計畫編號：BN06-00

計畫名稱：量子科學與工程研究中心

計畫主持人：朱時宜

計畫摘要(中)：

本整合型研究計畫含總計畫及五項子計畫。在總計畫中我們計畫建立「量子科學與工程研究中心」 (Center for Quantum Science and Engineering (簡稱 CQSE). CSQE 將是台大也是台灣第一個跨領域及尖端的量子中心。其主要目標分述如下：

- 促進前沿量子理論科學各方面的發展。
- 鼓勵理論和實驗物理學家之互動及合作，開發新穎的量子科技來研究超細尺度與超快量子動力學。
- 促進台大量子科學和工程學之研究員及中央研究院原分所之研究員的跨學科互動，建立世界一流的量子中心。
- 聘用優秀的量子科學與工程學研究人員。
- 促進和全世界科學家的交流與合作。
- 提供智力激發的環境，來培養學生在先進量子科技方面的學習及研究。

總計畫亦將負責行政協調及研究整合事項，而各子計畫的重點發展項目如下：

子計劃一 “原子分子與光學嶄新科技”將透過新的非微擾理論、阿秒雷射科技和新穎的非線性光學科技來研究超強且超短雷射場的原子分子物理、量子控制、實時電子動態、奈米電子學和奈米光學、以及多光子螢光與倍頻現象之應用等尖端課題。

子計畫二“量子計算與量子資訊/通信”研究量子計算與量子資訊/通信跨學門研究領域各種重要的研究課題。透過本計劃之研究，我們期望能有新的與令人激賞的科學能被發現和被深入的瞭解；同時能提升人們對自然界的量子性質的操控能力；並能進一步促進目前已被提出之各項有趣且重要的量子實驗的實現。

子計劃三“理論量子物理前沿”的主要目的是探索不同尺度的物理理論（高能理論及凝態理論）間的關係，尋求一個統合的理論架構。本計畫將透過在高能理論發展出來的量子場論來研究 BEC/BCS 跨越的新非微擾物理現象、拓墣量子計算、二維系統中的自旋流干涉等。

子計劃四“凝態理論高等研究”的主要目的是本研究選擇目前

凝態理論最有挑戰性的兩個課題進行研究。分別是 1. 在凝態物理中架構出一個整體理論來解決空間與時間的多尺度現象。2. 使用現代場論的方法來研究奇異的拓樸有序態、量子傳輸及自旋-軌道所引發的 Yang-Mills 場在二維電子氣中的影響及其相關行為。

子計畫五“計算科學及工程”的目的是要建立一個跨學門的研究群來探討先進的運算法，以及它們在計算科學與計算工程方面的應用。我們將集中發展新的演算法及佈置計算設施來解決量子物理在不同尺度下的計算問題----從量子色動力學到強關聯電子系統，原子分子及光子科學，及量子資訊科學等領域 (它們都是各子計畫中的研究主題)。

計畫摘要(英)：

The proposed program consists of a main project and five subprojects. In the main project, we propose to establish a state-of-the-art new center entitled “Center for Quantum Science and Engineering (CQSE)”. This will be the first interdisciplinary and forefront quantum center at NTU and in Taiwan. The primary goals of CQSE are as follows:

To advance progress in frontier quantum theoretical science on all scales.

To stimulate the interaction among theorists and experimentalists for the development of novel quantum technologies for probing ultra-fine scale and ultra-fast quantum dynamics.

To foster cross-disciplinary interaction among active researchers in quantum science and engineering at NTU and at the Institute of Atomic and Molecular Science (IAMS) of the Academia Sinica to build a world class quantum center.

To recruit outstanding quantum researchers to the center.

To promote international exchange and cooperation with global scientists.

To provide an intellectually stimulating environment for the training of students in advanced quantum science and technology.

The main project will also manage the administrative affairs and program integration. The focus of each subproject is as follows:

Subproject 1, “Atomic, Molecular, and Optical Science and Frontier Technology”, investigates cutting-edge topics of intense and

ultrashort laser field physics, quantum control, real-time electron dynamics, nanoscale electronics and nanophotonics, and application of multiphoton autofluorescence technology. The investigation is through the new nonperturbative theoretical formalisms, attosecond laser technology, and newly developed novel nonlinear optical technology.

Subproject 2, “Quantum Computing and Quantum Information/ Commutation (QCQI/C)”, investigates various important topics in the interdisciplinary field of QCQI/C. Through the studies of this subproject, we hope that new and exciting science can be understood, our ability to control the quantum aspects of nature can be greatly enhanced, and the implementation of fascinating quantum experiments that have been proposed can be facilitated.

Subproject 3, “Frontier of Theoretical Quantum Physics”, aims to provide a coherent theoretical study of, and to make links between high energy theory and condensed matter physics at different scales. Through quantum field theory developed in high energy physics, nonperturbative physics of the BEC/BCS crossover, topological quantum computing, and spin current interference in two dimensions will be investigated.

Subproject 4, Advanced Studies in Condensed Matter Theory”, focuses on two challenging areas of condensed matter theory: (1) developing a coherent numerical model to study the response of multiple spatial and time scales in condensed matters and (2) applying modern field theoretical methods to study the exotic topologically ordered states, quantum transport, and phenomena of spin-orbital induced non-Abelian gauge field in two-dimensional electronic systems.

Subproject 5, “Computational Science and Engineering”, aims to establish an interdisciplinary study of advanced computational algorithms and their applications in large scale computations in science and engineering. It focuses to develop new computationally-efficient numerical algorithms and enhance computing facilities for solving quantum physics problems at all energy scales, ranging from quantum chromodynamics, strongly correlated electron systems, atomic, molecular and optical science, and quantum information science, addressed in the other subprojects.

計畫編號：BN06-01

計畫名稱：原子分子與光學嶄新科技

計畫主持人：朱時宜

計畫摘要(中)：

原子分子和光學物理（AMO Physics）是 21 世紀最活躍的科學研究領域中的其中一項。特別在超快科學發展至阿秒(attosecond)階段和精準頻率梳激光科技的發明，是量子物理學中最令人振奮的最新進展。這個原子分子與光學嶄新科技計畫的目標是要建立一個智力激發平台，以促進跨學科合作，來探索在超快科學與量子控制科技中，這些令人振奮的新的科學契機。

研究團隊將由台灣大學、中央研究院原分所，以及交通大學的理論科學家和實驗物理學家所組成。

更具體來說，在本計畫中，我們將採用在原分所和台大所研發的新的非微擾理論、阿秒雷射科技與頻率梳激光科技，來探討以下的尖端課題：

1. 強激超短(阿秒)激光場的原子分子物理。
2. 研究高次諧波(high-order harmonic generation)，在 VUV/XUV 區域下的頻率梳狀結構和凝聚。
3. 原子分子與光學反應和凝態反應的量子控制。
4. 研究凝態系統和化學反應之電子動態。
5. 研發新穎的非線性光學技術及其應用。

本計劃的另一項特點是拓展與新的國內外的 AMO 學者共同研究合作，並加強我們與世界各國原子分子與光學研究中心既有的合作關係。我們計劃在台灣舉辦國際會議，來探討嶄新的原子分子與光學物理。本中心還將贊助國際知名訪問科學家和博士後計劃，以及小型研討課程。加入本研究計畫的博士後研究員和學生將能參與國際性的研究團隊，共同探討超快原子分子與光學之嶄新科技。

計畫摘要(英)：

Atomic, molecular, and optical (AMO) science is one of the most active scientific research fields in the 21st century. In particular, the development in ultrafast science into the attosecond (10-18 second) regime and the invention of the precision frequency comb laser technology are among the most exciting latest advancements in quantum physics. The goal of this AMO Science and Frontier Technology project

is to build an intellectually stimulating platform to facilitate the interdisciplinary collaborations on the exploration of these exciting new scientific opportunities in ultrafast science and quantum control technology.

The research team will consist of both leading theorists and experimentalists in National Taiwan University (NTU), Institute of Atomic and Molecular Science (IAMS) of the Academia Sinica (AS), and National Chiao Tung University (NCTU).

More specifically, in this project, we will investigate the following cutting-edge AMO topics by means of new nonperturbative theoretical formalisms, attosecond, and frequency comb laser technologies, etc., developed at IAMS and NTU:

1. Atomic and molecular physics in intense and ultrashort (attosecond) laser fields
2. Frequency comb structure and coherence in the VUV/XUV regimes via high-order harmonic generation
3. Quantum control of AMO and condensed matter processes
4. Study of real-time electron dynamics in atomic, molecular, and condensed matter systems and in chemical reaction.
5. Development and application of novel nonlinear optical technology.

An additional feature of the project is the ability to initiate new domestic and international collaborations and enhance our established collaborations with the major AMO research centers worldwide. We plan to organize international workshops/ conferences on frontier AMO science in Taiwan. The center will also sponsor visiting scientist and postdoctoral programs as well as mini-schools and mini-courses. Postdoctoral fellows and students participating in this research project will be joining an international research team working at the frontiers of ultrafast AMO science and technology.

計畫編號：BN06-02
計畫名稱：量子計算與量子資訊/通信
計畫主持人：郭斯彥
計畫摘要(中)：

量子計算與量子資訊/通信是以量子力學準則為運算與工作基礎

去研究、發現和進而設計出更有效的、更快速的或傳統電腦不可能達成的運算與資訊處理方法的新興且跨學門的研究領域。本子計畫之重要與創新之處即在於以廣泛之眼光來探索引人入勝的量子物理和在跨領域的量子計算與量子資訊/通信研究學門中的新穎與具挑戰性的應用。透過本計劃之研究，我們期望能有新的與令人激賞的科學能被發現和被深入的瞭解；同時能提升人們對自然界的量子性質的操控能力；並能進一步促進目前已被提出之各項有趣且重要的量子實驗的實現。

本計劃有關量子計算與資訊的研究主題包括：

1. 以矽半導體為基本材料的量子電腦元件的模擬計算
2. 對各種量子電腦提案中量子閘運算的最佳化研究
3. 固態量子位元的連續量子測量及量子回饋控制的研究
4. 量子系統受外部環境影響的非馬可夫消相干及退糾纏的動態的研究
5. 在介觀/巨觀物理系統中觀測出量子現象的研究與量子技術在精密測量的應用
6. 設計並建立一個可處理量子態資訊的網路，使得量子資訊能經由交換網路來傳送
7. 有關量子通信方面的應用研究，包括量子密碼學、量子分散式計算、多方量子通信等

本計劃的特色之一在於具有建立新的以及促進已經建立的與國際主要量子計算與量子資訊研究團隊間往來和共同合作研究的能力。我們也計畫未來幾年間在台灣舉辦量子計算與量子資訊的國際研討會。這些國際合作研究以及研討會的活動將提供更多國內接觸最先進的量子計算與量子資訊科技的平台和機會，因此將能進而促進此一令人興奮的科技能轉移到台灣。參與此計劃之博士後研究及博士生將加入的是一個從事尖端量子奈米科學研究的國際研究團隊。

計畫摘要(英)：

Quantum Computing and Quantum Information/Communication is a rapidly growing and interdisciplinary research field that explores and exploits quantum effects to compute and process information based on quantum principles in ways that are much faster or more efficient than or even impossible on conventional computers or information processing devices. The significant and innovative aspects of this subproject thus

relates to a large vision of exploring intriguing quantum physics as well as novel and challenging applications in this interdisciplinary field. Through the studies of this subproject, we hope that new and exciting science can be understood, our ability to control the quantum aspects of nature can be greatly enhanced, and the implementation of fascinating experiments that have been proposed can be facilitated.

The research topics that will be investigated in the quantum computing and quantum information/communication subproject include:

1. Device modeling of silicon-based quantum computer architectures
2. Optimizing quantum gate operations for various quantum computer proposals
3. Continuous quantum measurement and quantum feedback control of solid-state qubits
4. Non-Markovian decoherence and disentanglement dynamics of quantum systems in external environments
5. Study of observing quantum phenomena in mesoscopic (macroscopic) physical systems and applications of quantum technologies in precision measurements
6. Design and implementation of quantum-aware networks in which quantum phenomena such as superposition and entanglement can be processed and routed through a switching based architecture
7. Development of new communication-related applications, including quantum cryptography, quantum distributed computing and multiparty quantum secure communication

A feature of the subproject is the ability to initiate new international collaborations and enhance our established international collaborations with the major quantum computing and quantum information research groups worldwide. We also plan to organize and hold international workshops/conferences on quantum computing and quantum information in Taiwan in the next few years. These international collaborations and workshop/conference activities will give us access to state-of-the-art quantum computing and quantum information technologies, thus facilitating transfer of the exciting technologies to Taiwan. Postdoctoral fellows and PhD students participating in this research subproject will be joining an international research team working at the frontiers of quantum nanoscience.

計畫編號：BN06-03
計畫名稱：理論量子物理前沿
計畫主持人：賀培銘
計畫摘要(中)：

本計劃的目的是探索不同尺度的物理理論的關係，尋求一個統合的理論架構。 高能和凝態物理之間交互影響的一個著名的例子是凝態物理中重整群的概念，後來在高能物理中佔了極關鍵的地位（1982年諾貝爾獎）。反之，弦論中引伸出的非交換幾何被應用於量子霍爾效應的描述，矩陣模型被用來計算蛋白質的摺疊問題。最近，chiral anomaly 的概念也被應用於石墨薄片的研究中。

我們的主要數學工具是量子場論。 除了大家所熟知的量子場論應用，如量子霍爾效應，超導現象等，拓墣場論近來也被應用於量子電腦的研究中。BEC/BCS 跨越是另一個近年來受到注意的重要問題，而弦論中的 AdS/CFT 對偶性可能可以提供一個新的非微擾的研究途徑。我們也將研究二維系統中的自旋流干涉及其他量子計算中的問題。

我們的理論研究的主要概念之一是拓樸。拓樸在自然界中扮演一個極其重要的角色。量子物理中一些最有趣的物理現象，包括量子霍爾效應（1985 年諾貝爾獎）、分數量子霍爾效應（1998 年諾貝爾獎）、石墨薄片的新奇性質（近來是奈米科技及凝態物理最熱門的問題）、QCD 中 U(1)問題的解決、以及標準模型中手則畸異的抵消（這使我們得以對高能實驗的結果有精確的理論預測（1999 年諾貝爾獎 ）)，都與拓樸有密切的關係。

計畫摘要(英)：

The aim of this proposal is to provide a coherent theoretical study of, and to make links between physics at different scales. In particular, we apply techniques developed in high energy physics to condensed matter physics and quantum computation. As a famous example of the significant interplay between high energy and condensed matter theories, the idea of renormalization group learned from condensed matter physics turned out to be of utmost fundamental importance in high energy physics

(Nobel 1982). Conversely, the mathematical notion of noncommutative geometry in string theory, was applied to quantum Hall effect. Matrix models were used to describe protein folding. Recently, chiral anomaly also found its application to condensed matter physics in the study of graphene. This sub-project will serve as a platform on which experts in different areas come together, focus on the same problem, and benefit from each others’ expertise.

Quantum field theory (QFT) will be the main mathematical framework for our study. Our group members have considerable experience in application of QFT to various problems. In addition to well known topics in QFT such as quantum Hall effect, superconductivity, etc., topological field theory is recently applied to quantum computers. The BEC/BCS crossover is another important problem receiving a lot of attention these years. Application of AdS/CFT duality in string theory may open a brand new way to understand the nonperturbative physics behind it. We will also study spin current interference in two dimensions and other topics in quantum computation.

A central notion in our theoretical study will be topology. Topology plays a most important role in Nature. Its manifestations in quantum science leads to some of the most interesting physical phenomena such as the quantum Hall effect (Nobel prize 1985), the fractional quantum Hall effect (Nobel prize 1998), the novel graphene (recently the hottest topic in nanotechnology and condensed matter physics), the resolution of U(1) problem in QCD, and the anomaly cancellation in the Standard Model resulting in a renormalizable quantum field theory which gives precise theoretical predictions of measurements in high energy experiments (Nobel prize 1999).

In this sub-project, we will investigate the following topics:

(1) The role of chiral anomaly in two-dimensional condensed matter system such as graphene. (related to sub-project 2).

(2) Applications of topological quantum numbers, e.g. Berry phase, to quantum computing and information (sub-project 2), and to spin-orbital induced non-Abelian gauge in tow dimensional electronic system (sub-project 4).

(3) To determine the topological susceptibility in QCD and the mass of flavor singlet, and its potential realizations in condensed matter systems. (related to sub-project 4)
(4) To understand the relationship between the topological quantum numbers in condensed matter system (e.g., quantum Hall effect) and the axial anomaly and topological charge in quantum field theory. (related to sub-project 4)
(5) To understand the topological origin of BCS, and possibly BEC, and also to find an underlying theme for both low and high temperature superconductors, with AdS/CFT correspondence as a tool for the analysis of the BCS/BEC crossover. (related to sub-project 4)

計畫編號：BN06-04

計畫名稱：凝態理論高等研究

計畫主持人：張慶瑞

計畫摘要(中)：

科技的進展，使得人們可以合成 具有新的性質及在奈米尺度的材料。要能了解這些材料的機制，發展理論方法來研究這些系統中的多體效應是非常重要的。本研究選擇目前凝態理論最有挑戰性的兩個課題進行研究。

1. 凝態物理中的多尺度模擬

電腦的計算能力快速進步使得複雜系統的分析成為可能，而第一原理的計算幾乎已不需任何可調參數。本子項目主要在利用泛函密度理(DFT)論與量子蒙地卡羅(QMC)來研究奈米尺寸的物性， 如何解決在空間與時間的多尺度現象，而能有一個整體理論成為凝聚理論中重要的挑戰。本項目的重要目標是結合能帶理論，格林函數與 Boltzmann 方程式來了解奈米系統的多尺度響應，而研究的範圍會集中在團簇，單分子與二維電子氣。 我們也會發展有效數值方法來處理強關聯系統內的問題。

2. 奇異量子態及量子傳輸

強關聯量子系統總是帶來驚奇。在過去的二十年間，人們已經認識到奇異量子態，如分數量子霍爾態，是超越了傳統的 Landau 對稱破壞和費米液體的典範所可以描述的。拓撲序的概念被提出來描述這些奇異態。 嶄新的拓樸有序態在凝態系統中出現，並遠較對稱破壞態更有趣。我們對這些奇異態，例如具有不同規範對稱性的自旋液

體，以及價鍵固體等的了解仍然是非常有限的。現代場論的方法是研究這些這些奇異態異不可或缺的工具，這也顯示這是凝態理論研究令人興奮的新方向。

奈米結構下的電子傳輸中的物理，是非常的豐富，低溫下，量子力學的行為變得重要。我們的研究將側重於理解和控制的量子特性，在自旋極化結構中的電子傳輸。我們利用非平衡格林函數來了解奈米尺寸的量子輸運，特別是 Landauer-Keldysh 法用來了解有自旋的傳輸現象。次微米尺寸時，粒子的擴散性使得 Boltzmann 傳輸方程式變成可行 。近日的自旋量子 Hall 效應，更使得此一研究有新的意義，我們使用量子場論來研究自旋相關傳輸及其相關的自旋-軌道所引發的 Yang-Mills 場在二維電子氣中的影響及其相關行為。

我們希望啟動跨學科之間的不同子領域的互相交流，並建立更強的國際合作研究。我們計劃舉辦先進題目的研討會，以激發新的想法和新的合作關係。此外，學生，博士後和本地科學家將能夠獲益於國外訪客計畫。這些活動將使我們的凝聚態理論研究，保持在最前列。

計畫摘要(英)：

With advancing technology it is now possible to synthesize nanoscale materials with novel properties. In order to understand the physics of these materials it is essential to develop new theoretical methods of studying many-body effects in these systems. In this project we focus on two challenging areas of condensed matter theory.

1. Multiscale modeling in condensed matter:

The fast progress of computation power makes the numerical simulations in complex systems become feasible. Recent ab initio calculations in electronic structure systems have become almost parameter-free. The primary aim of this research direction is the study of nanomaterials by Density Functional Theory and Quantum Monte Carlo methods. However, the multiple spatial and time scales contained within the theory present great challenges. The ultimate goal of this study is to combine the band theory calculation, Green's function and Boltzmann transport equation to understand the multiscale response in condensed matters systems. We intend to focus our study on clusters, single molecules and two-dimensional electronic gas. We shall also focus on developing efficient numerical methods to solve the realistic situation in

strongly correlated electron systems.

2. Exotic quantum states and quantum transport

Quantum systems with strong correlations always bring surprises. In the past two decades, it has been realized that exotic quantum states, such as the fractional quantum Hall states, are beyond the description of conventional Landau symmetry-breaking and Fermi-liquid paradigms. A new kind of order, the topological order, has been proposed to describe these new states. Topologically ordered states emerge in a new class of materials, and prove to be even richer than symmetry breaking states. Our understanding of these exotic states, such as spin liquids with different gauge symmetries is still limited. Modern field theoretical methods are essential to study these exotic states, and this is an exciting new direction for condensed matter theory.

The physics of electron transport in nanostructures is incredibly rich, and at low temperatures, quantum mechanical behavior emerges. Our research will focus on understanding and controlling the quantum properties of structures in spin-polarized transport system. Non-equilibrium Green's function method will be applied to study the quantum transport behavior on nanoscale. In particular, the Landauer-Keldysh method can be used to study the spin-polarized transport phenomena. For the submicron scale, the diffusive nature of the electrons makes the Boltzmann transport equation a feasible approach. Interdisciplinary collaboration between field theorists and condensed matter theorists is crucial for the understanding of phenomena of spin-orbital induced non-Abelian gauge in two-dimensional electronic systems.

We hope to initiate interdisciplinary communication among the different subfields, and build a stronger international collaboration. We plan to organize workshops on advanced subjects to inspire new ideas and collaborations. In addition, students, post-docs and local scientists can benefit from foreign visitor programs. These activities will keep our research in condensed matter theory at the forefront of current research

計畫編號：BN06-05

計畫名稱：計算科學及工程

計畫主持人：許文翰/ 趙挺偉

計畫摘要(中)：

本計畫的目的是要建立一個跨學門的研究群來探討先進的運算法，以及它們在計算科學與計算工程方面的應用。這個研究群是台大迫切需要的，但是一直以來並未成立。所以我們希望能藉著這個計畫來提供一個平台，讓從事計算科學及計算工程的專家可以聚在一起，在一個共同的目標下去發展新的演算法，希望能互相激發靈感而彼此受益。因為量子場論與許多在量子科學及工程的問題都有密切關係，所以我們將集中發展新的演算法來解決量子場論在不同尺度下的計算問題－從量子色動力學到強關聯電子系統，原子分子及光子科學，及量子資訊科學等領域 (它們都是在 1－4 各子計畫中的研究主題)。透過本子計畫的研究，我們希望可以發展新的數值演算法及特別方針來解決與本卓越研究中心研究主題相關的大型計算。簡言之，我們要透過先進的計算途徑，來達到發現新科學的目標。

我們希望可以藉這個計畫，能在台大建立一個計算科學與工程的卓越研究群。為了達到這個目的，我們計畫聘請 1 位全職的研究助理，3 位博士後研究員(或訪問學者)。同時我們會購買一些特別的硬體(例如：GPU 及三度空間虛擬實境工作站)，來進行 N-body, lattice QCD 及量子自旋系統的大型數值模擬及分析數據的三度空間顯示。此外我們會開啟國際合作的研究，以增強與世界主要研究群既有的國際合作研究關係。自從 2006 年，以台大為基地的台灣 QCD 研究團隊(TWQCD)與日本格點 QCD 研究團隊(JLQCD)已開啟合作關係。這是一個非常成功的合作研究，因為我們已經獲得幾個世界一流的研究成果。參加 TWQCD 研究群的博士後研究員跟研究生，也同時是國際研究團隊的一員(例如：JLQCD)，進行格點 QCD 的前緣研究。這些國際合作研究將有助台大進入全世界 100 名頂尖大學的行列。

計畫摘要(英)：

The aim of this subproject is to establish an interdisciplinary study of advanced computational algorithms and their applications in large scale computations in science and engineering, which has been long overdue at NTU. It will provide a platform for experts in computational science and engineering to get together, to develop new algorithms of common interests, and to benefit from each other’s expertise. Since Quantum Field Theory (QFT) is relevant to many problems in Quantum

Science and Engineering, we will focus our efforts in developing new algorithms and enhance computing facilities for solving QFT at all energy scales, ranging from quantum chromodynamics (QCD), strongly correlated electron systems, atomic, molecular and optical (AMO) science, and quantum information science, which are addressed in the respective subprojects 1, 2, 3, and 4. Through the studies in this subproject, we hope to develop new computationally-efficient numerical algorithms and paradigms which