A new system of library code is proposed and initiated. It is emphasized that the same terminologies as we find in our textbooks should be used for class names in the library code. The language C# invented by Microsoft is adopted in this project. Several rules of thumb are suggested in order to obtain easy-readable coherent codes. As a first step, we present the library code for exact diagonalization in physics. When we build codes, we clearly distinguish between model independent and dependent parts, and we use familiar terminologies like Hamiltonian, HilbertSpace, GroundState, etc as class names. As an explicit example, we calculate ground state energy of a quantum dot, showing the triplet-singlet transition.

I. INTRODUCTION

In Feb. 2002, Microsoft launched a new program language named C#, which is strongly object-oriented. It is argued that C# language has three characteristic features, 1. C# is as elegance as Java, 2. C# is as powerful as C++, 3. C# is as productive as Visual Basic. Although it is still questionable whether or not C# is useful for scientific computing in academic area, we here adopt C# because of its strong character of object-oriented language.

Reusability is always one of main concerns in the area of software. Scientific computing also should require reusability seriously. We notice many efforts to improve reusability. The web site managed by Troyer is remarkable. The library code for density matrix renormalization group method invented by White is also well known. These library codes are written in C++. There are many fortran codes in netlib. It is clear that there is a general trend of transition from non object-oriented to object-oriented language.

The main advantage of C# over C++ is efficiency in making Windows applications. Since computer users are addicted by Windows operating system, user friendly programs would be Windows applications. As far as end users need more user friendly programs, C# can be useful. One good point is that so called Mono project is carried on to develop the C# compiler for Linux. After successful finish of Mono project, we guess that C# will become more popular.

In this article, we propose a new way of making library codes with C# as a preparation for the battle between C# and C++, which will take place soon. At present, C++ is the most powerful. However, after someone makes ease access to parallel computing in loosely connected Windows operating systems using XML web services, we expect that C# can compete with C++ even in scientific computing.

II. SUPERCODE

In order to improve the power of scientific computing, we have to consider the three factors: CPU time, REM memory, and Coding time. For some complicated problems, the main factor is nothing but coding time. In this situation, someone want to use Standardized Reusable Components (SRC). When we say Hamiltonian, everyone in physics community can understand the meaning of it. Hence, there must be a class called Hamiltonian. At this moment, we should notice the usefulness, when we use the same terminology as we find in our textbooks. All library codes must be organized like our textbooks and our library. The system of library codes should not be in simple alphabet order, but would be in subject-based order. This subject-based integration of library codes will result in high correlations between codes, in other words, it will need more coherence between codes. It is not an easy task to make classification in each category of our knowledge. We may need a big discussion on this matter. At any rate, this library codes can be called Supercode. As we see in usual real library, we can divide Supercode as Biology, Chemistry, ElectricalEngineering, Mathematics, MechanicalEngineering, Physics, etc.

In scientific computing, programmers always want to know results as quickly as possible. Because of this hurry habit, program codes become less structural, and reusability is lost. In order to enhance reusability, it is strongly proposed that scientists should make program codes in distinguishing model-independent and model-dependent parts. The model-independent parts are properly organized and will be upgraded in the future. Numeric workers should be familiar with the whole structure of model-independent parts, and should handle model-independent and model-dependent parts simultaneously. In order to emphasize the way of coding, we denote HANA, which is abbreviation for “Handle All aNd All”, where the first “All” means model-independent parts and the second “All” means model-dependent parts. We define HANA project as efforts to make Supercode. We are summing up some rules of thumb for Supercode:

1. Divide and Conquer. Do not exceed the total num-
We here omit to show the present codes of Physics0.01. All detailed codes are freely open in the author’s home page. This prototype object-oriented programming for physics is invented mainly only for exact diagonalization. We expect that Monte Carlo and Maxwell equation will be included. Hence upgrade Physics0.02 will appear soon.

IV. EXAMPLE: GROUND STATE ENERGY IN 2D PARABOLIC QUANTUM DOT

In order to present the general procedure of HANA project, we consider the problem of evaluating ground state energy in a two-dimensional parabolic quantum dot. In this problem, the second quantized Hamiltonian is written as

\[
H = \sum_{n,l,\sigma} (\hbar \omega (2n + \vert l \vert + 1) - \frac{1}{2} \hbar \omega c l - g \hbar \omega c \sigma \sigma^+ c^\dagger_{n l \sigma} c_{n l \sigma})
\]

\[+ \frac{1}{2} \sum_{n_1, n_2, n_3, n_4, k, l, m} V_{n_1 n_2 n_3 n_4}(k, l; m) \times \sum_{\sigma, \sigma'} \epsilon_{n_1, k, l, \sigma} \epsilon_{n_2, l + m, \sigma'} C_{n_1 \sigma} c_{n_2 \sigma} c_{n_4 k + m \sigma}, \tag{1}
\]

where one-particle creation operators \( c_{n l \sigma}^\dagger \) have three quantum numbers. The principal quantum number \( n \) runs as 0, 1, 2, 3, \( \cdots \), while the angular momentum quantum number \( l \) is given by \( 0, \pm 1, \pm 2, \pm 3, \cdots \), and the spin index \( \sigma = \pm 1 \). Note that the confining potential is related to \( \omega_0 \) in the usual way, and \( \omega = \sqrt{\omega_0^2 + \frac{1}{4}\omega_C^2} \), where the so-called cyclotron frequency is proportional to the strength of magnetic field \( B \) as \( \omega_C = eB/m^*c \). It is straightforward to calculate the Coulomb matrix elements:

\[
\frac{1}{2} V_{n_1 n_2 n_3 n_4}(k, l; m) = \frac{1}{2} C_{n_1 n_2 n_3 n_4} (k, l; m)
\]

\[= \hbar \omega \frac{58.47}{\kappa} \sqrt{\frac{m^*}{m}} \sqrt{\frac{m}{\hbar}} \frac{1}{\omega C} C_{n_1 n_2 n_3 n_4} (k, l; m), \tag{2}
\]

where \( \kappa \) is a dielectric constant, and \( C_{n_1 n_2 n_3 n_4} (k, l; m) \) are dimensionless numbers. With the usual bulk values, \( m^* = 0.07m \) and \( \kappa = 13 \), the overall factor of the Coulomb interaction becomes 58.47/13 * 0.07 = 1.19. However, since the used quantum dot looks two-dimensional, it seems that the values of dielectric constant and effective mass are not known. Thus, it is needed to take the overall factor as an input parameter. The value of \( \omega_0 \) is also an input parameter. In fact, the side gate is used in order to control the confining potential. In consequence, this calculation has four input parameters: number of electrons, the overall factor, \( \omega_0 \), and \( \omega_C \). We take 20 lowest energy states as \( 2n + \vert l \vert + 1 \leq 4 \) in this exact diagonalization. Only the main parts of the code are presented as follows.
using QM=Physics.QuantumMechanics;
using H=Physics.QuantumMechanics.Hamiltonian;
using HS=Physics.QuantumMechanics.HilbertSpace;
using OP=Physics.QuantumMechanics.Operator;

int Ne = Convert.ToInt32(textBox2.Text); \ input number of electrons
double factor = Convert.ToDouble(textBox3.Text); \ input the overall factor
double omega0 = Convert.ToDouble(textBox4.Text); \ input omega0
double omegac = Convert.ToDouble(textBox5.Text); \ input omegac

int half = (numberOfElectrons + (numberOfElectrons % 2))/2; \ At half, S_z=0

QM.Space i1 = new QM.Space(7,2); \ 14 sites
QM.Space i2 = new QM.Space(3,2); \ 6 sites
QM.Space ii = new QM.Space(i1,i2); \ add Space i1 and i2, so 20 states

QM.QuantumNumber qn = new QuantumNumberForModel(ii); \ assign n, l and spin
QM.Coupling u = new CouplingForModel0(qn,omega0,omegac); \ one body spectrum
QM.Coupling w = new CouplingForModel1(qn,factor,omega0,omegac); \ Coulomb matrix

OP.FermionCreation cdagger = new OP.FermionCreation(ii);
OP.FermionAnnihilation c = new OP.FermionAnnihilation(ii);

H.Hamiltonian h0 = new H.FermionOneBody(u, cdagger, c);
H.Hamiltonian h1 = new H.FermionTwoBody(w, cdagger, cdagger, c, c);
H.TotalHamiltonian h = new H.TotalHamiltonian(h0,h1);
h.ZeroPointEnergy = 0.0;

OP.Number nop = new OP.Number(numberOfElectrons);
for(int ta = 0; ta < 3; ta++){
    for(int ts = half; ts < half+2; ts++){
        QM.ConservedQuantity totalAngularMomentum = new QM.ConservedQuantity(qn,1,ta);
        QM.ConservedQuantity totalSpin = new QM.ConservedQuantity(qn,2,ts);

        HS.HilbertSpace hil1 = new HS.Fermion(cdagger, nop);
        HS.HilbertSpace hil2 = new HS.Reduction(hil1,totalAngularMomentum);
        HS.HilbertSpace hil = new HS.Reduction(hil2,totalSpin);

        QM.GroundState psi = new QM.GroundState(h,hil);
textBox1.Text = Convert.ToString(psi.Energy);}}

Note that the classes of model-independent parts are in specific directories. The model-dependent parts consist of QuantumDot.cs, QuantumNumberForModel.cs, CouplingForModel0.cs and CouplingForModel1.cs. The user friendly simulation program runs in Windows operating system. Giving the four input parameters, we simply click a button to find the ground state energy. The final result of ground state energy is printed on the screen.

We present the result of calculation related to the triplet-singlet transition[10], when the strength of confining potential is increased in the dot containing six electrons. We let the overall dimensionless factor be 2, and $\omega_c = 0$. We find the transition near $\hbar\omega_0 = 1.14$ meV as shown in Table II. We expect that someone observe this transition using the side gate voltage in the future.

V. CONCLUSION

We proposed a library code system, emphasizing that class names should be the same as we find in textbooks.
TABLE I: The ground state energy in each sector. We notice that there is the triplet-singlet transition between 1.1 and 1.2.

| Sector | Ground State Energy |
|--------|---------------------|
|        | $\hbar \omega_0 = 1.1$ | $\hbar \omega_0 = 1.15$ | $\hbar \omega_0 = 1.2$ |
| 0 0    | 59.7012              | 61.4422              | 63.1693              |
| 0 1    | 59.7247              | 61.4975              | 63.2490              |
| 1 0    | 59.7012              | 61.4759              | 63.2299              |
| 1 1    | 59.7247              | 61.4975              | 63.2490              |

Like an well known idiom in algorithm, “Divide and conquer”, we introduced “Handle all and all” for this library system. The first “all” means library codes and the second “all” means our specific project codes. Hence, there are only two folders: one is library and the other is our specific model dependent project. As the library grows, we expect that each class becomes strongly correlated with others. To change codes is not an easy task because of coherence between codes. However, experts can freely change the codes, and thus invent the upgrade version with fixing the first number such as Physics1.03 from the mother version Physics1.00. For instance, if someone feel that the class Symmetry can be improved, then change the code. If this change is worthwhile for everyone, then it should be reflected in the next version of Physics with clear notification of contributors. Along this line, the prototype library code, Physics0.01, will be upgraded soon.

We know that nowadays many theoretical physicists spend more time in complicated computing, which is however conceptually trivial. We agree that physicists need to do philosophical and conceptual thinking more. The author likes to imagine that a higher version of Physics will reduce the time of computing for all physicists.

Acknowledgment

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