Research activities in condensed matter theory spanned diverse areas such as the physics of nanomaterials, mesoscopic systems, molecular motors, heavy fermion systems, nonlinear Schrodinger equation, complex systems namely unzipping of DNA, sandpile models etc., phase transition in 2D extended XY-spin model, and electronic properties of hetero-structures. More specifically, Raman scattering intensity has been calculated for nano structures to study the interplay of the electronic and vibrational properties of such systems. The structure and stability of atomic clusters has been studied. Studies have been performed of the interplay of antiferromagnetism and superconductivity in heavy fermion systems and correlated superconductors. In mesoscopic systems at equilibrium, current enhancement effects have been demonstrated. Dephasing in mesoscopic systems, specifically in the Aharonov-Bohm ring, has been studied. Using stochastic energetics method, the efficiency of frictional thermal ratchets (molecular motors) has been studied.

The dynamics of phase transition associated with the unzipping of DNA has been studied using a discrete lattice model. The time evolution of unzipping is found to obey scaling laws, and the relevant dynamic exponents have been determined. Studies have been made of the universality class of noisy pulled fronts. Interfacial fluctuations in a sandpile have been studied as a limiting case of a class of one dimensional self-organized critical models. Studies have been made of certain discrete nonlinear Schrodinger equations and propagating solitary solutions have been shown to exist in such systems. The symmetry properties of these equations have been studied. Dark Current in AlGaAs/GaAs based hetero-structures has been studied, and different processes responsible for the escape of electrons from a biased single rectangular quantum well based on the Al_x $Ga_{1-x}As/GaAs$ heterojunctions have been considered. Investigations have been performed of the first-order transition in the classical 2D extended XY-spin model using Monte Carlo simulations and it has been demonstrated that the energy as a function of temperature exhibits a 'S'-shape at the first-order transition.

S. N. Behera

Atomic clusters, cluster assembled materials and nanostructures in general: Collaborative work on both the theoretifcal and experimental aspects of cluster assembled nanomaterials has been carried out duirng the year under consideration.

One of the most important aspects of physics of nanomaterials is determining their electronic as well as lattice vibrational properties. Since these nanomaterials quite often manifest as low dimensional systems such as quantum wires and quantum dots it is possible that these exhibit a strong interplay of their electronic and vibrational properties. Such an interplay is expected to be seen experimentally in metallic quantum nanowires and carbon nanotubes with diameters of a few nanometers and lengths extending to microns. These being one dimensional metallic systems, their electronic collective excitations, the plasmons are known to exhibit accoustic and optical like branches. The optical plasmons can have frequencies at the zone centre which are comparable to the optical phonons. Hence in a Raman scatterning experiment it is possible to study the interplay of these two modes. Keekping this in mind the Raman scatterning intensity is calculated which predicts clearly such an interplay between the two modes.

In the case of atomic clusters their structure and stability is determined by the electronic structure. Earlier a parametrized orthogonal tight binding molecular dynamics simulation method was adopted to calculate the structure and stability of samall silicon clusters consisting of upto 19 atoms. In order to check the reliability of these calculations, the results are compared with those obtained from other methods.

A phonomenological liquid drop model of nanoparticle is used to explain the lattice contraction of nanometer sized Sn and Bi particles.

Interplay of Magnetism and super-conductivity in Heavy Fermion Systems and correlated superconductors: The study of the interplay of magnetism and superconductivity is probably as old as the discovery of superconductivity itself. However, the coexistance of antiferromagnetism and superconductivity in systems like Rare earth Rhodium Borides and other ternary compounds dates back to about three decades. Subsequently the same coexistence was also found in some heavy fermion syperconductors, organic superconductors and more recently in Rare earth Nickel Borocarbide. The interplay, of these two long range orders, is probably at its best in these Borocarbides because of the availability of systems in which the superconducting (T_c) and antiferromagnetic (T_N) ordering transition temperatures are close to each other. These anomalies manifest as suppression of T_c on alloying as anomolous temperature dependence of the upper critical field and also in the temperature dependence of the phonon spectra as observed by inelastic neutron scattering. In order to understand these anomalies, a model (proposed earlier for explaining the observed heavy fermnion behaviour of certain high T_c superconductors) was adopted for the borocarbides. The model accounts for staggered sub-lattice antiferromagnetism and superconductivity by the itenerant conduction electrons, arising from the transition metal atoms; while the heavy fermion like behaviour is accounted for by the localized f-level of the rare-earth atom hybridizing with the itinerant electrons. The interplay of antiferromagnetism (AFM) and superconductivity (SC) was investigated by studying the temperature dependence of the respective order parameters. For a suitable choice of the parameters, the temperature dependence of the superconducting order parameter exhibits features similar to that observed in the temperature dependence of the upper critical field of some borocarbide superconductors in which AFM and SC coexist.

Theoretical calculations are performed of the Raman spectra of some heavy fermion superconductors. The system is represented by the Periodic Anderson Model, to account for the heavy fermion behaviour to which a mean field BCS term is added to represent superconductivity. Besides, the electrons are coupled to the phonons through the hybridization as well as the localized orbitaals. A detailed study of the Raman intensities and their variation with varying parameters of the model is presented. The study also provides a detailed review of the properties of heavy fermion, Kondo lattice and Kondo insurating systems.

S.M.Bhattacharjee

Dynamics of Unzipping of DNA by force: It is now well established that unzipping of DNA by a force is a genuine phase transition. A double stranded DNA remains bound until the force exceeds a critical value.

The dynamics of this unzipping transition has been studied using a discrete lattice model for DNA. The analytical solution of the equilibrium behaviour gives the phase diagram of the model exactly. The dynamics of unzipping can then be studied in various phases and also on the phase boundary. The time evolution of unzipping is found to obey scaling laws.

The relevant "dynamic" exponents have been determined. These scalings can be understood from the plausible mechanisms of unzipping and denaturation, except for the very high temperature region. For example, on the phase boundary, the time scales for unzipping one base pair at the contact point should be the same as the time required for the new kink released to diffuse out of the unzipped strand. This then tells us that the length m(t) of the unzipped strand should grow with time t as $m(t) \sim t^{1/3}$. Since the scaling form depends on the thermodynamic phase of the system, it could play a role in the mechanism to separate unzipped region from thermally denatured regions in real systems.

A. M. Jayannavar

Thermal ratchets (Molecular motors): It is known that molecular motors extract energy out of nonequilibrium enviroment and perform useful work (carrying cargo). Moreover they move in a unidirectional motion in absence of bias, which is ruled out under thermal equilibrium condition. Molecular motors thus acts as a engines, rectifying fluctuations into work. It is therefore necessary to quantify the efficiency of these engines working away from equilibrium (unlike conventional heat engines, fluctuations play the primary role).

For this we studied the efficiency of frictional thermal ratchets (motors) using stochastic energetics method, driven by finite frequency driving force and in contact with a heat bath. The efficiency exhibits varied behavior with driving frequency. Both nonmonotonic and monotonic behavior have been observed. Unlike the conventional heat engines, the magnitude of efficiency of thermal ratchets in finite frequency regime may be more than the efficiency in the adiabatic regime.

We are also studying the motion of two coupled overdamped Brownian motors moving in a flashing ratchet type potential. Besides the theoretical interest of studying the rectification properties of more complex system over a single particle system, these models have direct relevance to motion of double headed kinesin moving along cytoskeleton filaments. Coupled systems show several features like enhancement of diffusion and currents, noise induced stability, negative resistance, anomolous hysterisis, etc.

Time in Quantum mechanics: The subject of time in quantum mechanics is of perennial interest especially because there is no observable for the time taken by a particle to transmit (or reflect) from a given region of interest.The problem is essentially due to the fact that there is no hermitian operator to calculate this time in quantum mechanics. This problem has been beset with a lot of controversies. Several methods have been proposed based on scattering phase shifts and using different quantum clocks, where the time taken is clocked by some external input or indirectly from the phase of the scattering amplitudes. In our work we give a general method for calculating conditional sojourn times based on wave attenuation. In this approach clock mechanism does not couple to the Hamiltonian of the system. We emphasize that this time should satisfy certain criteria, which are -(a) It should be real, (b) It should add up for non-overlapping regions, (c) It should be causally related to the region of interest and (d) tend to correct classical limits. Our proposed clock satisfies all these aforesaid criteria as opposed to several earlier studies.

We have obtained an expression for the conditional time for the reflection of a wave from an arbitrary potential barrier using the WKB wavefunction in the barrier region. For this we have used the analogy with Bohmian picture of quantum mechanics. Our result indicates that the conditional times for transmission and reflection are equal for a symmetric barrier within the validity of the WKB approach.

Current enhancement effect in mesoscopic systems at equilibrium: We have studied a multiply connected mesoscopic system in both its open and closed form variations but in equilibrium using quantum theory. This system exhibits remarkable features, in its open form variation we see current enhancement, hitherto seen only in non-equilibrium systems in absence of magnetic flux. In its closed form analog parity effects are broken. Further we have analysed the global and local current densities of our system and shown that the orbital magnetic response of the system calculated from the current densities (and inherently linked to the topological configuration) is qualitatively not same as that calculated from its eigenenergy spectra or from theory of equilibrium statistical mechanics.

Dephasing in mesoscopic physics: The Aharonov-Bohm ring has been the mainstay of mesoscopic physics research since its inception. In our work we have dwelt on the problem of dephasing of AB oscillations using a model based on stochastic absorption. Dephasing or decoherence implies the loss of quantum mechanical interference due to coupling of an interfering particle with its surrounding environment. Complete dephasing erases the interference pattern. Thus quantum mechanical system behaves as though it were described by classical probability theory. We have calculated the conductance of Aharonov-Bohm ring by reformulating sequential transport. We have shown that conductance is symmetric under flux reversal (Onsager's relation) and visibility of AB oscillations decay to zero as a function of the incoherence parameter thus signalling dephasing in the system. We also see that this method of stochastic absorption/wave attenuation is better than the optical potential model which has also been used to simulate dephasing.

K. Kundu

Solitary Wave Like Solutions In Discrete Nonlinear Schödinger Equations: A new set of 1D discrete nonlinear Schrödinger Hamiltonians is introduced which includes the Ablowitz-Ladik system as a limit. The symmetry properties of these systems and their relationship with the Davydov-Holstein models for transport in biophysical systems are discussed. Proposed models are shown to possess propagating localized solutions. These propagating solutions exhibit nontrivial interactions, and, therefore, do not have the usual soliton properties.

A Study Of A New Class Of Discrete Nonlinear Schrödinger Equations: A new class of 1D discrete nonlinear Schrödinger Hamiltonians with tunable nonlinerities is introduced, which includes the integrable Ablowitz-Ladik system as a limit. A new subset of equations, which are derived from these Hamiltonians using a generalized definition of Poisson brackets, and collectively refered to as the N-AL equation, is studied. The symmetry properties of the equation are discussed. These equations are shown to possess propagating localized solutions, having the continuous translational symmetry of the one-soliton solution of the Ablowitz-Ladik nonlinear Schrödinger equation. The N-AL systems are shown to be suitable to study the combined effect of the dynamical imbalance of nonlinearity and dispersion and the Peierls-Nabarro potential, arising from the lattice discreteness, on the propagating solitary wave like profiles. A perturbative analysis shows that the N-AL systems can have discrete breather solutions, due to the presence of saddle center bifurcations in phase portraits. The unstaggered localized states are shown to have positive effective mass. On the other hand, large width but small amplitude staggered localized states have negative effective mass. The collison dynamics of two colliding solitary wave profiles are studied numerically. Notwithstanding colliding solitary wave profiles are seen to exhibit nontrivial nonsolitonic interactions, certain universal features are observed in the collison dynamics. Future scopes of this work and possible applications of the N-AL systems are discussed.

There is at least one continuous nonlinear equation, ϕ^4 equation, which can have either solitary wave solutions or "kink-like" solutions with permanent profile. On the contary, to the best of my knowledge there is no known analogy of ϕ^4 type of equation in the discrete case. So, here an extended nonintegrable version of the Ablowitz-Ladik discrete nonlinear Schrödinger equation (ALDNLSE), with a "tunable" nonlinearity is proposed. The form of nonlinearity in this equation is such that it can allow solitary wave like solutions, as seen in ϕ^4 equation. This equation for $m \varepsilon Z$ is

$$F_j(\psi_m, g_o^j) = g_0^j \left[(\psi_m^* \psi_{m+j} + \psi_{m+j}^* \psi_m)\psi_{m+j} + (\psi_m^* \psi_{m-j} + \psi_{m-j}^* \psi_m)\psi_{m-j}\right] \tag{1}$$

$$F(\psi_m, \lambda) = (1 + \lambda|\psi + m|^2) \sum_{j=1}^{l} F_j(\psi_m, g_o^j) \tag{2}$$

$$i\psi_m - 2j\psi_m + J(1 + \lambda|\psi + m|^2)(\psi_{m+1} + \psi m - 1) = -F(\psi_m, \lambda). \tag{3}$$

When $l = 1$, the system has an extra nearest-neighbor coupling in hopping with coupling constant, . In the $\lambda =$ w limit, this particular form of nonlinearity can be obtained by using the standard off-diagonal quasiparticle-phonon interaction theory and an antiadiabatic approximation. This equation also has an intimate relationship with Davydov-Holstein models for transport in biophysical systems.

The new discrete nonlinear Schrödinger equation enables us to show the existence of discrete nonintegrable nonlinear equations which can allow certain localized states to travel without experiencing any Peierls-Nabarro pinning from the lattice discreteness. It is also found that at least the interaction of two soliton-like solutions in nonintegrable systems has universal features. On the whole, this study offers a very significant insight into the transport properties of the well known Davydov-Holstein model for biological transport, and transport properties of localized states in soft molecular chains.

S. G. Mishra

Dark Current in AlGaAs/GaAs Based Hetero-structures: Long-wavelength infrared detectors, based on inter subband absorption in quantum well structures are being rapidly developed. The efficiency of a detector is high when the dark current in it is extremely small compared to the photocurrent. In order to understand the key parameters for reducing the dark current, it is essential to calculate it taking different escape mechanisms which contribute to it.

Different processes responsible for the escape of electrons from a biased single rectangular quantum well based on the Al_x Ga_{1-x} As/GaAs hetero-junctions have been considered. The direct tunneling rate due to the barrier lowering as a result of the applied electric field is studied. It is found to be temperature independent and exponential in nature. The indirect tunneling rates due to interaction of carriers with collective modes in the system are calculated using the Fermi golden rule where the interaction Hamiltonians are expressed in Frohlich form. While the acoustic phonon-assisted tunneling rate has negligible contribution at all field strengths and temperatures, the optic phonon- and plasmon-assisted tunneling rates turn out to be significant at room temperatures. While the phonon and plasmon assisted tunneling currents are weak, the dark current is governed by currents arising from the direct tunneling and thermionic processes.

S. B. Ota

Microcanonical Monte Carlo Simulations: The first-order transition in finite systems has induced notable scrutiny in recent years. Alder and Wainwright were the first to report a 'S'-shape in the phase-transition region of a two-dimensional (2D) system consisting of 870 hard-disk particles. Jellinek et al have simulated the solid-liquid phase change of 13 Argon particles using molecular dynamics. They have reported that when the caloric curve is constructed from averages over a long run, its form is smooth and monotonic showing no trace of the 'loop' that is observed with much shorter molecular dynamics run. The temperature dependence of energy for these systems, however, shows a 'S'-shape at the first-order transition in many computer simulations in microcanonical ensemble. There is substantial contemporary study on atomic clusters, in which, this element is also manifested in the temperature dependence of system energy. It is, however, not understood clearly, why the 'S'-shape arises in first-order transitions. Simulations in microcanonical ensemble implies that the system is not in contact with a heat bath or explicitly: 'isolated'. We have investigated the first-order transition in the classical 2D extended XY-spin model using Monte Carlo simulations. The simulations have been carried out on a system with 100 spins in the microcanonical ensemble, which represents a finite-isolated system. The energy as a function of temperature is found to exhibit a 'S'-shape at the first-order transition. We conclude that the observed phenomena at the first-order transition should be interpreted as the equilibrium response of a finite-isolated system.

G. Tripathy

Fluctuations of a pulled front: In continuation of an earlier work suggesting that fronts propagating into an unstable state should not be in the standard Kardar-Parisi-Zhang (KPZ) universality class, an effective field equation for this class of problems is introduced. It is shown on the basis of this equation that noisy pulled fronts in $d+1$ bulk dimensions should be in the universality class of the *((d+1)+1)*D KPZ equation rather than the $(d+1)D$ KPZ equation. Our scenario ties together a number of heretofor unexplained results in the literature, and is supported by earlier numerical results.

Interfacial fluctuations in a sandpile: Surface fluctuations of the Bak-Tang-Wiesenfeld (BTW) model were studied as a limiting case of a class of one dimensional self-organized critical (SOC) models where the effect of inertia is incorporated in a simple way. We find that for small systems the nature of interfacial fluctuations are fully described by an appropriate modification of the standard Kardar-Parisi-Zhang (KPZ) theory. However, we also find that for larger systems roughness scales very differently from the KPZ prediction. This indicates that criticality of the BTW model is responsible for the anomalously large roughness exponent observed.