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From classical to quantum dynamics at Rokhsar–Kivelson points

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Abstract

For any classical statistical-mechanics model with a discrete state space, and endowed with a dynamics satisfying detailed balance, it is possible to generalize the Rokhsar–Kivelson point for the quantum dimer model. That is, a quantum Hamiltonian can be constructed (on the same state space) such that the ground state wavefunction coincides with the classical equilibrium distribution. Furthermore the excited eigenstates correspond to classical relaxation modes, which (in cases with a symmetry or conserved quantity) permits extraction of the dispersion law of long-wavelength excitations. The mapping is natural mainly when the states have equal weight, as is typical of a highly frustrated model. Quantum and classical correlation functions are related by analytic continuation to the imaginary time axis.

1. Introduction

The quantum dimer model [1] of Rokhsar and Kivelson (RK) was inspired by the resonating-valence-bond state of a quantum antiferromagnet, which had just been proposed as a starting point for the explanation of high-temperature superconductivity. That was not to be, but models of this type are of interest among the 'highly frustrated systems' [3] characterized by massive degeneracy (or near-degeneracy). Generalizations of the RK construction were used to construct the first concrete lattice models for dimension $d > 1$ that manifestly exhibit fractionalized excitations [2–6].

The quantum dimer model had one nontrivial parameter V/t (see equation (2.1), below); when it takes a special value ('RK point'), RK showed that the exact ground state wavefunction is an equal-weighted superposition of all dimer coverings. This had the same (critical) static correlations as the classical dimer ensemble, an exactly solved model [7, 8]. Thus the RK point is a rather special kind of quantum critical point.

Later the author noticed that, at the RK point, *excited* eigenstates correspond exactly to relaxation modes of the master equation for the natural Monte Carlo (MC) dynamics of the classical dimer ensemble [9, 10]. Furthermore, the dimer ensemble (on bipartite lattices) has

a natural coarse-graining via the height representation [11], whereby it maps to a (2 + 1)-dimensional interface model in its rough phase. Since the classical dynamics is easy to grasp, this mapping delivered the dispersion law for the quantum dimer model's elementary excitations at the RK point. (This dispersion was already understood variationally [1].)

The purpose of this paper is to generalize the RK construction to any (degenerate) classical ensemble, showing the correspondence for several simple classical models. I begin (section 2) by reviewing basic notions of the quantum dimer model [1, 9] including the way that the classical and quantum models are connected, and the way we can comprehend the quantum dispersion if we know the classical dispersion. Any discrete classical model (e.g. [12]) with a dynamics satisfying detailed balance can be 'Rokhsar–Kivelsonized' to produce a quantum model with the same mapping of the eigenfunctions to classical dynamics (section 3).

Some examples are

(i) Chakravarty's quantum six-vertex model [13].
(ii) A classical Ising chain with spin-exchange (Kawasaki) dynamics, for which the RK model is the spin-1/2 Heisenberg ferromagnet.
(iii) A spin-1/2 Ising model on the pyrochlore lattice [16].

The examples are built on a large basis set of essentially degenerate states. In that sense they are 'highly frustrated' models [14], whether or not the massive degeneracy arises from competing interactions.

Finally (section 4) it is verified that the classical and quantum correlation functions are related exactly by a rotation of real time into imaginary time (and thus might be extracted more easily from simulations).

2. Classical and quantum dimer model

The Hilbert space of the quantum dimer model consists of all complete dimer covering configurations. Its Hamiltonian is customarily written as

$$\mathcal{H} = -t \sum (|\square\!\square\rangle\langle=\!=| + \text{h.c.}) + V \sum (|\square\!\square\rangle\langle\square\!\square| + |=\!=\rangle\langle=\!=|). \tag{2.1}$$

for a square lattice. In the t term, by an abuse of notation, '$|\square\!\square\rangle\langle=\!=|$' actually runs over $|\beta\rangle\langle\alpha|$ for every possible pair of configurations (β, α), such that β differs from α only by the replacement of a vertical pair by a horizontal pair of dimers on one plaquette. This is the elementary 'flip move' for this model—the smallest possible change that turns one valid configuration into a different one (since the same four vertices are covered in either state). (For a dimer covering on a general bipartite lattice, flippable plaquettes are those around which every second edge has a dimer, and the flip move exchanges covered and uncovered edges.) The V term is diagonal in this Hilbert space, and can be rewritten as $V\mathcal{N}_{\text{flip}}$, where $\mathcal{N}_{\text{flip}}(\alpha)$ (dependent on the configuration) is the number of flippable plaquettes in configuration α.

RK noted that when $V = t$ (the 'RK point'), the ground state wavefunction is

$$|\Psi_0\rangle = \frac{1}{\sqrt{\mathcal{N}_s}} \sum_{\alpha} |\alpha\rangle, \tag{2.2}$$

where the sum is over all valid dimer configurations. Thus, the probability weight is $\text{Prob}(\alpha) = \mathcal{N}_s^{-1}$, the same for each of the $\mathcal{N}_s$ states, just as in the classical ensemble.

Any discrete classical model's dynamics is described by the master equation

$$\dot{p}_\alpha(\tau) = \sum_{\beta[\beta\neq\alpha]} (W_{\alpha\beta}\, p_\beta(\tau) - W_{\beta\alpha}\, p_\alpha(\tau)). \tag{2.3}$$

Here $p_\alpha(\tau)$ is the instantaneous probability of being in configuration α at time τ, and $W_{\alpha\beta}$ is the rate of transition to state α, given that the system is in state β.

If we define

$$W_{\alpha\alpha} \equiv -\Gamma_\alpha \equiv -\sum_{\beta[\beta\neq\alpha]} W_{\beta\alpha}, \tag{2.4}$$

(total rate of transition out of α), then (2.3) can be rewritten as a matrix equation:

$$\dot{\mathbf{p}}(\tau) = \mathbf{W}\mathbf{p}(\tau). \tag{2.5}$$

Then the time evolution can obviously be decomposed into eigenmodes of the $\mathbf{W}$ matrix, labelled by eigenvalue $-\lambda$ where $\lambda \geqslant 0$:

$$p_\alpha(\tau) = \sum_\lambda c_\lambda \mathrm{e}^{-\lambda\tau}\phi_\alpha^{(\lambda)} \tag{2.6}$$

where $\phi_\alpha^{(\lambda)}$ is the (normalized) eigenvector.

We actually are concerned only with the states that are connected by flips to a given initial state; within this component we can invoke a variant of the Perron–Frobenius theorem to assert that there is a unique steady state distribution, $P_\alpha^{(0)}$, characterized in matrix notation by $\mathbf{W}\mathbf{P}^{(0)} = 0$ (this distribution is just $\phi^{(0)}$ with the sum of the components normalized to unity, not the sum of squares).

Furthermore, say the classical model has a Hamiltonian $\overline{\mathcal{H}}(\alpha)$ (we take a dimensionless $\overline{\mathcal{H}}$ which has already been divided by the temperature). Then the steady state should be the Boltzmann distribution,

$$P_\alpha^{(0)} = \mathrm{e}^{-\overline{\mathcal{H}}(\alpha)}/\mathcal{Z}, \tag{2.7}$$

where $\mathcal{Z} \equiv \sum_\alpha \mathrm{e}^{-\overline{\mathcal{H}}(\alpha)}$ is the partition function. Observe that $\mathcal{H}$ and $\overline{\mathcal{H}}$ are *not* related, at least not in the usual sense of taking the classical limit of a quantum dynamics.

Of course, the dynamics should satisfy detailed balance,

$$W_{\beta\alpha}P_\alpha^{(0)} = W_{\alpha\beta}P_\beta^{(0)}. \tag{2.8}$$

For the quantum dimer model, and also the generalized Rokhsar–Kivelsonized models, we will specialize to

$$\overline{\mathcal{H}} = 0, \tag{2.9}$$

i.e. the allowed configurations are all degenerate. In this case, $P^{(0)}(\alpha)$ is the same for every α and so (2.8) reduces to saying $W_{\beta\alpha} = W_{\alpha\beta}$, i.e. the rate matrix is symmetric. Next observe that if the classical model's flip rate is always w (whenever a flip is possible), i.e. $W_{\alpha\beta} = w$ or 0, then the matrix elements from (2.1) are $\mathcal{H}_{\alpha\beta} = -\frac{t}{w}W_{\alpha\beta} + \frac{V}{w}\Gamma_\alpha\delta_{\alpha\beta}$. Thus, at the RK point, the quantum Hamiltonian matrix is proportional to the classical rate matrix:

$$\mathcal{H} \equiv -\frac{t}{w}\mathbf{W}. \tag{2.10}$$

It follows, of course, that all the eigenvectors of the quantum matrix are the same as those of the classical matrix, and the eigenenergies are given by

$$E_\lambda = \frac{t}{w}\lambda. \tag{2.11}$$

This is the key result of the present paper. The quantum ground state eigenfunction (2.2) is just the special case which has $\lambda = 0$: its identity with the classical stationary state, denoted originally by RK [1], follows since $\mathbf{P}^{(0)}$ is a null vector of $\mathbf{W}$.

3. Generalizations and examples

Now consider *any* classical model with discrete configurations with null Hamiltonian (2.9). Define a set of allowed 'flips' (connecting two configurations) and endow the model with a Monte Carlo dynamics (in continuous time) such that every possible flip has rate w. Furthermore, on the Hilbert space $\{|\alpha\rangle\}$, define a quantum-mechanical Hamiltonian that includes those same flips (with amplitude t), as well as a term $V\mathcal{N}_{\rm flip}$ that penalizes a configuration once for every possible flip move. At the RK point $t = V$, the Hamiltonian and master-equation matrices are proportional, so as before the eigenvectors are the same and (2.11) holds.

In many cases, one can construct a coarse-grained field from these configurations and infer the relaxational dynamics of the classical model at long wavelengths. Thus by the mapping, one also understands the low-energy excited states of the quantum model, a nontrivial problem if it were approached directly.

3.1. Discrete models with 'height' representations

The quantum dimer model belongs to a class of models that are coarse-grained via a microscopic mapping of each microstate to an interface $\{h(\mathbf{r})\}$ in an abstract (2+1)-dimensional space [9, 11, 17]. The interface is in its roughened phase, so the classical model is described by an effective free energy density $\propto|\nabla h(\mathbf{r})|^2$. The normal modes of the classical master equation are simply capillary modes of this interface with eigenvalues $\lambda(\mathbf{q}) \propto |\mathbf{q}|^2$. Hence [9, 18] the quantum excitations are bosons with dispersion

$$\hbar\omega(\mathbf{q}) \propto |\mathbf{q}|^2. \tag{3.1}$$

Height models have conserved quantities, often called 'winding numbers' but most transparently understood as the components $(\nabla_x h, \nabla_y h)$. Local flip moves cannot change the global 'interface' slope ∇h. Hence the configuration space is partitioned into subspaces, each of which has a steady state under the classical dynamics and a corresponding RK quantum ground state with zero energy. So, just as a Goldstone mode follows from a symmetry, the dispersion (3.1) is related to the degeneracy under changes of ∇h.

The earliest quantum height model (*not* then recognized as such) was the Anderson–Fazekas [19] approach to the $s = 1/2$ triangular-lattice antiferromagnet from the Ising limit. The basis is the Ising ground states, which essentially map to the dimer coverings of a honeycomb lattice. (The triangular Ising antiferromagnet in a transverse field maps directly to the honeycomb quantum dimer model [3]. A more interesting spin model that maps to the square-lattice quantum dimer model is the nearly Ising $s = 1/2$ antiferromagnet on the 'checkerboard' lattice [3, 18].)

Chakravarty has introduced a 'quantum six-vertex' (Q6V) model [13], a generalization of a speculative state in which spontaneous orbital currents develop along the lattice edges, as was proposed for the pseudogap phase of cuprates. The currents define arrow variables, which satisfy an ice rule at vertices. The minimal flip move is to reverse all four arrows around a plaquette, provided they all point in the same clock sense[1]. The six-vertex configurations have a height representation [20], and the whole $T = 0$ behaviour is strictly parallel to the QDM of RK [1] (assuming that analogous terms are included in the Hamiltonian!) In particular, when $V = 0$, a 'flat' phase with gapped excitations occurs; in it, the arrows have long-range alternating order of the so-called 'd-density wave' type [13], though with fluctuations. At the

[1] This is equivalent to the transverse field with a projector in (16) and (17) of [13].

RK point $V = t$; however, a critical phase is predicted with dispersion (3.1). Quantum height models at the RK point will be further discussed in [18].

3.2. Spin exchange

Say that our classical model is a set of Ising spins on a lattice of N sites in any dimension, with a zero Hamiltonian. Adopt the spin-conserving 'Kawasaki' dynamics; i.e. the flip move is to exchange any nearest-neighbour pair.

It might appear that this example is so trivial that it is not worth the observation that it may be considered a Rokhsar–Kivelson model. Some of the reasons that it may be of interest are

(i) it adds weight to the conjecture that the RK point is typically a critical point and that the dispersion there is generically q^2 if there is a conserved quantity;
(ii) a one-dimensional chain of this sort is the simplest example of the extension of the RK idea to the case where the classical states are unequally weighted (section 3.4, below);
(iii) the Kagomé quantum dimer model of Misguich *et al* [15] maps to this model (see below).

The corresponding spin-1/2 quantum Hamiltonian is

$$\mathcal{H}_{\rm FM} = -t\sum(|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + \text{h.c.}) + V\sum(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow|) \tag{3.2}$$

(with same abuse of notation as in (2.1)). Converting to the notation of spin operators, each term becomes

$$-t\,(S_i^+S_j^- + S_i^-S_j^+) + V[(\tfrac{1}{2}+S_i^z)(\tfrac{1}{2}-S_j^z) + (\tfrac{1}{2}-S_i^z)(\tfrac{1}{2}+S_j^z)], \tag{3.3}$$

where i, j are nearest neighbours; thus

$$\mathcal{H}_{\rm FM} = \sum_{\langle ij\rangle} -J_\perp(S_i^xS_j^x + S_i^yS_j^y) - J_z(S_i^zS_j^z - \tfrac{1}{4}), \tag{3.4}$$

where $J_z \equiv 2V$ and $J_\perp \equiv 2t$. This is the ferromagnet with 'XXZ' exchange anisotropy and the RK point here is the isotropic Heisenberg chain.

Let us adapt (2.2) to this case. The sum over states runs over every possible sequence of up or down spins; thus the $\mathcal{N}_{\rm s} = 2^N$ terms can be grouped as a direct product of single-site terms, namely

$$|\Psi_0\rangle = \left(\frac{|\uparrow\rangle + |\downarrow\rangle}{2}\right)^N = |\rightarrow\rightarrow\rightarrow\cdots\rightarrow\rightarrow\rangle, \tag{3.5}$$

the ferromagnetic state with moments aligned in the $+x$ direction.

Since the model is isotropic, we know there are degenerate ferromagnetic states with moments in other directions[2]. This model conserves spin, so the quantum ground state is degenerate, as explained at the end of section 2. Indeed, the sum in a wavefunction (2.2) should only run over the mutually accessible configurations with $(1+\cos\theta)N/2$ up spins and $(1-\cos\theta)N/2$ down spins. In the thermodynamic limit this is essentially the direct product generalizing (3.5),

$$(\cos\tfrac{1}{2}\theta|\uparrow\rangle + \sin\tfrac{1}{2}\theta|\downarrow\rangle)^N, \tag{3.6}$$

a coherent state in which all spins are rotated from the z axis by an angle θ.

Now, the classical relaxation dynamics is simple diffusion. The diffusion constant is easily obtained if we re-imagine the dynamics as exchanging *all* neighbour pairs of spins at

[2] For an alternative viewpoint on $|\Psi_0\rangle$, note that (2.8) is perfectly compatible with $\overline{\mathcal{H}} = -h\sum_i S_i^z$ in place of (2.9): then $P^{(0)}(\alpha)$ directly maps to (3.6); in general, $\overline{\mathcal{H}}$ could be any conserved quantity.

a rate w. (If both spins point the same way, this has no effect.) For example, on a chain a marked spin executes a simple random walk with a total hopping rate of w to the right and w to the left. The long-wavelength behaviour is diffusion, $\mathrm{d}\sigma(x,\tau)/\mathrm{d}\tau = D\partial^2\sigma(x,\tau)/\partial x^2$, where $\sigma(x,\tau)$ is the spin density, and $D \equiv w$. The eigenvalues of this diffusion equation are $\lambda(q) \cong Dq^2 \equiv wq^2$ for small wavevectors q. Hence, via (2.10), the quantum model's excitations have dispersion $\hbar\omega(q) \cong tq^2 \equiv \frac{1}{2}J_\perp q^2$. But this is just the familiar formula for ferromagnetic spin waves!

The same classical model, if endowed with a *single*-spin-flip dynamics, maps under Rokhsar–Kivelsonization to noninteracting spins in a transverse field—a trivial, gapped quantum model. Now, one of the most interesting RK models is that of [15]. Its Hilbert space consists of all dimer coverings of the Kagomé lattice, which (it has been shown) correspond one-to-one to the possible s_z spin configurations on the triangular Bravais lattice (modulo a global spin reversal). Every 'hop' in the Hamiltonian of [15] rearranges dimers around one hexagon, and this simply corresponds to flipping exactly one Ising spins: this model is precisely that transverse-field model. (Since every state is flippable, the V term is trivial in this case.)

The above insight, that (3.2) is the RK map of the classical ferromagnet, suggests a modification of the Kagomé dimer model, by adopting a hop move that *exchanges* two 'Ising' spins (corresponding to a dimer rearrangement around two hexagons). But—since the conservation of S_z has no particular meaning in the dimer geometry—we could make a similarity transform $\mathcal{H}_{\mathrm{FM}} \to U\mathcal{H}_{\mathrm{FM}}U$, where U is S_{jy} for a particular y, or a product of such factors for any set of sites. Thus one has a family of 2^N distinct quantum dimer models, each with a hop move rearranging two hexagons, and each with *gapless* excitations labelled by a q^2 dispersion; it might be interesting to investigate these models.

A similar model to (3.2) that may be Rokhsar–Kivelsonized is a classical, noninteracting lattice gas. In the same fashion as the above spin model, it maps to a quantum model of hard-core bosons with a nearest-neighbour attraction V. In fact it *is* that spin model, using a well-known correspondence in which up (respectively down) spins are transcribed to occupied (vacant) sites.

3.3. Pyrochlore model

Hermele and Fisher [16] have developed a quantum spin-1/2 model on the pyrochlore lattice, which is the Rokhsar–Kivelsonization of the ground state ensemble of the pyrochlore Ising antiferromagnet. It is well known that those configurations map to those of the diamond-lattice ice model, with arrows along lattice edges. The appropriate order parameter for long wavelengths is the polarization, the coarse-graining of the ice-model arrow field, which is analogous to ∇h in the height models and is conserved in the dynamics. Thus the classical dynamics is described by a diffusion equation and the dispersion is (3.1) at the RK point. This contrasts with the $\omega \sim |\mathbf{q}|$ dispersion elsewhere in the phase diagram, which [16] have called 'light'. It indicates that, even in this model, the RK point is a quantum critical point. The q^2 dispersion is generic at RK points, if there is a conserved quantity in the classical model, even in the absence of a height representation.

3.4. Classical dynamics with nontrivial Hamiltonian

The RK mapping is possible even when the classical ensemble has unequal weights. The matrix $\tilde{\mathbf{W}}$ having elements

$$\tilde{W}_{\alpha\beta} \equiv P_\alpha^{(0)\,-1/2} W_{\alpha\beta} P_\beta^{(0)\,1/2} \equiv W_{\alpha\beta} \mathrm{e}^{(1/2)[\overline{\mathcal{H}}(\alpha)-\overline{\mathcal{H}}(\beta)]} \tag{3.7}$$

is symmetric, on account of detailed balance (2.8); furthermore, since $\tilde{\mathbf{W}}$ is a similarity transform of $\mathbf{W}$, they share the same eigenvalues. The eigenvectors are related by $\tilde{\phi}_\alpha^{(\lambda)} \equiv \phi_\alpha^{(\lambda)}/\sqrt{P_\alpha^{(0)}}$, where $\phi^{(\lambda)}$ refers to a *right* eigenvector of $\mathbf{W}$. The corresponding quantum Hamiltonian matrix must be proportional to $\tilde{\mathbf{W}}$.

Let us work through a case of Metropolis dynamics, letting $W_{\alpha\beta} = w$ if $\overline{\mathcal{H}}(\alpha) < \overline{\mathcal{H}}(\beta)$, or $w \exp[-\overline{\mathcal{H}}(\alpha) + \overline{\mathcal{H}}(\beta)]$ otherwise. Hence by (3.7), for $\beta \neq \alpha$,

$$\tilde{W}_{\alpha\beta} = w\mathrm{e}^{-(1/2)|\overline{\mathcal{H}}(\alpha)-\overline{\mathcal{H}}(\beta)|}. \tag{3.8}$$

The quantum hopping matrix element (t term) must be proportional to $\tilde{W}_{\alpha\beta}$. This depends only on the immediate environment of the flip location, provided that $\overline{\mathcal{H}}$ is a sum of local terms. However, the t term appears elaborate even in the simplest case, the model of section 3.2 on a one-dimensional chain with $\overline{\mathcal{H}} = -K\sum S_i^z S_{i+1}^z$. Flips that change $\overline{\mathcal{H}}$ are multiplied by $\mathrm{e}^{-|K|/2}$. Equation (3.4) is replaced by $\mathcal{H}_{\mathrm{FM}} = \sum_i -(J_\perp + J_\perp' S_{i-1}^z S_{i+2}^z)(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - (J_z + J_z' S_{i-1}^z S_{i+1}^z)(S_i^z S_{i+1}^z - \frac{1}{4})$ where $J_\perp = t(1+\mathrm{e}^{-|K|/2})$, $J_z = V(1+\mathrm{e}^{-|K|/2})$, $J_\perp' = t(1-\mathrm{e}^{-|K|/2})$ and $J_z{}' = V(1-\mathrm{e}^{-|K|/2})$.

4. Dynamic correlations

An amusing (and perhaps useful) corollary of equation (2.10) is that for any generalized RK model, one can relate the quantum correlation function

$$C_{BA}(\tau) \equiv \langle \hat{B}(\tau)\hat{A}(0)\rangle \tag{4.1}$$

to the similar classical one $C_{BA}^{\mathrm{class}}(\tau)$. For the latter to make sense, the operators must be diagonal in Hilbert space, $\langle\alpha|\hat{A}|\beta\rangle = A_\alpha\delta_{\alpha\beta}$, and similarly $\hat{B}$.

Quite generally in a classical discrete system (starting in equilibrium)

$$C_{BA}^{\mathrm{class}}(\tau) = \sum_\alpha B_\beta p_\beta(\tau|\alpha) A_\alpha P_\alpha^{(0)}, \tag{4.2}$$

where $p_\beta(\tau|\alpha)$ is the conditional probability, given that the state at $\tau = 0$ was α (which had probability $P_\alpha^{(0)}$). First, $p_\beta(0|\alpha) = \delta_{\alpha\beta}$; then (2.6) says $p_\beta(\tau|\alpha) = \sum c_\lambda \mathrm{e}^{-\lambda\tau}\phi_\beta^{(\lambda)}$; and orthonormality of the eigenvectors (since $\mathbf{W}$ or $\tilde{\mathbf{W}}$ is symmetric) implies $c_\lambda = \phi_\alpha^{(\lambda)}$. The latter formula (with a *right* eigenvector) holds even for the case of section 3.4 where the master-equation matrix $\mathbf{W}$ is nonsymmetric.

Using $P_\alpha^{(0)} = 1/\mathcal{N}_{\mathrm{s}}$, the final result is

$$C_{BA}^{\mathrm{class}}(\tau) = \sum_\lambda \mathrm{e}^{-\lambda\tau}\tilde{A}_\lambda\tilde{B}_\lambda, \tag{4.3}$$

where $\tilde{A}_\lambda \equiv \mathcal{N}_{\mathrm{s}}{}^{-1/2}\sum_\alpha A_\alpha\phi_\alpha^{(\lambda)}$ (similarly $\tilde{B}_\lambda$).

A quantum correlation function is computed using a similarity transform by the time-evolution operator to convert $\hat{B}(\tau) \to \mathrm{e}^{\mathrm{i}\hat{\mathcal{H}}\tau}\hat{B}\mathrm{e}^{-\mathrm{i}\hat{\mathcal{H}}\tau}$, an operator acting at the same time as $\hat{A}$, and taking the expectation in the ground state wavefunction:

$$C_{BA}(\tau) = \langle 0|\mathrm{e}^{\mathrm{i}\hat{\mathcal{H}}\tau}\hat{B}\mathrm{e}^{-\mathrm{i}\hat{\mathcal{H}}\tau}\hat{A}|0\rangle. \tag{4.4}$$

Insert a complete set of states $\sum|\lambda\rangle\langle\lambda|$ on either side of the exponential between $\hat{B}$ and $\hat{A}$, and note that $\langle\lambda|\hat{A}|0\rangle = \tilde{A}_\lambda$ (similarly for $\hat{B}$). This equality follows from $|\lambda\rangle = \sum\tilde{\phi}_\alpha^{(\lambda)}|\alpha\rangle$. (And it holds even in the case where the state weights are unequal; section 3.4.) We obtain

$$C_{BA}(\tau) = \frac{1}{\mathcal{N}_{\mathrm{s}}}\sum_\lambda \mathrm{e}^{-\mathrm{i}(E_\lambda - E_0)\tau}\tilde{A}_\lambda\tilde{B}_\lambda = C_{BA}^{\mathrm{class}}\left(\frac{\mathrm{i}t}{\hbar w}\tau\right) \tag{4.5}$$

where I used (2.11). Thus, the quantum correlations are the *classical correlations in imaginary time*. An obvious application is that any dynamic correlation, measured via classical Monte Carlo with sufficient precision, may be converted by analytic continuation to a quantum correlation function without the need to understand or compute the eigenfunctions. (Normally, for non-RK systems the same classical correlation function must be obtained from a quantum Monte Carlo simulation, based on a path integral and carried out in a space one dimension higher.)

It is fairly surprising to obtain the simple correspondence (4.5). It is true that the two evolution equations do have a corresponding time dependence, $e^{-\lambda\tau}$ and $e^{-iE_\lambda\tau/\hbar}$ respectively, and the classical and quantum eigenfunctions are the same. Yet the quantities which evolve according to these exponentials, and which are represented in the vector space spanned by those eigenfunctions, are *probability deviations* on the classical side, but *amplitudes* (which must be *squared* to obtain probabilities) on the quantum side.

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