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Quasiclassical Methods in Spin Dynamics*

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We present an extension of the concept of the Wigner distribution to include spin. The results are then used to indicate a method by which classical approximations to spin dynamics emerge naturally from the exact quantum theory, and estimates of the accuracy of these classical approximations can be computed.

I. INTRODUCTION

IN recent years, a number of calculations have been performed by various authors[1–7] in which spin dynamics were treated classically. These calculations have been concerned with predicting magnetic properties of materials. The use of classical spin dynamics considerably simplified the computations over comparable computations using quantum dynamics.[3,4]

The approximation involved in using classical spin dynamics has been rather difficult to evaluate. The approximation is known to be valid for large spins.[1] However, even when it is applied to spins of $\frac{1}{2}$ or 1, classical theory seems to give quite reasonable results.

Here we present a computational technique in which a classical approximation emerges quite naturally from the exact quantum theory, and by which the approximations made in using classical dynamics can be accurately estimated. This technique is just an extension of the use of the Wigner distribution familiar in computations involving position and momentum.[8–11] The method can be generalized to arbitrary spin. However, for simplicity we consider here only spin $\frac{1}{2}$.

II. SINGLE-PARTICLE SYSTEM

In order to illustrate the general technique, we shall first treat a single particle with spin $\frac{1}{2}$. The density matrix for this case can be written as

$$D(t)=\tfrac{1}{2}+\mathbf{d}(t)\cdot\mathbf{S}, \tag{1}$$

where $\hbar\mathbf{S}$ is the spin angular momentum operator, and the components of $\mathbf{d}(t)$ are c numbers.

We define a Wigner distribution in terms of $\mathbf{d}(t)$ and a unit vector $\mathbf{\Omega}$ by

$$\rho_w(\mathbf{\Omega})=1+3\mathbf{d}(t)\cdot\mathbf{\Omega}. \tag{2}$$

The components of $\mathbf{\Omega}$ are also c numbers.

We can use this distribution function to compute the expected values of any operator $A(\mathbf{S})$ by finding an appropriate Wigner equivalent of $A(\mathbf{S})$. That is, we need a function $A_w(\mathbf{\Omega})$ such that

$$\frac{1}{4\pi}\int d\mathbf{\Omega}\,\rho_w(\mathbf{\Omega})A_w(\mathbf{\Omega})=\mathrm{Tr}D(t)A(\mathbf{S}). \tag{3}$$

As was the case with $D(t)$,we can write $A(\mathbf{S})$ in the form

$$A(\mathbf{S})=a_0+\mathbf{a}\cdot\mathbf{S}, \tag{4}$$

where a_0 and the components of $\mathbf{a}$ are c numbers.

If we take the Wigner equivalent to be

$$A_w(\mathbf{\Omega})=a_0+\tfrac{1}{2}\mathbf{a}\cdot\mathbf{\Omega}, \tag{5}$$

then a trivial calculation shows that (3) is satisfied.

Suppose we have another operator $B(\mathbf{S})$, where

$$B(\mathbf{S})=b_0+\mathbf{b}\cdot\mathbf{S}, \tag{6}$$

then we can construct the Wigner equivalent of $B(\mathbf{S})$ in the same way,

$$B_w(\mathbf{\Omega})=b_0+\tfrac{1}{2}\mathbf{b}\cdot\mathbf{\Omega}. \tag{7}$$

We could also use (4) to compute the Wigner equivalent of the product $A(\mathbf{S})B(\mathbf{S})$ by noting that

$$A(\mathbf{S})B(\mathbf{S})=(a_0b_0+\tfrac{1}{4}\mathbf{a}\cdot\mathbf{b})+(\tfrac{1}{2}i\mathbf{a}\times\mathbf{b}+a_0\mathbf{b}+b_0\mathbf{a})\cdot\mathbf{S}. \tag{8}$$

It is more convenient to note that there is a Groenewold rule[9] which expresses the Wigner equivalent of the product $(A(\mathbf{S})B(\mathbf{S}))_w$ in terms of the Wigner equivalents A_w and B_w .This rule turns out to be the following:

$$(A(\mathbf{S})B(\mathbf{S}))_w=A_w(\mathbf{\Omega})GB_w(\mathbf{\Omega}), \tag{9a}$$

where

$$G=1+i\overleftarrow{\mathbf{L}}\cdot\mathbf{\Omega}\times\overrightarrow{\mathbf{L}}-\overleftarrow{\mathbf{L}}\cdot\overrightarrow{\mathbf{L}}, \tag{9b}$$

and $\overleftarrow{\mathbf{L}}$ and $\overrightarrow{\mathbf{L}}$ are vector differential operators acting to the left and right, respectively. The components of $\hbar\overleftarrow{\mathbf{L}}$ and $\hbar\overrightarrow{\mathbf{L}}$ are just the components of the orbital angular momentum operators $-i\hbar\mathbf{r}\times\nabla$, where $\mathbf{\Omega}=\mathbf{r}/r$.

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The proof of (9a) follows most easily when we note that

$$\Omega_\mu G\Omega_\nu = \delta_{\mu\nu} + i\epsilon_{\mu\nu\alpha}\Omega_\alpha. \tag{10}$$

Of course μ, ν, and α refer to Cartesian components and $\epsilon_{\mu\nu\alpha}$ is the totally antisymmetric tensor.

Consider the Heisenberg operator $A(t)$ such that

$$\frac{d}{dt}A(t) = \frac{i}{\hbar}[HA(t) - A(t)H]. \tag{11}$$

Then the Wigner equivalent $A_w(t)$ must satisfy

$$\frac{d}{dt}A_w(t) = \frac{i}{\hbar}[H_w G A_w(t) - A_w(t) G H_w] \tag{12a}$$

$$= -(2/\hbar)[H_w \overleftarrow{\mathbf{L}} \cdot \mathbf{\Omega} \times \overrightarrow{\mathbf{L}} A_w(t)], \tag{12b}$$

where H_w is the Wigner equivalent of the Hamiltonian H.

If we take $H = -\hbar\mu\mathbf{B}\cdot\mathbf{S}$, then for $\mathbf{\Omega}(t)$ Eq. (8) gives

$$\frac{d}{dt}\mathbf{\Omega}(t) = -\mu\mathbf{B}\times\mathbf{\Omega}(t). \tag{13}$$

Equation (13) can be thought of as a restatement of the Ehrenfest theorem.

We have now, however, the capability of using an equation of the form of (13) and Eq. (9a) to compute the fluctuations in the spin components.

Consider for example a system of spins with a magnetic field B applied along the z axis. In a resonance experiment the out-of-phase susceptibility is given by[12]

$$\chi''(\omega) = S_{xx}(\omega)\hbar\pi\mu^2(1 - e^{\beta\hbar\omega}), \tag{14}$$

where

$$S_{xx}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t}\langle S_x S_x(t)\rangle_T, \tag{15}$$

and $\langle\ \rangle_T$ indicates a thermal average.

Using our earlier results, we can rewrite the thermal average in (15) as

$$\langle S_x S_x(t)\rangle_T = \frac{1}{4\pi}\int d\mathbf{\Omega}\, \rho_w(\mathbf{\Omega})\tfrac{1}{4}[\Omega_x G \Omega_x(t)] \tag{16}$$

and we recall that there are no approximations in (16). To describe the time dependence of $\Omega_x(t)$, we will use the Bloch equations[13] for $t>0$ and

$$\langle S_x S_x(t)\rangle_T = \langle S_x S_x(-t)\rangle_T^*,$$

$$\frac{d}{dt}\Omega_x(t) = \mu B \Omega_y(t) - \frac{\Omega_x(t)}{T_2}, \tag{17a}$$

$$\frac{d}{dt}\Omega_y(t) = -\mu B \Omega_x(t) - \frac{\Omega_y(t)}{T_2}. \tag{17b}$$

The last terms in these equations are included to account for spin-spin relaxation. Equations (17) give, for $\Omega_x(t)$,

$$\Omega_x(t) = e^{-|t|/T_2}(\Omega_x \cos\omega_0 t + \Omega_y \sin\omega_0 t), \tag{18a}$$

$$\omega_0 = \mu B. \tag{18b}$$

Using this result in (16) we have

$$\langle S_x S_x(t)\rangle_T = \tfrac{1}{4}(\cos\omega_0 t)e^{-|t|/T_2} + \tfrac{1}{4}i\langle\Omega_Z\rangle\, e^{-|t|/T_2}\sin\omega_0 t, \tag{19}$$

where

$$\langle\Omega_z\rangle = \frac{1}{4\pi}\int d\mathbf{\Omega}\, \rho_w(\mathbf{\Omega})\Omega_z = 2\,\mathrm{Tr} DS_z. \tag{20}$$

Now we use (19) in (14) to obtain

$$\chi''(\omega) = \tfrac{1}{8}\mu\hbar(1 - e^{\beta\hbar\omega})\left[(1 - \langle\Omega_z\rangle)\frac{T_2}{1 + (\omega - \omega_0)^2 T_2^2} + (1 + \langle\Omega_z\rangle)\frac{T_2}{1 + (\omega + \omega_0)^2 T_2^2}\right]. \tag{21}$$

The absorptive processes in resonance experiments are given by the first term in (21). For high temperatures, we can expand $e^{\beta\hbar\omega}$ and approximate the average $\langle\Omega_z\rangle = 0$. Then the first part of (21) can be written in the usual form

$$\chi''(\omega) \equiv \tfrac{1}{8}(\hbar^2\mu^2\beta\omega)T_2/[1 + (\omega - \omega_0)^2 T_2^2]. \tag{22}$$

These results are meant only to illustrate the technique. They can be derived by other methods.

III. MANY-PARTICLE SYSTEMS

In this case, we take the spin angular momentum operator for the jth particle to be $\hbar\mathbf{S}_j$. The density matrix for an N spin system can be written as

$$D(t) = 2^{-N} + \sum_{n=1}^{N} \sum_{j_1 < \cdots < j_n} \sum_{\nu_1 \cdots \nu_n} \rho_{j_1 \cdots j_n}{}^{\nu_1 \cdots \nu_n}(t) \times S_{j_1\nu_1} \cdots S_{j_n\nu_n}. \tag{23}$$

Then we define the Wigner distribution as

$$\rho_w(\mathbf{\Omega}_1 \cdots \mathbf{\Omega}_N) = 1 + \sum_{n=1}^{N} \sum_{j_1 < \cdots < j_n} \sum_{\nu_1 \cdots \nu_n} \rho_{j_1 \cdots j_n}{}^{\nu_1 \cdots \nu_n} 3^n 2^{N-n} \times \Omega_{j_1\nu_1} \cdots \Omega_{j_n\nu_n}. \tag{24}$$

We can also write any function of the spins $A(\mathbf{S}_1 \cdots \mathbf{S}_N)$ in the form of (23)

$$A(\mathbf{S}_1, \ldots, \mathbf{S}_N) = a_0 + \sum_{n=1}^{N} \sum_{j_1 < \cdots < j_n} \sum_{\nu_1 \cdots \nu_n} a_{j_1 \cdots j_n}{}^{\nu_1 \cdots \nu_n} \times S_{j_1\nu_1} \cdots S_{j_n\nu_n}. \tag{25}$$

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Then the Wigner equivalent of A is

$$A_w(\mathbf{\Omega}_1\cdots\mathbf{\Omega}_N)=a_0+\sum_{n=1}^{N}\sum_{j_1<\cdots<j_n}\sum_{\nu_1\cdots\nu_n}2^{-n}a_{j_1\cdots j_n}{}^{\nu_1\cdots\nu_n}\times\Omega_{j_1\nu_1}\cdots\Omega_{j_n\nu_n}. \quad (26)$$

We can easily verify that

$$\mathrm{Tr}A(\mathbf{S}_1\cdots\mathbf{S}_N)D(t)=\frac{1}{(4\pi)^N}\int d\mathbf{\Omega}_1\cdots d\mathbf{\Omega}_N \times A_w(\mathbf{\Omega}_1\cdots\mathbf{\Omega}_N)\rho_w(\mathbf{\Omega}_1\cdots\mathbf{\Omega}_N). \quad (27)$$

Also we can show that a Groenewold rule can be used to compute Wigner equivalents of products

$$(AB)_w=A_w(\mathbf{\Omega}_1\cdots\mathbf{\Omega}_N)GB_w(\mathbf{\Omega}_1,\ldots,\mathbf{\Omega}_N), \quad (28a)$$

where

$$G=G_1\cdots G_N \quad (28b)$$

and G_j is in the form of (9b)

$$G_j=1-\overleftarrow{\mathbf{L}}_j\cdot\overrightarrow{\mathbf{L}}_j+i\overleftarrow{\mathbf{L}}_j\cdot\mathbf{\Omega}_j\times\overrightarrow{\mathbf{L}}_j. \quad (28c)$$

Since the Heisenberg operator $A(t)$ can be written in the form of (11), we can write an equation of motion for the Wigner equivalent again as

$$\frac{d}{dt}A_w(t)=\frac{i}{\hbar}\{H_wGA_w-A_wGH_w\}, \quad (29)$$

where G is given by (28b). Of course, in this case we cannot write Eq. (29) in the form of (12b). Consider G_j divided into two parts, namely,

$$G_j=G_{jc}+G_{jn}, \quad (30a)$$

$$G_{jc}=1-\overleftarrow{\mathbf{L}}_j\cdot\overrightarrow{\mathbf{L}}_j, \quad (30b)$$

$$G_{jn}=i\overleftarrow{\mathbf{L}}_j\cdot\mathbf{\Omega}_j\times\overrightarrow{\mathbf{L}}_j. \quad (30c)$$

Let us note that (29) can be written

$$\frac{d}{dt}A_w(t)=\frac{i}{\hbar}H_w(G-G^*)A_w(t), \quad (31a)$$

where

$$G^*=(G_{1c}-G_{1n})\cdots(G_{Nc}-G_{Nn}). \quad (31b)$$

We have then, for H_w at most bilinear in the $\mathbf{\Omega}_j$, (as, for example, in the Heisenberg model)

$$H_w(G-G^*)=2H_w\sum_{j=1}^{N}G_{jn}\prod_{j'\neq j}G_{j'c}, \quad (32)$$

where $\prod_{j'\neq j}$ indicates the product over all j' not equal to j. Equation (32) can be most easily seen by expanding (31b) in powers of the G_{jn} and noting that the next term in (32) is cubic in the G_{jn}'s, and it and all higher terms will vanish when H_w at is most quadratic in the $\mathbf{\Omega}_j$. Thus for the Heisenberg model

$$\frac{d}{dt}A_w(t)=\frac{2i}{\hbar}\sum_j H_wG_{jn}\{\sum_{j'\neq j}G_{j'c}\}A_w(t) \quad (33)$$

or

$$A_w(t)=\exp\left[\frac{2it}{\hbar}\sum_j H_wG_{jn}(\prod_{j'\neq j}G_{j'c})\right]A_w(0). \quad (34)$$

Now let us consider the special case

$$D(t)=2^{-N}, \quad (35a)$$

which implies

$$\rho_w=1. \quad (35b)$$

With these values (27) becomes

$$\mathrm{Tr}A(\mathbf{S}_1,\ldots,\mathbf{S}_N)=\frac{1}{(2\pi)^N}\int d\mathbf{\Omega}_1\cdots d\mathbf{\Omega}_N\,A_w(\mathbf{\Omega}_1,\ldots,\mathbf{\Omega}_N). \quad (36)$$

Frequently, we must obtain traces of operators. For example, consider the partition function

$$Z=\mathrm{Tr}e^{-\beta H}. \quad (37)$$

Using (36), we can write this as

$$Z=(2\pi)^{-N}\int d\mathbf{\Omega}_1\cdots d\mathbf{\Omega}_N(e^{-\beta H})_w. \quad (38)$$

Let us define z such that

$$z(\beta)=(e^{-\beta H})_w. \quad (39)$$

Then we can determine z by constructing a differential equation in β.

$$\frac{d}{d\beta}z(\beta)=(-He^{-\beta H})_w \quad (40a)$$

$$=-\tfrac{1}{2}(He^{-\beta H}+e^{-\beta H}H)_w \quad (40b)$$

$$=-\tfrac{1}{2}H_w(G+G^*)z(\beta), \quad (40c)$$

$$z(0)=1. \quad (40d)$$

For the Heisenberg model, the arguments we used to obtain (32) give

$$\tfrac{1}{2}H_w(G+G^*)=H_w(G_{1c}\cdots G_{Nc}+\sum_{j\neq j'}G_{jn}G_{j'n}\prod_{j''\neq j'\neq j}G_{j''c}). \quad (41)$$

Thus for the Heisenberg model (40c) becomes

$$\frac{d}{d\beta}z(\beta)=-H_w(G_{1c}\cdots G_{Nc}+\sum_{j\neq j'}G_{jn}G_{j'n}\sum_{j''\neq j'\neq j}G_{j''c})z(\beta). \quad (42)$$

The classical Heisenberg model results when we approximate the bracketed term by unity

$$(G_{1c}\cdots G_{Nc}+\sum_{j\neq j'} G_{jn}G_{j'n}\prod_{j''\neq j'\neq j} G_{j''c})\approx 1. \quad (43)$$

We can generate an iterative approximation scheme for $z(\beta)$ as follows:

$$z(\beta)=\sum_{n=0}^{\infty} z_n(\beta), \quad (44a)$$

where

$$z_0(\beta)=e^{-\beta H w} \quad (44b)$$

and

$$\frac{d}{d\beta}z_{n+1}(\beta)=-H_w(-\delta_{n0}+G_{1c}\cdots G_{Nc} +\sum_{j\neq j'} G_{jn}G_{j'n}\prod_{j''\neq j'\neq j} G_{j''c})z_n(\beta). \quad (44c)$$

Equations (44) can be used to determine the accuracy of classical approximations as for example in Ref. 2. Beyond these results this method can be used to determine the fluctuations in spin variables. For example, to determine the neutron, magnetic, scattering cross section, we must determine[14]

$$S_{\mu\mu}(t)=Z^{-1}\,\mathrm{Tr}e^{-\beta H}S_\mu S_\mu(t). \quad (45)$$

Using (36) we have

$$S_{\mu\mu}(t)=\frac{1}{(2\pi)\ Z}\int d\mathbf{\Omega}_1\cdots d\mathbf{\Omega}_N z(\beta)G \times\tfrac{1}{2}(\Omega\mu)G\tfrac{1}{2}[\Omega\mu(t)]. \quad (46)$$

The evaluation of (46) is rather more complicated than the example which we have presented. However, (46) is expressed in terms of continuous spin variables which satisfy classical equations.

[14] L. Van Hove, Phys. Rev. 95, 1374 (1954).

We can use (36) to avoid an explicit computation of ρ_w. Since (36) holds for any operator A, we can apply it to the operator BD where D is the density matrix

$$\mathrm{Tr}DB=(2\pi)^{-N}\int d\mathbf{\Omega}_1\cdots d\mathbf{\Omega}_N D_w G B_w. \quad (47)$$

We note that D_w is *not* equal to ρ_w. In fact, D_w must satisfy an equation analogous to (29):

$$\frac{d}{dt}D_w(t)=-\frac{i}{\hbar}[H_wGD_w(t)-D_w(t)GH_w]. \quad (48)$$

Thus, we have two possible methods for computing expected values—Eqs. (27) and (47).

IV. DISCUSSION

It should be a rather straightforward matter to extend these results to larger spins. This is accomplished by expanding the spin operators in terms of the trace orthogonal invariant tensors and using the spherical harmonics Y_{lm} as the coefficients in the Wigner distribution and Wigner equivalents. These results for higher spins will be important in descriptions of the effects of higher multipole moments. However, for simple systems such as the Heisenberg model the results presented here should be sufficient to determine the accuracy of quasiclassical methods.

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