THEORETICAL CALCULATION OF MUON SITE IN YBa$_2$Cu$_3$O$_x$

By

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We accept this thesis as conforming
to the required standard

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Abstract

The muon is a useful probe of magnetic fields in superconductors, but knowing the field seen by the muon is often of limited value until we know where the muon is in the crystal lattice. In this thesis I employ two independent theoretical methods to search for candidate muon sites: the potential energy field method, which seeks the minimum of the electrostatic potential of the $\mu^+$, and the magnetic dipolar field method, which compares the calculated magnetic field (due to the host electronic, atomic or nuclear dipolar fields) with the observed local fields at the muon.
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Chapter 1

Introduction

1.1 History of Muon Site Determination

The first $\mu^+$ site determination was performed in a single crystal of gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), in which the magnetic field due to the adjacent protons at fixed locations is well known. If the $\mu^+$ were mobile in the crystal, the dipolar fields of the protons would simply cause relaxation of the muon spin. However, if the muon replaces protons at fixed lattice sites, the Muon Spin Resonance ($\mu$SR) results should show exactly the same behavior as the proton NMR. The experiment showed the split-frequency muon precession expected for muons occupying proton sites, and thus gave the first positive identification of the $\mu^+$ site in a crystal. [1]

During the following years the $\mu$SR technique has been applied to metals, oxides, magnetic materials and superconductors to explore the internal magnetic and electronic structure. But without knowing the exact locations of the $\mu^+$ in the samples the information often has limited value.

The local magnetic field at a stopped $\mu^+$ site was measured in a single crystal of ferromagnetic cobalt as a function of temperature between 4 and 1100K by Graf. [2] The data are consistent with a relatively smooth temperature dependence of the hyperfine field only if it is assumed that the $\mu^+$ is at an octahedral interstitial site; the calculated local field at the tetrahedral site would imply a discontinuous hyperfine field. These facts lead to the conclusion that octahedral interstitial sites are preferred
by the $\mu^+$.  

The longlived metastable states of the $\mu^+$ in the magnetic oxide $\alpha$–Fe$_2$O$_3$ have also been studied. [3] Three separate frequencies were seen. This indicates that the muons are localized at three different local energy minima in the unit cell.  

Other muon site determinations have been performed on Cu, [5] Fe, [6] [7] and Si. [8] Lattice distortion plays a key role in determining the muon site in Alkali fluorides and semiconductors.  

One of the most interesting magnetic phenomena in a superconductor is the well known Meissner effect. When a type I superconductor is cooled in a magnetic field below its transition temperature, the magnetic flux is abruptly expelled, except for a thin surface layer where the field decays roughly exponentially on the scale of the London penetration depth $\lambda_L$. In a type II superconductor the magnetic flux penetrates into the interior of the sample in an array of “vortices” each carrying the flux quantum $\phi_0$ when the magnetic field is between $H_{c1}$ and $H_{c2}$. As a result, the internal magnetic field in the superconductor is inhomogeneous. The $\mu$SR technique can measure the mean magnetic field at the muon site (through the $\mu^+$ precession frequency) and its dispersion (through the $\mu^+$ relaxation rate).  

Experiments on superconducting GdBa$_2$Cu$_3$O$_7$ were performed in the temperature range from 30mK to 130K by A. Golnik. [9] In zero external field two different frequencies were distinguished, which correspond to internal magnetic fields of 33 and 52 mT, respectively. This shows that muons find two magnetically inequivalent stopping sites in the sample. Two types of muon stopping sites are in principle possible: interstitial sites and oxygen vacancy sites.  

So far there is no solid evidence to show the $\mu^+$ site in YBa$_2$Cu$_3$O$_7$. Our own TRIUMF [46] group predicts that $\mu^+$ stops primarily in a site close to the CuO$_2$ plane. The PSI [48] and Tokyo [47] groups claim that the $\mu^+$ stopping site is close to an oxygen
on the CuO chain. The only point of agreement is that the muon site is 1Å away from some oxygen ion.

So far no rigorous theoretical prediction has been made, due to the difficulties involved in evaluating electrostatic potentials and magnetic fields inside the superconductors. The current theoretical method is to apply the potential equation which best generates the \( \mu^+ \) sites in YBa\(_2\)Cu\(_3\)O\(_6\) to the case of YBa\(_2\)Cu\(_3\)O\(_7\). During the round-table discussion at the Vth International Conference on \( \mu \)SR in Oxford (1990), it became clear that one reason for the differences of opinion about the muon site in YBa\(_2\)Cu\(_3\)O\(_6\) is the uncertainty regarding the orientation of Cu magnetic moments which should lie in the Cu-O plane oriented along an \( \bar{a} \) or \( \bar{b} \) axis.

The initial approach taken to locating the muon site focussed on the antiferromagnetic (AFM) material YBa\(_2\)Cu\(_3\)O\(_6\), which has a magnetic structure consisting of strong nearest-neighbor correlated spins in adjacent copper planes which are aligned antiferromagnetically. This special case offers some hope of calculating the internal magnetic field at potential muon sites theoretically. The simulated results can be verified by comparing them with the experimental data.

The first study of local fields at muon sites in antiferromagnetic YBa\(_2\)Cu\(_3\)O\(_6+x\) was done by Nishida. [14] The experimental data show that there are at least two independent \( \mu^+ \) sites.

1.2 Space Group

A perfect crystal is constructed by an infinite regular repetition in space of identical structural units or building blocks. A space group, which consists of a Bravis lattice and a basis, displays all the symmetries of a crystal. Through the symmetry of the space group, one point generates several equivalent points at symmetric positions in a
Chapter 1. Introduction

Table 1.1: Transformations pmmm of YBa$_2$Cu$_3$O$_7$

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unit cell. Therefore, a space group fully represents a crystal structure. [10] [36] [13]

Neutron-diffraction experiments [12] have shown that YBa$_2$Cu$_3$O$_7$ has a pmmm structure and YBa$_2$Cu$_3$O$_6$ has similar structure but with 4 transformations instead of 8 for YBa$_2$Cu$_3$O$_7$. *i.e.*, every input ion site will generate 8 equivalent ion sites for YBa$_2$Cu$_3$O$_7$ and 4 equivalent ion sites for YBa$_2$Cu$_3$O$_6$, due to its antiferromagnetic structure.

In summary, the transformations of YBa$_2$Cu$_3$O$_7$ are pmmm and orthorhombic. Its startpoint, the origin of the cluster, is (0.0,0.0,0.0) which can be specified by users. The transformations of YBa$_2$Cu$_3$O$_6$ are p123 which is termed for convenience and tetragonal. Its startpoint is (0.0,0.0,0.0). Through such transformations, (1,1,1) represents a set of 4 sites at (1,1,1), (-1,-1,1), (1,-1,-1) and (-1,1,-1) for YBa$_2$Cu$_3$O$_6$ and a set of 8 sites at (1,1,1), (-1,-1,-1), (-1,-1,1), (1,1,-1), (1,-1,1), (-1,-1,1), (-1,1,-1), (-1,1,1), (-1,-1,1) and (1,-1,1) for YBa$_2$Cu$_3$O$_7$.

1.3 Muon Spin Resonance/Rotation/Relaxation ($\mu$SR)

The muon possesses a magnetic moment and a spin of $\frac{1}{2}$; hence it exhibits Larmor precession in a transverse magnetic field. After stopping inside the target, the implanted
Table 1.2: Transformations p123 of YBa$_2$Cu$_3$O$_6$

highly spin polarized positive muons, precess in the local field and decay ($\mu^+ \rightarrow e^+ + \nu_e + \bar{\nu}_\mu$) with a mean lifetime of 2.198$\mu$s. The decay positrons are emitted in directions correlated with the direction of the muon spin. Inhomogenenities of the local field will cause loss of muon spin ensemble polarization, termed depolarization, by dephasing.

In this case information about the internal or external field distribution can be derived from the experimental distribution of precession frequencies which are proportional to the local field. In general, the precession frequency $\omega$ and depolarization rate $\sigma$ are given by

$$\omega = \gamma_\mu H$$

$$\sigma = \gamma_\mu M_z^{\frac{1}{2}}$$

where $M_z \equiv \langle (H - \langle H \rangle)^2 \rangle$, $\omega = \langle H \rangle$ and $\gamma_\mu$ is the gyromagnetic ratio of the muon. Specific equations have to be derived for specific cases.

In this thesis two experimental techniques are referred to zero applied field (ZF) $\mu$SR and Level Crossing Resonance (LCR). In ZF-$\mu$SR the $\mu^+$ undergoes Larmor precession around the local magnetic field. For a local magnetic field given by $\vec{H} = (H_x, H_y, H_z)$ the muon spin initially polarized along the $z$ direction evolves as

$$P_z(t) = \frac{H_x^2}{H^2} + \frac{H_y^2 + H_z^2}{2H^2} \cos(\gamma_\mu H t)$$

$$= \cos^2 \theta + \sin^2 \theta \cos(\gamma_\mu H t)$$

(1.1)
where $\theta$ is the angle between $\vec{H}$ and the $\hat{z}$ direction. The internal field components are assumed to have a gaussian distribution

$$
\rho(H_i) = \frac{1}{\sqrt{(2\pi)\Delta}} \exp \left( -\frac{H_i^2}{2\Delta^2} \right), i = x, y, z
$$

where $\Delta^2 = \gamma^2 \langle H_i^2 \rangle$. The average of the polarization in the $z$ direction is

$$
P_z(t) = \int \int \int \rho(H_x) \rho(H_y) \rho(H_z) (\cos^2 \theta + \sin^2 \theta \cos \gamma \mu H t) d^3 H
$$

Evaluation of this equation leads to the well-known Kubo-Toyabe formula for the evolution of a static spin in zero field:

$$
P_z(t) = \frac{1}{3} + \frac{2}{3} (1 - \gamma \mu^2 \Delta^2 t^2) \exp \left( -\frac{1}{2} \gamma \mu^2 \Delta^2 t^2 \right)
$$

The application of LCR was first suggested by Abragam [15]; it quickly became one of the most valuable $\mu$SR techniques. The level-crossing occurs when the field strength is adjusted to match the energy splitting of the muon's Zeeman levels to those of the magnetic levels of the neighboring host nuclei (in this study, $^{17}$O), which are determined mainly by their quadrupolar interaction energies. Details of the LCR technique can be found in references [16] [17] [18] [19].
Chapter 2

Methods of Muon Site Determination

In this chapter two theoretical approaches are introduced to search for candidate muon sites: electrostatic potential mapping and dipolar magnetic field calculation.

2.1 Electrostatic Potentials

The principal interactions of the $\mu^+$ in ionic lattices are the static long-range Coulomb force and the overlap force, both of which are envisioned mainly as simple two-body forces; electronic polarization effects (in which an ion may be polarized by the resultant electric field due to other ions in the crystal) are considered to be less important. The $\mu^+$ interaction potential is the sum of all two-body interactions between the muon and other ions. The concept of an additive two-body interaction is only an approximation to reality; the wave mechanical calculations made by Lowdin [22] showed that an appreciable fraction of the lattice cohesive energy cannot be represented in terms of two-body interactions. Moreover, the effect of electronic polarization cannot be represented by a two-body interaction. However, the polarization effects are largely suppressed by the high symmetry of the structure so that the approximation is adequate for most purposes.

The Coulomb potential can be employed to describe the potentials of ions at distances much larger than their ionic radii; in insulating YBa$_2$Cu$_3$O$_x$ (as in most ionic oxides), this is a fair description of all the positive ions. In metallic YBa$_2$Cu$_3$O$_7$, attention should be paid to the screening effect of conduction electrons on the field due to
ions far away from the muon sites. For nearby ions, in this instance O$^{2-}$, the calculation is more difficult. I resort to a familiar approximation, namely the Morse-like potential, which is frequently used for quantum mechanical calculations in solid state physics to calculate the potentials between $\mu^+$ and O$^{2-}$:

$$V(r) = \frac{A}{r} + B \exp \left( -\frac{r - r_0}{\rho} \right) - \frac{\vec{r} \cdot \vec{p}}{r^3},$$  \hspace{1cm} (2.3)$$

where $A = Z e$ and $r$ is the $\mu^+\text{-}O^{2-}$ distance. The first term arises from the Coulomb interaction between $\mu^+$ and O$^{2-}$. The second term is the Morse-like potential, which represents the major part of the $\mu^+\text{-}O^{2-}$ potential. The semi-empirical constants $B$ and $\rho$ are determined by experiment, and $r_0$ is the equilibrium $\mu^+\text{-}O^{2-}$ bond length. The third term arises from the interaction of $\mu^+$ with the induced electric dipole moments by the muon on the O$^{2-}$ ions, $\vec{p}$.

The induced moment was determined from the following procedure. A unit dipole $p_0$ was placed on a test O$^{2-}$ ion giving a dipole moment of $\vec{p}_1 = p_0 \hat{i}$ on this ion, where $\hat{i}$ is a unit vector along $x$. The electric field at the test ion produced by these other dipole moments is given by $\vec{E}_1 = (E_{1x}, E_{1y}, E_{1z})$. This procedure was repeated with unit dipole moments along the $y$ and $z$ axes of the test ion, $\vec{p}_2 = p_0 \hat{j}$ and $\vec{p}_3 = p_0 \hat{k}$; the corresponding electric fields calculated at the test ion are given by $\vec{E}_2 = (E_{2x}, E_{2y}, E_{2z})$ and $\vec{E}_3 = (E_{3x}, E_{3y}, E_{3z})$. The net dipole moment at the O$^{2-}$ ion can be written

$$\vec{P} = p_0 \hat{i} + p_0 \hat{j} + p_0 \hat{k}$$

This moment is induced by the electric field due to the point charges of all the other ions $\vec{E}_0$ plus the electric field due to induced dipole moments on all the other O$^{2-}$ ions. Thus,

$$\vec{p} = \alpha_0[\vec{E}_0 + (1/p_0)(p_x \vec{E}_1 + p_y \vec{E}_2 + p_z \vec{E}_3)],$$

where $\alpha_0$ is the polarizability of O$^{2-}$ in YBa$_2$Cu$_3$O$_x$. The last two equations can be
Chapter 2. Methods of Muon Site Determination

written as a set of three simultaneous equations:

\[ p_x = \alpha_0[E_{0x} + (1/p_0)(p_x E_{1x} + p_y E_{2x} + p_z E_{3x})], \]  
(2.4)

\[ p_y = \alpha_0[E_{0y} + (1/p_0)(p_x E_{1y} + p_y E_{2y} + p_z E_{3y})], \]  
(2.5)

\[ p_z = \alpha_0[E_{0z} + (1/p_0)(p_x E_{1z} + p_y E_{2z} + p_z E_{3z})]. \]  
(2.6)

If \( E_0 \) and \( (1/p_0)(p_x \bar{E}_1 + p_y \bar{E}_2 + p_z \bar{E}_3) \) could be derived from a lattice-sum calculation, then these equations would be solved for \( p_x, p_y, \) and \( p_z. \)

In order to fix the parameters in Eq.(2.2), I simplified the model. First, no consideration was given to any screening effects, which would introduce a screening factor to the first term. However, one reference is given here for those interested in solving screening effects. Given the electron density, the charge distribution in the \( \mu^+ - O^{2-} \) could be estimated as for OH\(^-\), [20] and the screening factor could be fixed. Second, the dipolar part is suppressed by the high symmetry of the structure, so it was neglected.

Recent ZF-\( \mu S\bar{R} \) and wTF experiments on \( ^{17}\)O-doped YBa\(_2\)Cu\(_3\)O\(_7\) [21] place the \( \mu^+ \) approximately 1 \( \text{\AA} \) away from some oxygen ion; LCR-\( \mu S\bar{R} \) measurements suggest specifically the O(2, 3) oxygen in the CuO\(_2\) planes. Previous ZF-\( \mu S\bar{R} \) experiments [23] [24] on AFM YBa\(_2\)Cu\(_3\)O\(_6\) provide some constraints on the local field. Based on this foreknowledge, and assuming that the muon’s site preference will not be much affected by oxygen deficiency in YBa\(_2\)Cu\(_3\)O\(_6\), I narrowed my search down to a small ensemble of candidate sites within one unit cell. This allowed me to fix certain necessary parameters in the semi-empirical equations with which I calculated the crystal potential in superconducting YBa\(_2\)Cu\(_3\)O\(_7\) to better locate the muon sites,

\[ V_i(r) = \frac{Q}{r} + \frac{|Q|}{r_0} e^{(19.4 - 25r/\text{\AA})}, \]

where \( Q \) is the valence of the ion and \( r_0 \) is the ion’s hard core radius. The first term
Figure 2.1: Potential $V_i(r)$ vs $R$

is the Coulomb potential and the second term is the repulsive overlap potential. This choice of parameters ensures that the muon-oxygen bond length is $1 \text{ Å}$.

The total potential at the $\mu^+$ is in the form

$$V_{tot} = \sum_{i=1}^{N} V_i(r)$$

The summation has been carried out in two regions defined by a spherical boundary with finite radius. Upon the assumption of zero net charge in the unit cell, the coulomb contribution of ions outside this sphere goes to zero as long as the distance from that unit cell to the $\mu^+$ site is long enough compared with its dimensions, because this unit cell can be considered as a point with zero net charge. The contributions from included ions are simply summed. The exponential term is convergent. Therefore the
convergence of this sum is ensured by assuming that the net charge of the unit cell is zero.

Another general method for calculating the interionic potentials, based on the density functional approximation to the energy of an electron gas, is introduced here but not used in this thesis because of the difficulties of finding the electron densities in $\text{YBa}_2\text{Cu}_3\text{O}_x$. Gordon and Kim [26] assumed that the interatomic interactions between all charges must be evaluated from the additive atomic densities. For a pair of ions, $\text{AB}$, the total density $\rho_{\text{AB}}(r)$ is assumed to be the sum of the separated ion densities $\rho_A(r)$ and $\rho_B(r)$; the total energy is therefore given by

$$E_{\text{AB}} = E[\rho_{\text{AB}}] = E[\rho_A + \rho_B]$$

so that the interaction energy can be written as

$$E_{\text{int}} = E[\rho_A + \rho_B] - E[\rho_A] - E[\rho_B]$$

This is the essence of the approximation to the interionic potential.

The energy of an isolated, closed-shell ion is given by

$$E[\rho] = C_k \int [\rho(r)]^{5/3} dr + C_e \int [\rho(r)]^{4/3} dr - Z \int \rho(r)/rdr$$

$$\frac{1}{2} \int \int \frac{\rho(r)\rho(r')}{|r - r'|} drdr' + \int \epsilon_c[\rho(r)]\rho(r)dr$$

in which $Z$ is the nuclear charge, $\rho$ is the ion density and

$$C_k = (3/10)(3\pi^2)^{2/3} \quad \text{and} \quad C_e = -(3/4)(3/\pi)^{1/3}.$$  

The first four terms represent the kinetic, exchange and coulomb energies respectively, while the final term is an estimate of the electron pair correlation energy. The correlation energy density $\epsilon_c[\rho(r)]$ is simply an interpolation between the high and low density limits.
The Coulombic interaction of this pair is given by

\[ V_c = Z_A Z_B / R - Z_B \int \frac{\rho_A(r_1)}{r_{1B}} dr_1 - Z_A \int \frac{\rho_B(r_1)}{r_{1A}} dr_2 + \int \int \frac{\rho_A(r_1) \rho_B(r_2)}{r_{12}} dr_1 dr_2 \]  

(2.7)

The electron-gas contribution to the interatomic interaction is

\[ V_g = \int \{ [\rho_A(r) + \rho_B(r)] E_G[\rho_A(r) + \rho_B(r)] - \rho_A(r) E_G[\rho_A(r)] - \rho_B(r) E_G[\rho_B(r)] \} dr \]

The final form for \( E_{\text{int}} \) is thus,

\[ E_{\text{int}}(R) = Z_A Z_B / R - Z_B \int \frac{\rho_A(r_1)}{r_{1B}} dr_1 - Z_A \int \frac{\rho_B(r_1)}{r_{1A}} dr_2 + \int \int \frac{\rho_A(r_1) \rho_B(r_2)}{r_{12}} dr_1 dr_2 \]

\[ + \int \{ [\rho_A(r) + \rho_B(r)] E_G[\rho_A(r) + \rho_B(r)] - \rho_A(r) E_G[\rho_A(r)] - \rho_B(r) E_G[\rho_B(r)] \} dr \]

in which

\[ E_G[\rho(r)] = C_k[\rho(r)]^{2/3} + C_e[\rho(r)]^{1/3} + \epsilon_e[\rho(r)] \]

and \( r, r_{1A}, r_{1B} \) and \( r_{12} \) are functions of the internuclear separation, \( R \).

Here only nearest-neighbour interactions are included in the lattice summations. The next-nearest-neighbour interactions lead to an overestimate of the cohesive energy. Rae [27] pointed out that the exchange energy in the equation includes a self-energy contribution which, though negligible for an infinite electron gas, is significant for a small, finite number of electrons and leads to an overestimate of the exchange energy in the interaction of two light atoms or ions. A correction has been made by replacing the exchange term by a modified contribution,

\[ V_e(GKR) = V_e(GK)[1 - 8/3\delta + 2\delta^2 + 1/3\delta^4] \]
in which $\delta$ is a solution of

$$(4N)^{-1} = \delta^3(1 - 9/8\delta + 1/4\delta^3)$$

and $N$ is the number of electrons.

It has been concluded that for solids such as the alkali and alkaline-earth halides and the alkaline-earth oxides, which are largely ionic, the modified electron-gas approximation is a reliable non-empirical method for the calculation of interionic potentials. [28] [29] [30]

One different potential assumption is also used by W.K. Dawson et al. [32] They assume that the muon-oxygen bonding potential has the form

$$V = \left( -\frac{a}{r} + \frac{b}{r^6} \right) 14.4 eV$$

where $r$ is the $\mu^+-O^{2-}$ distance in Å and $a$, $b$, and $c$ are semiempirical constants ($a = +0.359, b = 0.0531, c = +8.32$). The calculations are carried out within a finite sphere of radius on the order of 50Å. Convergence of the lattice sum is ensured by assuming that the net charge of the unit cell is zero.

2.2 Dipolar Magnetic Fields

In the zero field (ZF) case, [31] the local magnetic field at the $\mu^+$ is usually split up into two contributions:

$$\vec{H} = \vec{H}_{hf} + \vec{H}_{dip}$$

where the dipolar field contribution is from the $\mu^+-O^{2-}$ interaction. The hyperfine field $\vec{H}_{hf}$ results from the contact interaction between the $\mu^+$ and any polarized electrons density at the muon site. When covalent bond effects occur as in muon-oxygen bond formation, $\vec{H}_{hf}$ is mostly due to these effects. Generally $\vec{H}_{hf} = \frac{8\pi}{3} [n^+(\vec{r}_\mu) - n^-(\vec{r}_\mu)]$, 
where \( n^+(\vec{r}_\mu) \) is the density of spin-up electrons at the \( \mu^+ \) and \( n^-(\vec{r}_\mu) \) the corresponding spin-down density. In the case of \( \alpha-\text{Fe}_2\text{O}_3 \) the hyperfine effect is due to electron spin transfer into unoccupied metal 3d-orbitals, which causes spin polarization of the oxygen 2p-orbitals. These 2p-orbitals overlap with the muon s-orbitals, resulting in a nonzero spin density at the muon site. In order to estimate \( \vec{H}_{hf} \) for a muon participating in a “muoxyl bridge”, Sawatzky [33] pictures a simple arrangement of one oxygen ion surrounded by metal ions; only those metal ions which form a direct link with the muoxyl bridge were taken into account. For this simple structure \( \vec{H}_{hf} \) is assumed to be the sum of the contributions of the linkages:

\[
\vec{H}_{hf} = C \cdot \sum_i [(A^2_\sigma - A^2_\pi) \cos^2 \theta_i + A^2_\pi] \vec{S}_i
\]

where \( \vec{S}_i \) is the unit vector of the magnetic moment of the metal ion, \( C \) is a constant, \( \theta \) is the angle between the metal-oxygen and muon-oxygen directions and \( A^2_\sigma \) and \( A^2_\pi \) are the magnitudes of the spin polarization of oxygen orbitals with \( \sigma \) and \( \pi \) symmetry. The spin density at the muon is proportional to \( (A^2_\sigma - A^2_\pi) \cos^2 \theta_i + A^2_\pi \).

Here I neglect \( \vec{H}_{hf} \) in the case of antiferromagnetic \( \text{YBa}_2\text{Cu}_3\text{O}_6 \), because of too small electron spin density at muon site, and assume that the field at the muon arises mainly from the dipolar magnetic fields of surrounding atoms. The dipolar field is

\[
\vec{H}_i = \left( \frac{\mu_i}{r^3_i} \right) [3(\hat{\mu}_i \cdot \hat{r}_i)\hat{r}_i - \hat{\mu}_i]
\]

where \( \vec{H}_i \) is the field generated by the \( i^{th} \) magnetic moment, \( \vec{r}_i \) is the vector distance from that magnetic moment to the muon and \( \hat{\mu}_i \) is a unit vector in the direction of the magnetic moment. The resultant magnetic field at any point is the sum of such contributions over the lattice. It is calculated by summing explicitly over the contributions from lattice points within a certain radius \( R \) (the “Lorentz sphere”) and replacing the summation over points beyond \( R \) by an integral. The accuracy of this
method obviously increases with the radius \( R \); an estimate of the error may be obtained by recording the variation of the calculated result with the value used for \( R \).

M. Bonn [34] has proved that a simple procedure for evaluating a sum

\[
S_n = \sum_l \frac{1}{|X(l)|^n}
\]

over a simple lattice is to obtain by direct summation the contributions by the lattice points \( X(l) \) within a certain radius \( R \) and to replace the summation over the points beyond this radius by an integral.

2.3 Conclusion

From the potential maps I was able to narrow down the areas of candidate \( \mu^+ \) sites in the sample and then apply the dipolar field calculations on these areas. The candidate muon sites are then those points which fall into the potential minima and have the correct magnetic field.
Chapter 3

Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

3.1 Potential Maps of AFM

Fig. 3.22 depicts a unit cell of the YBa$_2$Cu$_3$O$_6$ crystal. The positions and properties of the ions of YBa$_2$Cu$_3$O$_6$ are shown in Table 3.3. The ion positions are taken from T. Siegrist. [35] Hard core radii are from Handbook of Chemistry and Physics. [36] The valences of barium and yttrium can only be 2+ and 3+, but Cu can be 1+ or 2+. Copper ions on the Cu-O chain are thought to have no magnetic moments; they are therefore 1+ ions, and those on the Cu-O$_2$ plane are 2+ ions. [37] [38] [39] Cu2 has a slightly smaller radius than Cu1.

<table>
<thead>
<tr>
<th>ion</th>
<th>X-axis (a)</th>
<th>Y-axis (b)</th>
<th>Z-axis (c)</th>
<th>valence</th>
<th>hard core radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu1</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>1+</td>
<td>0.74Å</td>
</tr>
<tr>
<td>Cu2</td>
<td>0.5</td>
<td>0.5</td>
<td>0.143</td>
<td>2+</td>
<td>0.7Å</td>
</tr>
<tr>
<td>Y</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3+</td>
<td>0.893Å</td>
</tr>
<tr>
<td>Ba</td>
<td>0.0</td>
<td>0.0</td>
<td>0.314</td>
<td>2+</td>
<td>1.34Å</td>
</tr>
<tr>
<td>O1</td>
<td>0.5</td>
<td>0.5</td>
<td>0.347</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
<tr>
<td>O2</td>
<td>0.0</td>
<td>0.5</td>
<td>0.12</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
<tr>
<td>O3</td>
<td>0.5</td>
<td>0.0</td>
<td>0.12</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
</tbody>
</table>

Table 3.3: Properties and coordinates of ions in YBa$_2$Cu$_3$O$_6$. Here $a = b = 3.856Å$ amd $c = 11.666Å$. Origin is at Y(0,0,0).

The calculations are performed over one unit cell at the center of a finite sphere of more than 400 ions generated by a software package, ORTEP. Twenty planes intersecting the z axis at even intervals are chosen in the unit cell, and the potential is calculated on each plane. The deepest minima of the potential maps are the expected
muon sites. The exact positions can be decided by finely adjusting z values. The following are the potential maps at constant distance along the z direction. The two dimensional potential maps on each plane are represented graphically by single characters which stand for the value of the potential at that point, using the table below to decode the potential map. Generally * represents the highest potential, capital letters are the next highest and numbers are the lowest. The length scales are in units of the lattice constants $a = b = 3.856\text{Å}$ and $c = 11.666\text{Å}$. Coppers are at the four corners of the unit cell, oxygens are at the centers of edges and Yttrium is at $(0,0,0)$.

The graphs that follow indicate that there is a very large increase in potential energy close to the ions and that the potential has (naturally) the symmetry of the crystal. Surprisingly, a large region close to the Cu-O chain in $YBa_2Cu_3O_6$, which might make an attractive home for a muon, doesn’t have a potential minimum. Instead, the minima occur in two planes at $0.03c$ and $0.19c$. 
### Chapter 3. Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

<table>
<thead>
<tr>
<th>Value of Potential ($F$)</th>
<th>Character Printed</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F &gt; 36$</td>
<td>*</td>
</tr>
<tr>
<td>$35 &lt; F &lt; 36$</td>
<td>Z</td>
</tr>
<tr>
<td>$10 &lt; F &lt; 11$</td>
<td>A</td>
</tr>
<tr>
<td>$9 &lt; F &lt; 10$</td>
<td>9</td>
</tr>
<tr>
<td>$1 &lt; F &lt; 2$</td>
<td>1</td>
</tr>
<tr>
<td>$0 &lt; F &lt; 1$</td>
<td>0</td>
</tr>
<tr>
<td>$-1 &lt; F &lt; 0$</td>
<td>a</td>
</tr>
<tr>
<td>$-26 &lt; F &lt; -25$</td>
<td>z</td>
</tr>
<tr>
<td>$F &lt; -26$</td>
<td>!</td>
</tr>
</tbody>
</table>
Figure 3.2: Two dimensional potential map at $Z=0.02c$
Figure 3.3: Two dimensional potential map at $Z=0.03c$
Figure 3.4: Two dimensional potential map at $Z=0.05c$
Figure 3.5: Two dimensional potential map at Z=0.07c
Figure 3.6: Two dimensional potential map at $Z=0.10c$
Figure 3.7: Two dimensional potential map at $Z=0.15c$
Figure 3.8: Two dimensional potential map at Z = 0.17c
Figure 3.9: Two dimensional potential map at $Z=0.19c$
Figure 3.10: Two dimensional potential map at Z=0.20c
Figure 3.11: Two dimensional potential map at \( Z = 0.26c \)
Figure 3.12: Two dimensional potential map at $Z=0.30c$
Chapter 3. Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

Figure 3.13: Two dimensional potential map at Z=0.35c
Figure 3.14: Two dimensional potential map at $Z=0.38$.
Figure 3.15: Two dimensional potential map at $Z=0.40c$
Figure 3.16: Two dimensional potential map at $Z=0.42c$
Figure 3.17: Two dimensional potential map at \( Z = 0.45c \)
Figure 3.18: The Contour Potential Map of YBa$_2$Cu$_3$O$_6$ at Z=0.03c. Coppers are at the four corners. Larger number lines represent lower potentials.
Chapter 3. Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

The contour maps in Fig. 3.18 and Fig. 3.19 show the inverted muon potential energy $-U(x,y)$ in the $a-b$ plane (Cu ions at the four corners). Larger-numbered contour lines represent lower potential energy and indicate likely $\mu^+$ sites. The scales are in units of the lattice constants ($a$, $b$, $c$). Yttrium is at the center. Fig. 3.18 describes the plane 0.03Å away from Y plane and between the CuO$_2$ planes — and Fig.3.19 the plane 0.81Å below the CuO$_2$ planes — i.e., toward the CuO chains.

These contour maps confirm the strong $\mu^+O^2-$ attraction that binds all muons closely to oxygen ions. For convenience, I define the $z = 0.12c$ copper oxide plane as a reference plane; here yttrium is at (0,0,0). The first muon site (0.45$a$,0.06,0.03$c$) is 1.07Å “down” away from O2 in the plane. The other site is (0.3$a$,0.0$b$, 0.19$c$) which is 1.125Å “above” away from O2 in the same plane. There are another six sites at symmetric positions on these planes.

3.2 Dipolar Magnetic Field Calculations

For antiferromagnetic YBa$_2$Cu$_3$O$_6$ the large Cu ion paramagnetic moments dominate the dipolar magnetic field, which is thus $\sim 2000$ times larger than that from the nuclear moments. The magnetic structure consists of strong nearest-neighbor correlated spins in adjacent copper planes which are aligned antiferromagnetically. The moments are constrained to lie in the tetragonal $a-b$ plane; I assume that they point along either the $\hat{a}$ axis or the $\hat{b}$ axis. From neutron scattering measurements, the ordered moment on the Cu ions in the CuO$_2$ plane is estimated to be 0.66 $\mu_B$[40]. J.W. Lynn[41] reports that at lower temperatures the Cu moments in the oxygen-deficient CuO chain layers also order antiferromagnetically, with a moment that can be quite substantial (0.5 $\mu_B$); however, in my calculations I only consider the contributions from Cu moments in the CuO$_2$ planes.
Figure 3.19: The contour potential map of YBa$_2$Cu$_3$O$_6$ at Z=0.19c
The calculated results are in Table 3.4 and Table 3.5. Here the magnetic field
\[ B = \sqrt{B_x^2 + B_y^2 + B_z^2} \.

<table>
<thead>
<tr>
<th>X-axis</th>
<th>Y-axis</th>
<th>Z-axis</th>
<th>Field (Gauss)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.10</td>
<td>0.03</td>
<td>308.88</td>
</tr>
<tr>
<td>0.10</td>
<td>0.00</td>
<td>0.03</td>
<td>318.57</td>
</tr>
<tr>
<td>0.45</td>
<td>0.00</td>
<td>0.03</td>
<td>307.86</td>
</tr>
<tr>
<td>0.05</td>
<td>0.00</td>
<td>0.03</td>
<td>287.17</td>
</tr>
<tr>
<td>0.50</td>
<td>0.05</td>
<td>0.03</td>
<td>302.79</td>
</tr>
</tbody>
</table>

Table 3.4: The magnetic field at \( z = 0.03c \).

<table>
<thead>
<tr>
<th>X-axis</th>
<th>Y-axis</th>
<th>Z-axis</th>
<th>Field (Gauss)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>0.00</td>
<td>0.19</td>
<td>268.45</td>
</tr>
<tr>
<td>0.30</td>
<td>0.00</td>
<td>0.19</td>
<td>308.83</td>
</tr>
</tbody>
</table>

Table 3.5: The magnetic field at \( z = 0.19c \).

Only the points at which the local magnetic field has a magnitude of around 300G are listed here. Contour maps of the magnetic field strength on these two planes are shown in Fig. 3.20 and Fig. 3.21.
3.3 Comparison With Experimental Data

Experiments [14] on AFM YBa$_2$Cu$_3$O$_6$ below 100K obtain a dominant ZF-\(\mu S\) signal at about 4 MHz, which indicates an internal field of about 300 Gauss. Meanwhile, the LCR experiment shows that the muon sites in YBa$_2$Cu$_3$O$_7$ are 1 Å away from the O in the CuO$_2$ plane. If we assume that the muon occupies the same site regardless of oxygen deficiency, the overlap between the regions with potential minima and those with the magnetic field within uncertainty will be the candidate muon sites. Table 3.6 lists the muon sites in YBa$_2$Cu$_3$O$_6$.

<table>
<thead>
<tr>
<th>X-axis a</th>
<th>Y-axis b</th>
<th>Z-axis c</th>
<th>Distance Å</th>
<th>Field (Gauss)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.45</td>
<td>0.00</td>
<td>0.03</td>
<td>1.070</td>
<td>307.86</td>
</tr>
<tr>
<td>0.30</td>
<td>0.00</td>
<td>0.19</td>
<td>1.125</td>
<td>308.83</td>
</tr>
</tbody>
</table>

Table 3.6: Muon candidate site in YBa$_2$Cu$_3$O$_6$. Here \(a = b = 3.856\) Å and \(c = 11.666\) Å.
Figure 3.20: The contour plot of magnetic field at $Z = 0.03c$. It shows only a quarter of the plane. Coordinates are in the unit cell length.
Chapter 3. Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

Figure 3.21: Contour plot of magnetic field at 0.19c

300G line
Chapter 3. Explicit Calculations of Muon Sites In YBa$_2$Cu$_3$O$_6$

Figure 3.22: The crystal structure of antiferromagnetic YBa$_2$Cu$_3$O$_6$
Chapter 4

Calculations on YBa$_2$Cu$_3$O$_7$

4.1 Muon Site Decision Experiment

ZF- and WTF-$\mu$SR measurements were made on normal and $^{17}$O enriched samples of YBa$_2$Cu$_3$O$_7$ at a temperature of 103K. In the latter samples, 38% of the naturally abundant and spinless $^{16}$O was replaced by $^{17}$O. At this temperature the correlation time for muon hopping is much longer than the muon lifetime so that the nuclear dipolar fields seen by the muon are essentially static. The $\mu$SR time spectra for the $^{17}$O enriched sample are compared with corresponding spectra in the pure $^{16}$O control sample. The depolarization rate in the $^{17}$O substituted sample is enhanced in both ZF and wTF(24G), which suggests that the muon is close to an oxygen ion. The $rms$ internal field was estimated by fitting the wTF relaxation function to a sum of two Gaussians. The fitted results yield an $rms$ internal field $\langle B^2 \rangle^{1/2}$ along the applied field direction equal to 1.31G in the unsubstituted YBa$_2$Cu$_3$O$_7$ and 2.65G in the $^{17}$O enriched sample. If the muon is much closer to a single oxygen (i.e. if it forms an hydroxyl-like bond) such that the dipolar fields from other oxygens can be neglected, one obtains a powder averaged $\langle B^2 \rangle^{1/2}$ due to a single $^{17}$O equal to $\Delta_o = 3.64G$. The $^{17}$O nuclei then exert an effective static dipolar field on the muon given by $\vec{B}_{dip} = (\hbar \gamma \nu / r^3) S \cdot [3(\vec{r} \cdot \vec{q})\hat{r} - \vec{q}]$ where $S \cdot \vec{q}$ is the component of nuclear spin along the electric field gradient direction $\vec{q}$ and $\hat{r}$ is the unit vector between the muon and $^{17}$O nucleus separated by distance $r$. 

43
Averaging over all angles between $\vec{B}_{dip}$ and $\vec{z}$ yields

$$\Delta_0 = \frac{1}{3}(\hbar \gamma N/r^3)[S(S + 1)(3(\hat{\tau} \cdot \hat{q})^2 + 1)]^{1/2},$$

from which $r = 1.01\text{Å}$ can be estimated provided that the muon is bonded to a single oxygen and the bond axis is perpendicular to $\hat{q}$.

LCR was introduced in order to decide to which oxygen the muon is bonded. Principally, LCR is based upon the idea that when two systems are prepared so that an energy splitting in one system matches a splitting found in the second system, an exchange of energy or polarization may occur between levels of the two systems. In this study, the system consists of a spin 1/2 muon in an external field interacting with a spin 5/2 nucleus $^{17}$O in an electric field gradient plus external field. Whenever the Zeeman energy of the muon matches the quadrupolar level splitting of $^{17}$O, there may be a resonance. The spin Hamiltonian for a $\mu^+$ in the crystal is:

$$H = H_{dip} + H_Q + H_Z \quad (4.8)$$

$$H_{dip} = \frac{\hbar^2 \gamma \mu \gamma \nu}{r^3}[s_\mu \cdot I - 3(s_\mu \cdot \hat{r})(I \cdot \hat{r})] \quad (4.9)$$

$$H_Q = \frac{e^2 q}{4I(2I - 1)}[3(I_x^2 - I_y^2) + \delta(I_x^2 - I_y^2)] \quad (4.10)$$

$$H_Z = (u_\mu + u_O) \cdot \mathbf{H}_{ext} \quad (4.11)$$

where $H_{dip}$ is the dipolar interaction between muon and $^{17}$O, $H_Q$ is the quadrupolar interaction of $^{17}$O, $H_Z$ is the combined Zeeman energy of the muon and the $^{17}$O in the external field, $r$ is the separation between nucleus and $\mu^+$, $s_\mu$ and $I$ are the nuclear magnetic moments of $\mu^+$ and $^{17}$O and $\delta = (V_{xx} - V_{yy})/V_{zz}$. Here $V_{ij}$ is the electric field gradient (EFG) tensor. Due to the two splittings between $|1/2\rangle$ and $|3/2\rangle$ and between $|3/2\rangle$ and $|5/2\rangle$, two resonances are expected at approximately $B_r = \frac{3}{20}e^2 q Q/\gamma \mu \hbar$ and $2B_r$, assuming $\delta = 0$. 
Chapter 4. Calculations on YBa$_2$Cu$_3$O$_7$

From the data the best estimate of the average quadrupolar parameter is $e^2qQ/h = 6.6$ MHz, which is very close to that measured by NMR for the O(2,3) [42] planar sites in the absence of the muon[42]. These results suggest that the muon is bonded to an oxygen in the CuO$_2$ plane at a distance of 1Å.

4.2 Potential Map of Superconductor YBa$_2$Cu$_3$O$_7$

<table>
<thead>
<tr>
<th>ion</th>
<th>X(a)</th>
<th>Y(b)</th>
<th>Z(c)</th>
<th>Valence</th>
<th>Hard core radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3+</td>
<td>0.893Å</td>
</tr>
<tr>
<td>Ba</td>
<td>0.0</td>
<td>0.0</td>
<td>0.347</td>
<td>2+</td>
<td>1.34Å</td>
</tr>
<tr>
<td>Cu1</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>2+</td>
<td>0.74Å</td>
</tr>
<tr>
<td>Cu2</td>
<td>0.5</td>
<td>0.5</td>
<td>0.143</td>
<td>2.3+</td>
<td>0.7Å</td>
</tr>
<tr>
<td>O1</td>
<td>0.5</td>
<td>0.5</td>
<td>0.312</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
<tr>
<td>O2</td>
<td>0.0</td>
<td>0.5</td>
<td>0.12</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
<tr>
<td>O3</td>
<td>0.5</td>
<td>0.0</td>
<td>0.12</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
<tr>
<td>O4</td>
<td>0.5</td>
<td>0.0</td>
<td>0.5</td>
<td>2-</td>
<td>1.2Å</td>
</tr>
</tbody>
</table>

Table 4.7: The positions and properties of YBa$_2$Cu$_3$O$_7$. Here $a = 3.856$ Å, $b = 3.87$ Å and $c = 11.666$ Å.

Eq. 2.1 is used to generate the potential maps of YBa$_2$Cu$_3$O$_7$, which have a structure similar to those of YBa$_2$Cu$_3$O$_6$ except that there is no potential minimum between two Cu—O$_2$ planes. Furthermore a minimum-potential area appears around the bridging oxygen O4 due to the two extra negative ions on the Cu chain, which decrease the potential around that region. Further studies of region will be concerned with the dipolar magnetic field.

The plane at $z = 0.19c$ has a potential map similar to those of YBa$_2$Cu$_3$O$_6$. The contour plot of this plane shows that there is also a very strong interaction between the muon and the ions. Muons are evidently bonded to the oxygen ions in the copper-oxygen plane.
Chapter 4. Calculations on $YBa_2Cu_3O_7$

4.3 Dipolar Magnetic Field

For $YBa_2Cu_3O_7$ the dipolar fields are due to weak nuclear moments, primarily from $^{63}\text{Cu}$ and $^{65}\text{Cu}$ nuclei but with minor contributions also from Ba and Y nuclei. For $^{17}\text{O}$-doped samples the substantial contributions from $^{17}\text{O}$ nuclear moments must also be included. The spin-3/2 copper nuclear moments will precess about the electric field gradient, which is along the $c$-axis for Cu ions in the CuO$_2$ plane and along the chain for Cu ions in the CuO chains. This quadrupolar precession is assumed to average out all transverse field components; those remaining are all treated as static (i.e., any muon-nuclear “flip-flop” dynamics are neglected). Within these conditions, the nuclear moments are assumed to be oriented along the electric field gradient and the resultant local fields are characterized by a gaussian width $\Delta$ as usual.
Chapter 4. Calculations on YBa$_2$Cu$_3$O$_7$

<table>
<thead>
<tr>
<th>Ion</th>
<th>Nuclear Magnetic Moment $\mu_b$</th>
<th>Abundance %</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{63}$Cu</td>
<td>2.226</td>
<td>69.01</td>
</tr>
<tr>
<td>$^{65}$Cu</td>
<td>2.385</td>
<td>30.91</td>
</tr>
<tr>
<td>$^{17}$O</td>
<td>-1.8937</td>
<td>38</td>
</tr>
<tr>
<td>$^{135}$Ba</td>
<td>0.8365</td>
<td>6.59</td>
</tr>
<tr>
<td>$^{137}$Ba</td>
<td>0.9357</td>
<td>11.32</td>
</tr>
<tr>
<td>$^{89}$Y</td>
<td>-0.13682</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 4.8: The nuclear magnetic moments of ions in YBa$_2$Cu$_3$O$_x$.

The calculations indicate that the muon relaxation rate of $^{17}$O doped sample should be larger than that in the unsubstituted sample, which is consistent with the experiments. The minimum potential region at $z = 0.19c$ yields a theoretical value of $\Delta$ consistent with those measured experimentally. Other regions with potential minima don’t have dipolar magnetic fields of the right magnitude. Note that no consideration has been given to any lattice relaxation or hopping of muons, which would significantly affect the relaxation.

4.4 Conclusion

The combined results of potential maps and dipolar magnetic field calculations indicate that the most likely muon site is on the plane at $z = 0.19c$, which is between the Cu—O$_2$ plane and the Cu—O chain and 0.84Å “down” from the Cu—O$_2$ plane, which is indicated on Fig.4.4. All the other regions either have minimum potentials but wrong dipolar magnetic fields or have the correct magnetic field but don’t fall into the minimum potential areas. In conclusion, the most probable muon site is at $(0.3a, 0.0b, 0.19c)$ and corresponding symmetric sites.
Chapter 4. Calculations on YBa$_2$Cu$_3$O$_7$

Figure 4.23: The contour plot of the potential map at Z=0.19c
Chapter 4. Calculations on $\text{YBa}_2\text{Cu}_3\text{O}_7$

Figure 4.24: The crystal structure of superconducting $\text{YBa}_2\text{Cu}_3\text{O}_7$. 
Bibliography


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Appendix A

Programs

To determine the candidate muon sites a calculation consisting of three steps was performed. The first step is to generate a cluster of lattice points by using XTLPLOT; the second step is to produce potential maps on the planes at equal separation along the z-axis in a crystal unit cell to decide possible muon stopping regions; and the last step is to calculate the magnetic field on the different planes to verify that those possible muon stopping regions have the correct magnetic field. This initial introduction to the programs will emphasize the relationships between the programs. Details about the procedures followed in each program can be found in the corresponding manuals.

XTLPLOT provides information to another program ORTEP, which actually produces the model cluster. One of 230 different space groups has to be specified by users in order to generate a crystal structure. 10 space groups are available in the files USR2:[ALANA]*.SPG on the TRIUMF VAX cluster. A special space group can be generated by editing a *.SPG file in which the specific transformations are indicated.

Different radii have been employed to distinguish different ions on the plot because of the difficulty of labeling the ions. In this study two kinds of units are used: unit cell length and actual length. Positions are in the unit cell length, radius are in actual length.

POTENTMAP program generates electric potential maps of a crystal structure over the x - y plane at the fixed z values specified by the users, minima of which are likely muon sites. The potential maps are characterized by letters; each letter
Appendix A. Programs

represents potential levels, which can be decoded by the table in the documentation. POTENTMAP's preselection of candidate muon sites is very useful, because each calculation of the dipolar magnetic field consumes at least half an hour of CPU time on the VAX. From the potential maps it will be easy to decide where the magnetic field needs to be calculated. The Morse potential is used to calculate the interaction between muon and ions. No consideration was given to any lattice relaxation or charge screening effects. The calculation involves more than 400 ions in the cluster. Some modifications of POTENMAP can be made to generate output in a format suitable for input to PLOTDATA which can produce beautiful contour graphs or density maps. Both methods were employed in this thesis. The lettered maps show pseudo-three-dimensional structure and the contour map gives more detail of the two dimensional potential at every \( z \) value.

CLUSTSUM calculates the dipolar magnetic field caused by other magnetic dipole moments at a site. Because of the limit of the size of the cluster generated by XTLPLOT, the contribution from those outside the cluster will be replaced by an integral. The sum will vary with the radius of the cluster.

POTENMAP and CLUSTSUM read in cluster files generated by XTLPLOT. Because the cluster usually involves many more ions than on one plot, no plot should be drawn after one sees the prompt XTLPLOT\}. Also two kinds of clusters are optional: "unit-cell" shaped, to draw the entire structure of a unit cell; and "sphere", to look at the environment of a particular position. In the case of this thesis, the sphere is usually used. For POTENTMAP, a sphere centred on (0,0,0) is produced. For CLUSTSUM, a sphere centred on the candidate muon position is required.

The cluster file created will be in the proper format to be read by the two programs POTENMAP and CLUSTSUM. The only thing that must be done before they are run is that the appropriate ion property be included in lieu of the "*****" you will find
in the newly created file. For the program POTENMAP, this property would be the ion's hard core radius in your chosen length unit; for CLUSTSUM, it would be the ion's dipole moment, in Bohr magnetons or nuclear magnetons, depending upon which dominates the field. In the case of YBa₂Cu₃O₆, Bohr magnetons are used; nuclear magnetons are used for YBa₂Cu₃O₇.

POSITION, PLOTPARAMETERS and XTLMAIN, subroutines of XTLPLOT, play the roles of reading in ion positions, plotting parameters and lattice constants respectively. It is possible to revise the programs for a batch job. One example is usr2:[qiang.thesis.program]li.for, which calculates the magnetic field at 100 evenly distributed points on the plane specified by the user in YBa₂Cu₃O₆ with the cluster generated automatically.