

Hartree-Fock-Bogoliubov calculation of r-process nuclei around A=130.

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Keyword: Hartree-Fock-Bogoliubov, Skyrme interaction, r-process, pairing correlation

Abstract: The ground-state properties of r-process nuclei are important in nuclear astrophysics. Neutron rich r-process nuclei have been studied under Hartree-Fock-Bogoliubov formalism. The Skyrme interaction SLY6 has been used to calculate the binding energy and ground state deformation along with other properties of nuclei important in the r-process whose peak occurs around mass number 130. Stable and unstable isotopes of Rhodium, Palladium, Silver, Cadmium and Indium have been investigated selfconsistently with SLY6 Hamiltonian. Potential energy surface (PES) has also been studied.

1. Introduction

Stars are born and when they die they eject their material back into the space. Therefore, there is an intricate relationship between the life cycle of stars and the nucleosynthesis of elements. Heavier elements are synthesized through neutron capture processes. The two main neutron capture processes are the slow (s) and the rapid (r) processes i.e the s and r processes. In the s process the neutron capture takes place in a time scale much longer than the mean time for β decay. In the case of the r process time to capture neutron is much smaller than the beta decay time. While the mean time for beta decay depends only on the nuclear species, but the neutron capture time depends strongly on the environment, particularly on a strong neutron flux.

The s-process is relatively well understood but it is difficult to measure the properties of the r-process nuclei due to their short life time and hence their properties are not certain. The site where the r-process take place is still controversial. The r process element formation requires high neutron density and temperature that are associated catastrophic events. The two potential candidates for the r -process are type II (corecollapse) supernova explosions and neutron star mergers. At present the astrophysical conditions of these two phenomena are not well understood.

An element with a given proton number should be able to capture many neutrons before undergoing β decay. In the scenario of high neutron fluxes the temperature is very high and therefore large quantities of gamma photons are released. The equilibrium abundances for a given isotopic chain will be determined by the neutron density, temperature and neutron separation energy through the Saha equation. This equilibrium implies that the maximum abundance of participating elements will be characterized by similar neutron separation energies. The neutron separation energy determines the maximum neutron abundance of each isotope. In r-process the neutron separation energy is of the order of 2-3 MeV.

To develop a model of the r-process we require a large number of nuclear informations which must include the various characteristics of light to heavy nuclei. Nuclei and their β decay branches between the valley of stability and near the neutron drip lines are crucial for r- process. Due to the extreme conditions required for r-process nuclei, they must be investigated with the help of theoretical route.

In decomposition of the solar abundances of heavy nuclides with respect to A into r-process double peaks occurs at $A \sim 130$ and 195. In this present work I have investigated the ground state properties of r-process nuclei around mass region $A=130$. The Hartree-Fock-Bogoliubov (HFB) is a reliable method to find the properties of r-process nuclei. In this work I have chosen the stable and unstable isotopes of the nuclei with $Z = 46 - 49$ that is Rhodium, Palladium, Silver, Cadmium and Indium. The paper can be outlined as follows. In section 2, I have described the theoretical approach. The Skyrme Hamiltonian is described in subsection 2.1. HFB formalism have been described in next subsection 2.2. HFB equations have been briefly given in subsection 2.2.1. In section 3, I have given results of my calculation. Section 4 and 5 are devoted to conclusion and acknowledgement.

2. Theoretical Approach

It is possible to find the exact solution when we have one nucleon system, but for more than two or many body system we have to satisfy with approximate solution. To get approximate solution we will search for some theoretical model and Hartree-Fock theory is one of the good choice. The standard Hartree-Fock theory is the successful theory in describing the nuclear properties of nuclei of closed shell, but it is not successful for nuclei having unfilled shells. With unfilled shells we find additional correlation i.e pairing correlations, between these particles. The Hartree-Fock (HF) theory based on the single particle picture does not incorporate the pairing correlations. This non inclusion of pairing correlation does not have large impact when dealing with nuclei close to stability, but pairing effects are stronger for nuclei near the driplines and they must be included efficiently. The pairing correlation generally incorporated with the help of the BCS approximation [1] for nuclei lying close to stability but BCS approximation becomes unreliable for nuclei lying close to the driplines because of the coupling between the bound and single particle states has not included properly. [2, 3, 4]. The Hartree-Fock-Bogoliubov (HFB) includes pairing correlation self consistently, allowing HFB to correctly treat the pairing effect. When there is no pairing effect then HFB theory gives the same result as with the result of the HF theory.

2.1. The Skyrme Hamiltonian

The Skyrme interaction is the effective interaction which has been investigated successfully to calculate the entire properties of nuclei lying in the wide range of nuclear chart. There are various choices of Skyrme forces are available in literature and SLY6 is the good choice for the neutron rich nuclei and nuclear matter. In present work I have used the SLY6 Skyrme force [5, 6] to gleaned the information of ground-state properties of nuclei around mass region 130. The total energy E of the system [7, 8] can be defined as

$$E = \int dr \left\{ \mathcal{H}_{kin}(\tau_q) + \mathcal{H}_{SK}(\rho_q, \tau_q, s_q, j_q, J_q, T_q) + \mathcal{H}_{pair}(\chi_q) + \mathcal{H}_C(\rho_p) \right\} - E_{CM} \quad (1)$$

It contains local time-even and time-odd densities, as well as the pairing density χ_q . Where ρ_q is of nucleon, τ_q is kinetic energy, s_q is spin, j_q is current, J_q is Spin-Orbit part, T_q is Spin kinetic energy, χ_q is pairing density and q denotes proton and neutron. The total densities ρ have no the index $\rho = \rho_p + \rho_n$. The different part of Eq(1) are Kinetic energy

$$\mathcal{H}_{Kin} = \sum_q \frac{\hbar^2}{2m_q} \tau_q(r) \quad (2)$$

Pairing -energy

$$\mathcal{H}_{pair} = \frac{1}{4} F(r) \sum_q V_{pair,q} \chi_q^*(r) \chi_q(r) \quad (3)$$

Coulom-energy part is

$$\mathcal{H}_C = \frac{e^2}{2} \int dr' \rho_p(r) \frac{1}{|r-r'|} \rho_p(r') - \frac{3}{4} e^2 \left(\frac{3}{\pi} \right)^{1/3} [\rho_p(r)]^{4/3} \quad (4)$$

and center of mass term

$$E_{CM} = \frac{\langle \hat{P}_{CM}^2 \rangle}{2mA} \quad (5)$$

The pairing interaction may be density dependent or not. If density dependent then Surface pairing with $F = 1 - \frac{\rho}{\rho_0}$ and $\rho_0 = 0.20113 \text{ fm}^{-3}$ and if not Volume pairing with $F = 1$ [9]. The main part of Eq(1) is the Skyrme Functional \mathcal{H}_{SK} which contains the term

$$\begin{aligned} \mathcal{H}_{SK}^{(even)} = & \frac{b_0}{2} \rho^2 - \frac{b'_0}{2} \sum_q \rho_q^2 + b_1 \rho \tau - b'_1 \sum_q \rho_q \tau_q \\ & - \frac{b_2}{2} \rho \Delta \rho + \frac{b'_2}{2} \sum_q \rho_q \Delta \rho_q + \frac{b_3}{3} \rho^{\alpha+2} - \frac{b'_3}{3} \rho^\alpha \sum_q \rho_q^2 \\ & - b_4 \rho \Delta J - b'_4 \sum_q \Delta J_q - \tilde{b}_1 J^2 - \tilde{b}'_1 \sum_q J_q^2 \end{aligned} \quad (6)$$

where $b_i, b'_i, \tilde{b}_i, \tilde{b}'_i$ are the force parameters.

2.2. The Hartree-Fock Bogoliubov Method

The Hartree-Fock approximation is inadequate to explain the nuclear properties of nuclei near drip line due to noninclusion of pairing correlation. The concept of mean field with a pairing field with Hartree-Fock-Bogoliubov (HFB) equations are introduced to incorporate these correlations. Pairing correlations are included by introducing the idea of independent quasiparticles defined by the Bogoliubov transformation (Ring and Schuck, 1980),

$$\hat{b}_n^+ = \sum_i (U_{in}\hat{a}_i^+ + V_{in}\hat{a}_i) \quad (7)$$

Where the creation operators for states i given as

$$\hat{a}_i^+ = \int d^3r \sum_{\sigma\tau} \psi_i(x)\hat{a}_x^+ \quad (8)$$

the independent-particle state can be described by $\hat{a}_i^+|\Phi\rangle = 0$ for occupied states ($1 \leq i \leq A$) and $\hat{a}_i|\Phi\rangle = 0$ for unoccupied states ($i > A$). Eq(7) connects single-particle states to quasiparticle states. In compact notation the transformation is

$$\begin{pmatrix} \hat{b} \\ \hat{b}^+ \end{pmatrix} = \mathcal{W}^+ \begin{pmatrix} \hat{a} \\ \hat{a}^+ \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad (9)$$

where the transformation matrix is unitary i.e $U^+U + V^+V = 1$, $UU^+ + V^*V^I = 1$, $U^IV + V^IU = 0$, and $UV^+ + V^*U^T = 0$. The ground state of the system by the quasiparticle vacuum condition is then given as ,

$$\hat{b}_n|\Phi\rangle = 0 \quad (10)$$

for all n . The quasiparticle states are described here in terms of fermion operators. Quasiparticle states can also be defined in terms of quasiparticle wave functions in coordinate space i.e

$$\phi_n = \begin{pmatrix} \phi_n^U(\mathbf{x}) \\ \phi_n^V(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \sum_i U_{in}\psi_i(\mathbf{x}) \\ \sum_i V_{in}\psi_i(\mathbf{x}) \end{pmatrix} \quad (11)$$

These states are orthonormal because of the unitarity of the quasiparticle transformation, i.e

$$\int dx \phi_n^+(\mathbf{x})\phi_m(\mathbf{x}) = \delta_{nm}, \quad \int dx = \int d^3r \sum_{\sigma\tau} \quad (12)$$

A firm description for an independent-particle state is provided by the introduction of one -body density matrices. This is specially useful for self-consistent mean-field models whose energy functionals are defined in terms of these densities. For independent quasi particle, we have to deal with two objects first one is a one-body density matrix ρ and a pair tensor κ , which are

$$\rho_{ij} = \langle \Phi | \hat{a}_j^+ \hat{a}_i | \Phi \rangle = (V^* V^T)_{ij} = \rho_{ji}^* \quad (13)$$

$$\kappa_{ij} = \langle \Phi | \hat{a}_j \hat{a}_i | \Phi \rangle = (V^* U^T)_{ij} = -\kappa_{ji} \quad (14)$$

These may be observed as the components of a generalied quasiparticle density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} \quad (15)$$

The representation of the density matrices in configuration space is equivalent to a coordinate space representaion i.e

$$\rho(\mathbf{x}, \mathbf{x}') = \langle \Phi | \hat{a}_x^+, \hat{a}_x | \Phi \rangle \equiv \sum_n \phi_n^{(V)}(\mathbf{x}) \phi_n^{(V)*}(\mathbf{x}') \quad (16)$$

$$\kappa(\mathbf{x}, \mathbf{x}') = \langle \Phi | \hat{a}_x, \hat{a}_x | \Phi \rangle \equiv \sum_n \phi_n^{(U)}(\mathbf{x}) \phi_n^{(V)*}(\mathbf{x}') \quad (17)$$

. Each of the three representation form i.e Eq(7,10),Eq(11) and Eq(15) represents an independent-quasiparticle state or Hartree-Fock-Bogoliubov state.

2.2.1. The Hartree-Fock Bogoliubov equation

The g.s $|\Phi\rangle$ of the Hartree-Fock-Bogoliubov (HFB) method is obtained by minimization of the total energy

$$\mathbf{E} = \langle \Psi | \hat{\mathbf{H}} | \Psi \rangle = E[\rho, \kappa, \kappa^*] \quad (18)$$

by applying the constraints on proton number and neutron number $\langle \Psi | \hat{N}_q | \Psi \rangle = N_q$. Any expectation value of an operator with an HFB state can be written in terms of the one-body densities only.

The minimization of the total Routhian $E^\lambda = E - \lambda_q \langle \Psi | \hat{N}_q | \Psi \rangle = N_q$ leads to the HFB equation, which can be expressed in terms of the U and V transformation matrices

$$\mathcal{H} \begin{pmatrix} U_n \\ V_n \end{pmatrix} = e_n \begin{pmatrix} U_n \\ V_n \end{pmatrix} \quad (19)$$

$$\mathcal{H} = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \quad (20)$$

The Lagrangian multipliers introduced to constrain the orthonormalization of the quasiparticle states. Here the quasiparticle energies e_n are Lagrangian multipliers. The Hamiltonian is defined in standard form $\hat{H} = \hat{T} + \hat{V}$ where \hat{V} is two-body interaction and \hat{T} is the kinetic energy part. The matrix elements of the mean-field and gap Hamiltonians are given as

$$h_{ij} = T_{ij} + \sum_{kl} V_{ikjl\rho l k}, \quad \Delta_{ij} = \frac{1}{2} \sum_{kl} V_{ijkl\kappa k l} \quad (21)$$

where $V_{ikjl\rho l k}$ is the antisymmetrized two-body matrix element and Δ_{ij} is the pairing field.. Equation (19) and (20) are the HFB equations.

The calculation of HFB method can be find out in two steps, fist diagonalization of \hat{h} and the solving the HFB equations in the basis. In my calculation I have used the deformed harmonic oscillator basis to get the solution of HFB equations. All the mathematical information of HFB have been taken from the [7] and the references therein.

3. Results

To completely understand the r- process, conditions such as temperature and neutron density in the associated astrophysical site are required in addition to the properties of a large number of extremely neutron-rich nuclei. These required conditions of r- process is a function of time during the process [14]. The temperature and neutron density for r- process is $T \gtrsim 10^9 K$ and $n_n \gtrsim 10^{20} cm^{-3}$ [15]. From previous studies it is known that for such high temperature and neutron density $(n, \gamma) \rightleftharpoons (\gamma, n)$ equilibrium is attained. It is also known that in this equilibrium, the abundance distribution in each isotopic chain at a specific proton number Z shows a sharp peak at one nucleus. This is known as waiting-point (WP) nucleus because, after reaching it, the r- process waits for it to β - decay before producing heavier nuclei. For this WP approximation to be valid neutron capture and photodisintegration reaction is no more followed, which very much simplifies the r- process calculation. The r- process path will then be defined by all the WP nuclei heavier than the seed nuclei and will be regulated by the β - decay of these WP nuclei. Critical waiting-point nuclei with N=82 and with A=130 are ^{130}Cd , ^{129}Ag , ^{128}Pd , ^{127}Rh . By studying the properties of these WP nuclei, condition required for r-process nucleosynthesis under WP approximation can be calculated. For a specific isotopic chain, the corresponding WP nucleus has the largest abundance and it can be determined by the partition functions and neutron separation energies of the relevant nuclei for fixed T and n_n . Due to establishment of the equilibrium between $(n, \gamma) \rightleftharpoons (\gamma, n)$, the ratio of abundance between two neighbouring isotopes is given by the Saha Equation [15, 16, 17, 18],

$$\frac{Y(Z, A+1)}{Y(Z, A)} = n_n \left(\frac{2\pi\hbar^2}{m_u kT} \right)^{\frac{3}{2}} \frac{G(Z, A+1)}{2G(Z, A)} \left(\frac{A+1}{A} \right)^{\frac{3}{2}} \exp \left[\frac{S_n(Z, A+1)}{kT} \right], \quad (22)$$

where Y represents number abundance, \hbar is the plank constant, m_u is the atomic mass unit, k is the Boltzman constant, (Z,A) indicates a nucleus with proton number Z and mass number A, and, G represents partition function and S_n denote the neutron separation energy of the appropriate nucleus. Exponential dependence on neutron separation energy can be seen from Saha-equation, hence neutron separation energy can be used to calculate the required temperature and neutron density for r- process. Maximum of Saha equation can be found at fixed temperature which comes out $S_n = kT$. Due to great impact of neutron separation energy in r- process

calculation, I have calculated the ground-state binding energy of chain of isotopes of r-process nuclei and from that binding energy, neutron separation energy of isotopic chain of r- process nuclei around neutron number 82 and mass number around 130 have been calculated.

So in this work ,numerical calculations have been done using axially deformed Harmonic Oscillator basis state expansion for solving the HFB equations. Computational code HFODD(V2.40h) have been used here [11].The number of shells taken into account are 15. The pairing force parameters used in my calculation -50.0 in MeV fm^3 for neutron as well as proton. The pairing cut-off energy is 60MeV. Table(1) and Table(2) shows the ground state binding energy of stable and unstable isotopes of nuclei under investigation. These data of g.s Binding energy and deformation have been achieved with unconstrained calculation. Data of stable isotopes have been compared with experimental binding energy. Values of binding energy of unstable isotopes have been compared with the binding energy obtained from the statistics from [12] As we know that nuclei which have either proton or neutron number equal to magic one, shows extra stability and they have zero deformation. From table(2) of unstable isotopes it is clear that all isotopic chain having neutron number around 82 have very small deformation and isotope with 82 neutrons have zero deformation. Deformation of these unstable nuclei have not been compared because deformation values are not available as these nuclei have not been created in laboratory.

From table(2) one neutron and two neutron separation energy can be easily calculated. In this work S_n and S_{2n} have been computed for isotopic chain of Rh, Pd, Ag, Cd, and In. One neutron separation energy from table(2) is in the range near about 2- 4 MeV which is close to the S_n of r- process calculation. I have used this one neutron separation energy in Saha-equation which gives the temperature $T = 10^{10}K$ which is close to temperature required for nuclearsynthesis of r-process nuclei. In this work I have also studied the Potential Energy Surface (PES) of unstable isotope (A=130) of silver which have 47 protons and 83 neutron which is near to magic number 82. As from figure(1) it can be seen that very small deformation about 0.06 is present and which is of prolate shape. The energy barrier is about 1.48 MeV. From the figure (1) shape coexistence can be seen as and it also shows the weak triaxial deformation.

Table 1: The ground-state binding energy and deformation of stable isotopes of Rh,Pd,Ag,Cd,In nuclei.

$Element_N^A$	(Cal)Binding Energy(MeV)	(Cal) Deformation	(Exp) B.E(MeV)	(Exp) Deformation [13]
Rh_{54}^{99}	-854.45	0.1749	-849.42	—
Rh_{56}^{101}	-872.10	0.1920	-867.38	—
Rh_{57}^{102}	-879.86	0.1898	-874.75	—
Rh_{58}^{103}	-887.62	0.1885	-884.15	—
Pd_{56}^{102}	-879.37	0.1985	-875.21	0.1390
Pd_{58}^{104}	-895.84	0.1930	-892.81	0.2090
Pd_{59}^{105}	-903.41	0.1858	-899.91	—
Pd_{60}^{106}	-910.33	0.2450	-909.46	0.1620
Pd_{62}^{108}	-925.37	0.2237	-925.23	0.2430
Pd_{64}^{110}	-939.65	0.2679	-940.18	0.2567
Ag_{60}^{107}	-918.92	0.1743	-915.25	—
Ag_{62}^{109}	-933.74	0.2147	-931.72	—
Cd_{58}^{106}	-908.65	0.1800	-905.13	0.1677
Cd_{60}^{108}	-926.27	0.1691	-923.40	0.1702
Cd_{62}^{110}	-942.84	0.1626	-940.63	0.1720
Cd_{63}^{111}	-950.49	0.1448	-947.60	—
Cd_{64}^{112}	-957.11	0.1995	-957.00	0.1818
Cd_{65}^{113}	-965.23	0.2195	-963.53	—
Cd_{66}^{114}	-972.91	0.2378	-972.59	0.1300
Cd_{67}^{115}	-979.98	0.2360	-978.73	—
Cd_{68}^{116}	-986.78	0.2352	-987.42	0.1351
In_{48}^{97}	-799.49	0.0870	-791.81	—
In_{49}^{98}	-814.63	0.0595	-806.54	—
In_{64}^{113}	-964.32	0.2739	-963.08	—
In_{66}^{115}	-980.94	0.2612	—	—

Table 2: The ground-state binding energy and deformation of unstable isotopes of *r*- process nuclei around $A=130$.

$Element_N^A$	(Cal)Binding Energy(MeV)	(Cal)Deformation	(Statistics [12]) B.E(MeV)
Rh_{80}^{125}	-1017.05	0.0876	-1015.87
Rh_{81}^{126}	-1020.16	0.0564	-1019.59
Rh_{82}^{127}	-1023.01	-0.0069	—
Rh_{83}^{128}	-1025.76	0.0666	—
Pd_{80}^{126}	-1033.60	0.0911	-1033.07
Pd_{81}^{127}	-1037.34	0.0648	-1036.44
Pd_{82}^{128}	-1040.28	0.0163	-1042.04
Pd_{83}^{129}	-1042.75	0.0650	—
Pd_{84}^{130}	-1044.75	0.1002	—
Ag_{80}^{127}	-1049.52	0.0844	-1046.81
Ag_{81}^{128}	-1053.96	0.0618	-1051.26
Ag_{82}^{129}	-1057.63	0.0152	-1056.63
Ag_{83}^{130}	-1059.63	0.0538	-1058.46
Ag_{84}^{131}	-1061.65	0.0900	—
Cd_{80}^{128}	-1064.90	0.0782	-1062.78
Cd_{81}^{129}	-1069.78	0.0564	-1067.21
Cd_{82}^{130}	-1074.44	-0.0007	-1073.25
Cd_{83}^{131}	-1075.55	0.0465	-1075.11
Cd_{84}^{132}	-1077.56	0.0682	-1078.17
Cd_{85}^{133}	-1079.60	0.0928	-1079.82
In_{80}^{129}	-1079.02	0.0610	-1075.60
In_{81}^{130}	-1084.82	0.0392	-1080.82
In_{82}^{131}	-1090.90	-0.0007	-1086.90
In_{83}^{132}	-1092.31	0.0319	-1089.39
In_{84}^{133}	-1094.05	0.0594	-1092.59
In_{85}^{134}	-1095.70	0.0723	-1094.91
In_{86}^{135}	-1097.44	0.0845	-1097.82

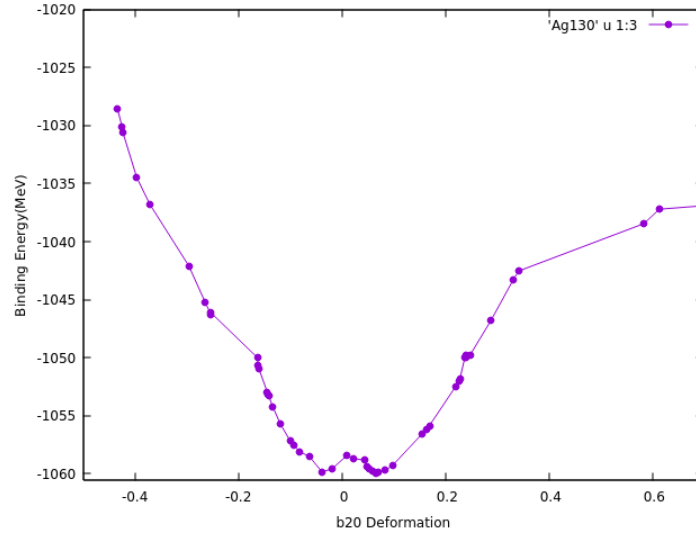


Figure 1: Potential Energy Surface of Ag^{130}

4. Conclusion

A long list of tasks remains to be undertaken in the near future, and this work can be viewed as a starting point for a more aspiring work. I can conclude from the result discussed above that a more systematic study is required to understand the properties of *r*- process nuclei with different Skyrme forces and pairing correlation. Systematic calculation of *r*- process nuclei with $N=50$, $N=126$ closed shell with peak at $A=80$ and 195 has to be performed for better understanding of required condition of temperature and neutron density which will be helpful in understanding of nucleosynthesis of heavier element in Solar pattern. Nuclear properties of extremely neutron rich nuclei are important in order to fully and more clearly the *r*- process which is responsible for nucleosynthesis of element heavier than Fe. Nuclear properties can be found by performing the constrained calculation of the isotopic chain of the nuclei. PES calculation may have given the shape coexistence clearly as

well as triaxial deformation. I intend to carry out parametric studies of r-process nuclei based on more detailed and more realistic nuclear astrophysical model with different Skyrme forces.

5. Acknowledgement

I express my sincere gratitude to my supervisors Prof.G.Gangopadhyay and Prof. Abhijit Bhattacharyya, Department of Physics, University of Calcutta, West Bengal. Prof. G.Gangopadhyay has helped and advised during this research work.

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