Exploiting the paradigm of quantum information in nanosystem modeling

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Abstract. We will discuss a recently introduced approach to modeling the electronic properties of nanosystems. It is based upon a special type of Hamiltonian dynamics associated with mixed states of composite systems. In particular, the formalism of this approach leads to the concept of nonlocal bonding. This paradigm has already proven useful in finding computationally implementable PDE models of quantum Hall systems in equilibrium. The discussion in this report will highlight the non-equilibrium evolution of such systems. In particular, we will discuss some preliminary indications of the relevance of the dynamics based on time-periodic Hamiltonian.

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1. INTRODUCTION

The progress of nanotechnology will in large measure depend on our ability to effectively model nanosystems. For one thing, parametric models of nanosystems are crucial in the development of systematic methods for the task of harvesting of information from nanosystem generated signals. The latter operation, in turn, may prove quite crucial in the nanofabrication process control and quality assurance. This is in addition, of course, to the fact that the ability to model nanosystems is certainly conducive to the deeper understanding of the fundamental physics of nanosystems. We note, however, that simulation of complex quantum systems within the framework of the *ab initio* paradigm is hardly ever feasible. This points to a need to develop novel methods for nanosystem modeling. Recently we have been able to construct a PDE model of quantum Hall systems, [1]. The model is based on a conceptual framework which involves the quantum information theory in addition to a hidden-variable type nonlinear quantum dynamics, [2]. Moreover it turns out that the paradigm we have assumed is in principle amenable to experimental testing; the most direct type of test would be based on the principle of quantum teleportation, [3]. At the same time, the model can be tested indirectly by observation of various phenomena it predicts. In this report we will review the foundational concepts and subsequently indicate potential novel predictions of the model. Namely, we will demonstrate that the model predicts self-induced time-periodic Hamiltonian dynamics. The specific properties of this dynamics will be addressed at a later date. However, already at this stage, we can speculate that this type of dynamics potentially leads to distinct observable phenomena, e.g. induced radiation phenomena, among other.

2. BIPARTITE QUANTUM SYSTEMS

Let $\widehat{\mathbf{H}}$ and $\mathbf{H}$ be finite-dimensional Hilbert spaces, of equal dimensions, representing two quantum systems. Consider a composite system confected of the two subsystems, which is represented by the tensor product space $\widehat{\mathbf{H}}\bigotimes\mathbf{H}$. The states of the composite system, [4], assume the form

$$|\Psi_{\text{combined}}\rangle = \sum_{m,n} K^*_{mn}|\varphi_m\rangle \otimes |\psi_n\rangle \in \widehat{\mathbf{H}}\bigotimes\mathbf{H}, \tag{1}$$

where $\{\varphi_n\}$ and $\{\psi_n\}$ are orthonormal bases. We will associate with $|\Psi_{\text{combined}}\rangle$ the operator

$$K = \sum K_{mn}|\varphi_m\rangle\langle\psi_n|. \tag{2}$$

In particular, if the subsystem corresponding to $\mathbf{H}$ were found in the state, say, $\psi \in \mathbf{H}$, then the other subsystem would collapse onto the state $K\psi \in \widehat{\mathbf{H}}$. Let us define the density operators of both subsystems in the usual way, i.e.

$$\begin{aligned} \rho &= \mathrm{Tr}_{\widehat{\mathbf{H}}}\left(|\Psi_{\text{combined}}\rangle\langle\Psi_{\text{combined}}|\right), \\ \hat{\rho} &= \mathrm{Tr}_{\mathbf{H}}\left(|\Psi_{\text{combined}}\rangle\langle\Psi_{\text{combined}}|\right). \end{aligned} \tag{3}$$

One readily finds

$$\rho = K^*K, \qquad \hat{\rho} = KK^*. \tag{4}$$

This outlines the basic structure for a quantum-mechanical description of a composite system.

3. THE CONCEPT OF NONLOCAL BONDING

We wish to consider the energy functional of the form

$$\mathrm{Tr}\left(H\rho\right) + \mathrm{Tr}\left(\hat{\rho}\hat{H}\right) + \beta\mathrm{Tr}\left(f\left(\rho\right)\right), \tag{5}$$

where f is a suitable analytic function. In view of the fact that ρ can vary, it may be appropriate in some contexts to restrict f to the Hardy class H^1, [5], but other functions are also admissible, such as the important example of the logarithm. As it turns out, substituting the decomposition (4) into (5) leads to interesting Hamiltonian dynamics. Indeed, consider

$$\Xi(K) = \mathrm{Tr}\left(KHK^*\right) + \mathrm{Tr}\left(K^*\hat{H}K\right) + \beta\mathrm{Tr}\left(f\left(K^*K\right)\right). \tag{6}$$

The gradient flow of this functional is found to assume the form of a *Hamiltonian* evolution equation

$$-i\hbar\dot{K} = KH + \hat{H}K + \beta Kf'(K^*K), \tag{7}$$

cf. [3], [6] for more details and relevant calculations. It is interesting to postulate that this equation describes the evolution of the composite state (1). A straightforward calculation shows that if $K = K(t)$ is a solution of (7), then the corresponding density operators (4) satisfy the quantum mechanical law of evolution, i.e. the Heisenberg equation. Namely,

$$i\dot{\rho} = [H,\rho], \quad \text{and} \quad i\dot{\hat{\rho}} = [\hat{\rho},\hat{H}]. \tag{8}$$

Therefore, evolution prescribed by (7) remains hidden if it is analyzed via the prism of component-wise observation. Note that we have fermionic-type symmetry here, i.e. switching the two subsystems will alter the signs in their evolution equations. Note also that equations (8) directly imply

$$\frac{d}{dt}\mathrm{Tr}\left(\rho\right) = 0 = \frac{d}{dt}\mathrm{Tr}\left(\hat{\rho}\right). \tag{9}$$

Thus, once the variable K is normalized at time zero, so as to ensure $\mathrm{Tr}\left(\rho\right) = 1 = \mathrm{Tr}\left(\hat{\rho}\right)$, the density operators will remain normalized for all times.

The stationary-state equation corresponding to (7) is

$$KH + \hat{H}K + \beta Kf'(\rho) = \nu K. \tag{10}$$

this equation has been discussed in [2] for $f(z) = log(z)$. It is demonstrated that in case of two-level subsystems with $\hat{H} = H = \mathrm{diag}(h_1,h_2)$, the model predicts a nonlocal molecule assuming two discrete energy states an energy gap

$$\Delta E = \sqrt{\beta^2 + (h_1 - h_2)^2} - \beta.$$

4. THE SEMICLASSICAL LOOP IN SYSTEMS WITH AMBIENT MAGNETIC FIELD

Thus far our discussion of the composite system has been symmetric with respect to the two subsystems. (Note that $\beta \mathrm{Tr}(f(\hat{\rho})) = \beta \mathrm{Tr}(f(\rho))$.) In some cases it may be appropriate to give up this symmetry. Indeed this is what we have proposed in relevance to the Quantum Hall Effect, [1]. Namely, the quantization of Hall resistance is captured by a certain system of nonlinear PDE, which stems from (10) (with $f \equiv \log$) on one hand, and a description of the electron in the magnetic field via the Landau Hamiltonian on the other. We now wish to consider a possible generalization of that model. More specifically, let us take the magnetic-field system as a hatted subsystem with trivial evolution $\hat{H} = 0$. Let us also take an electronic subsystem with nontrivial evolution prescribed by $H = H_A = \nabla_A^* \nabla_A$. The coupling between the two subsystems will be asymmetrical. First, if the electronic subsystem is in a state ψ then the magnetic system is postulated to be in the state $K\psi$. Second, the feedback from the magnetic field to the electronic subsystem is via the magnetic flux density $B = R_H |K\psi|^2$. (R_H is the necessary normalizing factor.) This leads to the following system of PDE:

$$\begin{cases} *dA &= R_H |K\psi|^2 \\ -i\hbar \dot{K} &= KH + \beta K f'(K^*K) \\ i\hbar\dot{\psi} &= H_A \psi \end{cases} \tag{11}$$

We wish to understand what possible observable phenomena can take place when the system undergoes evolution of this type. The exact properties of solutions to this system will require further research, but we shall be able to make a few interesting observations already now.

5. TIME-PERIODIC HAMILTONIAN DYNAMICS IN QUANTUM HALL SYSTEMS

Consider (11), and substitute $\varphi = K\psi$. A straightforward calculation shows that the system is equivalent to

$$\begin{cases} *dA &= R_H |\varphi|^2 \\ i\dot{\varphi} &= \beta f'(\hat{\rho})\varphi \\ -i\hbar \dot{K} &= KH + \beta K f'(K^*K) \\ i\hbar\dot{\psi} &= H_A \psi \end{cases} \tag{12}$$

Moreover, since $\hat{H} = 0$, (8) implies that the density $\hat{\rho}$ is frozen in time, i.e. $\hat{\rho}(t) = \hat{\rho}(0) = K(0)K(0)^*$. Therefore, the electronic system does not affect the magnetic component during the evolution time $t > 0$. At the same time, the independently evolving magnetic field will have an effect on the electronic subsystem. Recall that (in suitable units) the magnetic Hamiltonian assumes the form

$$H_A \psi = \frac{1}{2}\left(-\Delta\psi + 2i\langle A, d\psi\rangle - i(\delta A)\psi + |A|^2\psi\right).$$

Now, the vector potential A is determined by the wavefunction

$$\varphi(t) = e^{-i\beta f'(\hat{\rho}(0))t/\hbar}\varphi(0)$$

via equation $*dA = R_H|\varphi|^2$. The vector potential, in turn, feeds to the electronic Hamiltonian $H_A = \nabla_A^*\nabla_A$.

Consider a possible scenario in which $f'(\hat{\rho})$ has commensurate eigenvalues, so that $\varphi(t)$, and therefore automatically the magnetic flux density as well, will be a periodic pulse. Hamiltonian dynamics with periodic magnetic field is an interesting and nontrivial object. It has been considered from the point of view of direct operator analysis, e.g. [7]. Periodic Hamiltonians in general have been the subject of research involving semiclassical methods, especially in the context of chaotic flows, [8]. Remarkably, time-periodic systems, the kicked rotators, have been considered in the context of Anderson localization relevant to solid state systems, [9]. Finally, time-periodic magnetic Hamiltonian typically implies radiation phenomena [10]. Of course, more research in theory and simulation will be necessary before we can draw final conclusions as to the exact nature of dynamics in our scenario. However, we are induced to propose, as a working hypothesis, that spontaneous radiation phenomena may occur in non-equilibrium quantum-Hall type systems. We emphasize that the periodic magnetic field is not imposed externally, but rather forms spontaneously under the conditions of the quantum-Hall regime. In this regime, the external magnetic field is imposed as a strong constant field, and its spatial and time variability are the result of feedback from the electronic subsystem.

6. CONCLUSION

We have discussed a specific approach to the task of modeling of the quantum Hall nanosystems. We view quantum Hall systems as prototypical nanosystems, and believe that many of the principles relevant to this field will prove relevant to nanophysics in general. In this spirit, we have shed some light on the relation of the assumed paradigm to the fundamental principles of quantum mechanics. We have also justified some new hypotheses for further research into the properties of quantum Hall systems. A satisfactory resolution of the questions of interest will require a synergetic effort in the areas of theory and computer simulation, as well as experiment.

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