of this equation we have expressed the time derivative of the $v_{\kappa,m}$ term in terms of the external flux as this proves to be convenient for computational purposes, in that $\dot{\Phi}_x(t)$ can be expressed analytically and $\partial v_{\kappa,m}/\partial\Phi_x(t)$ is just a simple division in the code.

Expressing the magnetic flux in terms of Φ_0 using the notation $\varphi = \Phi/\Phi_0$. Now for convenience we define a lookup table function $\mathcal{L}$ that contains all the elements that we can get from the previous TISE calculation.

$$\mathcal{L}_{\lambda,\kappa} = \sum_{m=0}^{\infty} v_{\lambda,m}\left(\alpha\left(v_{\kappa,m+1}\sqrt{m+1} - v_{\kappa,m-1}\sqrt{m}\right) - \frac{\partial v_{\kappa,m}}{\partial\varphi_x(t)}\right) \quad (16)$$

where

$$\alpha = \frac{1}{\hbar\Phi_0}\sqrt{\frac{\hbar\omega_0 C}{2}} \quad (17)$$

rearranging equation (11) we get

$$i\hbar\frac{\partial}{\partial t} b_\lambda(t) = b_\lambda E_\lambda(t) - \sum_{\kappa=0}^{\infty} b_\kappa(t)\left(\frac{\partial}{\partial t}\Phi_x(t)\left\langle\lambda(t)\left|Q\right|\kappa(t)\right\rangle + i\hbar\left\langle\lambda(t)\left|\frac{\overrightarrow{\partial}}{\partial t}\right|\kappa(t)\right\rangle\right) \quad (18)$$

so that

$$\frac{\partial}{\partial t} b_\lambda(t) = -\frac{i}{\hbar} b_\lambda E_\lambda(t) + \frac{i}{\hbar}\frac{\partial\Phi_x(t)}{\partial t}\sum_{\kappa=0}^{\infty} b_\kappa(t)\left(\left\langle\lambda(t)\left|Q\right|\kappa(t)\right\rangle + i\hbar\sum_{m=0}^{\infty} v_{\lambda,m}\frac{\partial v_{\kappa,m}}{\partial\Phi_x}\right) \quad (19)$$

which we can express in the more compact and useful form

$$\frac{\partial}{\partial t} b_\lambda(t) = -\frac{i}{\hbar} b_\lambda E_\lambda(t) + \frac{\partial\varphi_x(t)}{\partial t}\sum_{\kappa=0}^{\infty} b_\kappa(t)\,\mathcal{L}_{\lambda,\kappa}(\varphi_x(t)) \quad (20)$$

The solution to the problem is now reduced to finding the coefficients b_κ in equation (20). This is just a set of first order coupled differential equations. Because we have to solve these equations numerically we must take only a finite number of coefficients in all the expansion given. In equations (9) and (16) typical limits are approximately the first 30 terms and we typically use 4 eigenstates of the ring Hamiltonian in equation (20). Note that the choice of the number of simple harmonic oscillator states used to solve the rings eigenproblem is key to the calculations as it sets the number of simple harmonic oscillator states used in setting up the instantaneous eigenstates that we use as a basis. As we have deliberately chosen this basis because it is very efficient. Hence, any error will propagate though the rest of the computation.

C. EXPECTATION VALUES OF OBSERVABLES

1. We are mainly interested in the expectation value of two observables, firstly the energy as this is essential to understanding the physics of the system, and secondly the screening current, because it is though the screening current that we model the interaction of the SQUID with the classical measurement device (the tank circuit) [Bossche, et al (1995); Clark et al (1998).]the expectation value of the energy is simply

$$\langle H \rangle = \langle \Psi \mid H \mid \Psi \rangle = \langle \psi \mid V^{\dagger} H V \mid \psi \rangle = \sum_{\kappa=0}^{\infty} |b_{\kappa}(t)|^2 \, E_{\kappa}(\Phi_x(t)) \qquad (21)$$

as seen in the pervious chapter, the screening current operator is defined to be

$$I_s = -\frac{\partial H}{\partial \Phi_x} = \frac{\Phi - \Phi_x(t)}{\Lambda} \qquad (22)$$

and this has an expectation value given by

$$\langle I_s \rangle = \left\langle \Psi \left| \frac{\Phi - \Phi_x(t)}{\Lambda} \right| \Psi \right\rangle = \left\langle \psi \left| V^{\dagger} \left(\frac{\Phi - \Phi_x(t)}{\Lambda} \right) V \right| \psi \right\rangle = \frac{1}{\Lambda} \langle \psi \left| \Phi \right| \psi \rangle \qquad (23)$$

but in the algorithm we use to solve the TDSE we expand ψ in terms of the instantaneous energy eigenstates of the operator $V^{\dagger} H V$ which in turn is expanded in terms of simple harmonic oscillator basis states, i.e.

$$|\psi\rangle = \sum_{\kappa=0}^{\infty} b_{\kappa} |\kappa(t)\rangle = \sum_{\kappa=0}^{\infty} b_{\kappa} \sum_{\kappa=0}^{\infty} v_{\kappa,n} |n\rangle \qquad (24)$$

from this an the fact that

$$\langle m \mid \Phi \mid n \rangle = \sqrt{\frac{\Lambda \hbar \omega_0}{2}} \left(\sqrt{(n+1)} \delta_{m,n+1} + \sqrt{n} \delta_{m,n-1} \right) \qquad (25)$$

we obtain

$$\langle I_s \rangle = \sqrt{\frac{\hbar \omega_0}{2\Lambda}} \sum_{\lambda=0}^{\infty} \sum_{\kappa=0}^{\infty} \sum_{n=0}^{\infty} b_{\lambda}^{*} b_{\kappa} \left(\sqrt{n+1} v_{\lambda,n} v_{\kappa,n+1} + \sqrt{n} v_{\lambda,n} v_{\kappa,n-1} \right) \qquad (26)$$

We have now expressed the energy and screening current operators in terms of quantities that we obtain trough solving the time dependent Schrödinger equation for the system.

CONCLUDING REMARKS :

In this paper we have set out a number of tips and tricks on dealing with the numerical analysis of simple SQUID rings. We have presented sufficient information to allow the reader to begin to tackle both time independent and time dependent problems. We hope that it will be of use to any reader wishing to start working in this area.

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حلول عددية لمعادلة شرودنجر فى المواد فائقة التوصيل

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الملخص

نقدم فى هذا البحث بعض الوسائل الرياضية والحسابية للتحليل العددي للمواد فائقة التوصيل للتيار الكهربى . العديد من نتائج فى هذا البحث مستقاة عن أطروحتي الخاصة والقائمة على بعض نتائج الآخرين، وهذا بالتالي لا يحتوي على جوهر البحث(وعلى حد علمي أن هذه المعلومات لم تنشر بعد) وعوضاً عن ذلك تقدم الورقة لمحة سريعة للذين يرغبون في النمذجة العددية للمواد فائقة التوصيل للتيار الكهربائي. وسوف نقدم هذه الورقة كدعم للباحثين للبدء السريع فى موضوع النمذجة الرياضية والمبنية على المواد فائقة التوصيل للتيار الكهربى.