Sign of the Coupling between T-Violating Ground States in Second-Order Perturbation Theory

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We consider the coupling between two T-violating systems by a non-T-violating interaction. We show that the configuration in which the signs of the T breaking in the two systems are opposite generally has lower energy. In the context of those theories of the cuprate superconductors which postulate breaking of T invariance in the CuO_2 planes, a crude estimate of the Coulomb-induced "antiferromagnetic" coupling for reasonable domain sizes indicates that it is an "edge" effect but at least competitive with the "ferromagnetic" one due to Josephson and magnetic effects.

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There is current interest in time-reversal- (T-) violating systems, mostly due to the realization that the charge carriers in the CuO planes of the high-T_c superconductors may be fractional statistics quasiparticles [1,2] (anyons [3]). Other T-violating possibilities in this context are the so-called "flux phases" [4], or ^{3}He "ABM"-type phases [5]. Theoretical treatments of this problem concentrate mainly on a single plane, whereas in predicting observable quantities in the *bulk* system it is important to have a picture of the ordering of the signs of the (spontaneous) symmetry breaking in different planes. We will call "ferromagnetic" (FM) the configuration in which T is broken with the same sign in different layers, and "antiferromagnetic" (AFM) that in which the sign of T alternates between adjacent layers. Recent numerical studies of finite clusters [6] show that if a Coulomb-type interaction is included between layers, the AFM configuration is favored, and this picture seems to be consistent with experiments in reflection of polarized light [7,8].

With this motivation we consider the general situation of two distinguishable systems, each of them breaking T, and coupled via a T-even interaction. We show that up to second-order perturbation theory, the AFM configuration has lower energy in most physically interesting cases. We briefly discuss the applicability of our result in the high-T_c context.

Consider two subsystems 1 and 2 with identical T-conserving Hamiltonians, and assume that in the absence of coupling T invariance is spontaneously broken; i.e., for each subsystem j ($j=1,2$) there exists a pair of ground states $|O\rangle, |\tilde{O}\rangle$ related by $|\tilde{O}\rangle \equiv \hat{T}|O\rangle$. Suppose that the coupling between the subsystems can be written schematically in the form

$$\hat{V} = \int^1 d\mathbf{r} \int^2 d\mathbf{r}' f(\mathbf{r},\mathbf{r}') \hat{\Omega}_1(\mathbf{r}) \hat{\Omega}_2(\mathbf{r}') , \tag{1}$$

where $\hat{\Omega}_j(\mathbf{r})$ is a Hermitian operator which is even under $\hat{T}$ [$\hat{T}\hat{\Omega}_j(\mathbf{r})\hat{T}^{-1} = \hat{\Omega}_j(\mathbf{r})$], and $f(\mathbf{r},\mathbf{r}') \equiv f(\mathbf{r}',\mathbf{r})$. For example, for the Coulomb case, $\hat{\Omega}(\mathbf{r}) \equiv \hat{\rho}(\mathbf{r})$, the single-particle density operator, and $f(\mathbf{r},\mathbf{r}') \equiv e^2/|\mathbf{r}-\mathbf{r}'|$. Note, however, that in the general case $\mathbf{r}$ is an abstract label and does not necessarily have the significance of a single-particle coordinate.

In view of the evenness of $\hat{\Omega}(\mathbf{r})$ under $\hat{T}$, it is clear that the first-order term in V cannot split the FM and AFM states. Clearly this is a consequence of the fact that we are considering the systems to be disconnected, the particles in subsystem 1 can be distinguished from those of system 2, and there are no exchange terms between the two systems. A familiar case in which the first-order term in perturbation theory favors a "ferromagnetic" configuration is Hund's rule in atomic physics (states with maximum L minimize the Coulomb repulsion). However, that situation corresponds to indistinguishable particles and the exchange terms are crucial.

To discuss the second-order term, we note that by a suitable choice of eigenfunctions $\varphi_n(\mathbf{r})$ we can always rewrite the perturbation (1) in the form [9]

$$\hat{V} = \sum_n V_n \hat{\Omega}_n^{(1)} \hat{\Omega}_n^{(2)\dagger} \equiv \sum_n V_n \hat{\Omega}_n^{(1)\dagger} \hat{\Omega}_n^{(2)} , \tag{2}$$

where V_n is real and $\hat{\Omega}_n^{(j)} \equiv \int^j \hat{\Omega}(\mathbf{r}) \varphi_n(\mathbf{r}) d\mathbf{r}$.

The general form of the second-order correction is given by [we suppress for simplicity the index i ($=1,2$) in $\hat{\Omega}_n^{(i)}$]

$$\Delta E = -\sum_{n,m} \sum_{j_1,j_2} V_n V_m \frac{\langle O_1|\hat{\Omega}_n^\dagger|j_1\rangle\langle j_1|\hat{\Omega}_m|O_1\rangle\langle O_2|\hat{\Omega}_n|j_2\rangle\langle j_2|\hat{\Omega}_m^\dagger|O_2\rangle}{E_{j_1}+E_{j_2}} \tag{3}$$

$$\equiv -\sum_{n,m} \sum_{j_1,j_2} V_n V_m \frac{\langle O_1|\hat{\Omega}_m|j_1\rangle\langle j_1|\hat{\Omega}_n^\dagger|O_1\rangle\langle O_2|\hat{\Omega}_m^\dagger|j_2\rangle\langle j_2|\hat{\Omega}_n|O_2\rangle}{E_{j_1}+E_{j_2}} , \tag{4}$$

where $|O_i\rangle$ and $|j_i\rangle$ are, respectively, the (T-violating) ground state and excited states of subsystem i. Note that (4) is obtained from (3) by interchanging 1 and 2.

Let us define

$$\chi_1^{(n,m)}(\omega)=\sum_{j_1}\langle O_1|\hat{\Omega}_n^\dagger|j_1\rangle\langle j_1|\hat{\Omega}_m|O_1\rangle\delta(E_{j_1}-\omega)\,, \tag{5}$$

$$\chi_2^{(n,m)}(\omega)=\sum_{j_2}\langle O_2|\hat{\Omega}_n|j_2\rangle\langle j_2|\hat{\Omega}_m^\dagger|O_2\rangle\delta(E_{j_2}-\omega)\,. \tag{6}$$

Then (3) is

$$\Delta E=-\sum_{m,n}V_nV_m\int_0^\infty d\omega\int_0^\infty d\omega'\frac{\chi_1^{(m,n)}(\omega)\chi_2^{(m,n)}(\omega')}{\omega+\omega'}\,. \tag{7}$$

Now, in view of the property $\hat{T}\hat{\Omega}(\mathbf{r})\hat{T}^{-1}=\hat{\Omega}(\mathbf{r})$, we have quite generally $\hat{T}\hat{\Omega}_n\hat{T}^{-1}=\hat{\Omega}_n^\dagger$. Hence $\chi_2^{(m,n)}(\omega)$ can be written

$$\chi_2^{(n,m)}(\omega)=\sum_{j_2}\langle TO_2|\hat{\Omega}_n^\dagger|Tj_2\rangle^*\langle Tj_2|\hat{\Omega}_m|TO_2\rangle^*\delta(E_{j_2}-\omega) \tag{8}$$

because of the antiunitarity property of the time-reversal operator (if $|\psi'\rangle=T|\psi\rangle$ and $|\phi'\rangle=T|\phi\rangle$, then $\langle\psi'|\phi'\rangle=\langle\psi|\phi\rangle^*$ [10]).

Now, in the *antiferromagnetic* arrangement $T|O_2\rangle$ is simply $|O_1\rangle$, and moreover (because of the T invariance of H_0) $T|j_2\rangle$ corresponds to a particular $|j_1\rangle$. Thus, in this case we have

$$\chi_2^{(n,m)*}(\omega')\equiv\chi_1^{(n,m)}(\omega')\quad\text{(AFM case)}\,. \tag{9}$$

On the other hand, in the *ferromagnetic* case $\chi_2^{(n,m)*}(\omega')$ is in general different from $\chi_1^{(n,m)}(\omega')$, corresponding to the spectral densities of the "time-reversed" operator. Let us call it $\chi_T^{(n,m)}(\omega)$, and denote $\chi_1^{(n,m)}(\omega)$ simply by $\chi^{(n,m)}(\omega)$. Taking also (4), we find that the difference in energy $\tilde{\Delta}E$ between the FM and the AFM configurations up to second order in V can be written in the compact form

$$\Delta E_{\mathrm{FM}}-\Delta E_{\mathrm{AFM}}=\frac{1}{2}\sum_{n,m}V_nV_m\int_0^\infty d\omega\int_0^\infty d\omega'\frac{f_{n,m}(\omega)f_{n,m}^*(\omega')}{\omega+\omega'}\,, \tag{10}$$

with

$$f_{n,m}(\omega)\equiv\chi^{(n,m)}(\omega)-\chi_T^{(n,m)}(\omega)\,. \tag{11}$$

Although $f_{n,m}$ is a complex function, the double integral can be proven positive, because

$$\begin{aligned}\int_0^\infty d\omega\int_0^\infty d\omega'\frac{f_{n,m}(\omega)f_{n,m}^*(\omega')}{\omega+\omega'}&=\int_0^\infty d\alpha\int_0^\infty d\omega\int_0^\infty d\omega' f_{n,m}(\omega)f_{n,m}^*(\omega')e^{-\alpha(\omega+\omega')}\\&=\int_0^\infty d\alpha\left|\int_0^\infty d\omega f_{n,m}(\omega)e^{-\alpha\omega}\right|^2\equiv|g_{n,m}|\,.\end{aligned} \tag{12}$$

Thus, provided V_n is uniform in sign, the AFM configuration has lower energy. This condition on V_n does not seem so restrictive, and is by the way satisfied in the Coulomb case.

An interesting special case is that in which the $\varphi_n(\mathbf{r})$ can be chosen to be eigenfunctions of some symmetry operator which commutes with the subsystem Hamiltonian $\hat{H}_0$. For example, in the Coulomb case, we can obviously choose $\varphi_n(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})$. Thus, provided that the symmetry in question is not itself spontaneously broken in the ground state, there is no coherence between the terms in (3) [or (4)] corresponding to $n\neq m$. In that case $f_{n,m}(\omega)=\delta_{n,m}f_n(\omega)$ is a real function, and also [see (12)] $|g_{n,m}|=\delta_{n,m}|g_n|$. We then have

$$\Delta E_{\mathrm{FM}}-\Delta E_{\mathrm{AFM}}=\tfrac{1}{2}\sum_n V_n^2|g_n|\,, \tag{13}$$

which is positive irrespective of oscillations in V_n, favoring the antiferromagnetic alignment.

However, one could ask when in general is $f_n(\omega)\neq0$? For a translationally invariant system one can label the states with some wave vector $\mathbf{k}$, and $f_{\mathbf{k}}(\omega)\neq0$ requires that $\chi_{\mathbf{k}}(\omega)\neq\chi_{-\mathbf{k}}(\omega)$. If despite the breaking of T, reflection invariance in the plane [the operation that brings (x,y) to $(-x,-y)$] is still a good symmetry, then $\chi_{\mathbf{k}}(\omega)=\chi_{-\mathbf{k}}(\omega)$. This happens, for example, for free particles in an external magnetic field (and also for the anyon case), in a geometry with no boundaries (periodic boundary conditions), and for densities such that an integer number of Landau levels is filled. In this case both the ground state and excited states can be labeled by $\mathbf{k}$, and since P is conserved $\chi_{\mathbf{k}}(\omega)=\chi_{-\mathbf{k}}(\omega)$. An analogous situation occurs for a T-violating BCS state [5]. The situation changes if one considers the boundaries, for in this case the perfect translational invariance is lost. For a two-dimensional layer there exists current-carrying states which are localized within approximately a cyclotron radius of the sample boundary [11]. For a given edge, it can be shown [12] that the dynamics of these states is approximately that of one-dimensional fermions which are only allowed to move in one direction. The dispersion law is linear in k and the direction of movement is determined by the sign of the magnetic field. The coupling between

two planes can then be approximated by that of two pairs of one-dimensional systems, one for each edge of the sample. Because of the fact that the fermions can move in only one direction, it is easy to see that, if the fermions propagate in the $+k$ direction, $\chi_{+k}(\omega)\neq 0$, whereas $\chi_{-k}(\omega)=0$, where χ is the spectral function of the operator that measures the charge near the edge of the sample. This result implies that the AFM configuration is favored by an amount proportional to the perimeter and not to the surface of the sample [13].

The asymmetry in the motion of one-dimensional fermions occurs also for a ring geometry that encloses a flux Φ. Let us discuss this case in some detail. In this example the T symmetry is broken externally. Our previous arguments are valid as long as for each state $|i\rangle$ for flux $\Phi=\phi$, there exists a $|i^*\rangle$ for $\Phi=-\phi$ with the same energy.

We consider the Hamiltonian of a *single* ring to be

$$H=\sum_m (\epsilon_m c_m^\dagger c_m + u_m \hat{\rho}_m^\dagger \hat{\rho}_m)\,, \tag{14}$$

with

$$\hat{\rho}_m=\sum_{m'} c_{m'-m}^\dagger c_{m'}\,, \tag{15}$$

and $c^\dagger$ a fermion creation operator. The kinetic energies are (in units of $\hbar^2/2mr^2$) $\epsilon_m=(m-\phi)^2$, where ϕ is the magnetic flux enclosed by the ring in units of the quantum flux. If we define the total angular momentum as

$$\hat{K}=\sum_m m c_m^\dagger c_m\,, \tag{16}$$

and the total particle number as

$$\hat{N}=\sum_m c_m^\dagger c_m\,, \tag{17}$$

we can write the Hamiltonian of a single ring in the presence of a field in terms of the Hamiltonian for $\phi=0$ as follows:

$$H(\phi)=H(\phi=0)-2\phi\hat{K}+\phi^2\hat{N}\,. \tag{18}$$

Because of the translational invariance of the potential, the eigenstates for $\phi=0$ can also be taken as eigenstates of $\hat{K}$, and therefore the eigenvalues for $\phi\neq 0$ are given by (the total particle number is obviously a good quantum number)

$$\varepsilon_i(\phi)=\varepsilon_i(\phi=0)-2\phi K_i+\phi^2 N\,, \tag{19}$$

where the subindex i refers to a many-body state of total angular momentum K_i and particle number N. Note that, as in the noninteracting case, the corresponding wave function $|\psi_i\rangle$ is the same for both $\phi=0$ and $\phi\neq 0$.

We now want to compute the spectral functions of $\hat{\rho}_m$, $\chi^{(m)}(\omega)$, and $\chi_T^{(m)}(\omega)$. We first note that although the eigenstates and eigenvalues for finite flux can be obtained directly from the values for zero flux, there are quite generally level crossings as the flux evolves, and the *ordering* of the levels is not necessarily the same for zero or finite flux. Let us call $|O_i\rangle\equiv|O_\phi\rangle$ the state which becomes the ground state for flux ϕ. Also, $K_i\equiv K_\phi$ and its energy is $\varepsilon_i(\phi=0)-2\phi K_\phi$ (we forget about the term $\phi^2 N$ because it is independent of the configuration).

The spectral function is given by [we use the notation $\varepsilon_j=\varepsilon_j(\phi=0)$]

$$\chi^{(m)}(\omega)=\sum_j |\langle j|\hat{\rho}_m|O_\phi\rangle|^2\delta(\omega-\varepsilon_j+\varepsilon_i-2m\phi) \tag{20}$$

and

$$\chi_T^{(m)}(\omega)=\sum_{j'} |\langle j'|\hat{\rho}_m^\dagger|O_\phi\rangle|^2\delta(\omega-\varepsilon_{j'}+\varepsilon_i+2m\phi)\,. \tag{21}$$

Now, the operator $\hat{\rho}_m$ has nonzero matrix elements only between many-body states whose total angular momenta differ in m (this follows from the commutation relation $[\hat{K},\hat{\rho}_m]=-m\hat{\rho}_m$). This implies that the states $\langle j|$ and $\langle j'|$ in (20) and (21) correspond to manifolds that for zero flux have different momentum ($K_\phi \pm m$) in modulus and sign. In general these manifolds are different, and so are their energies. This implies that in general $\chi^{(m)}(\omega)\neq\chi_T^{(m)}(\omega)$, and the AFM configuration of external fluxes has lower energy, unless some coincidence occurs that makes $f_n(\omega)=0$ for *all* n. But this seems rather pathological. A hint is given by the noninteracting case, where $f_n(\omega)$ can be computed easily. In this situation, there are no level crossings for $\phi<\phi_0$. So if, for example, we take N odd, $|O_\phi\rangle\equiv|O_{\phi=0}\rangle$ has total angular momentum equal to zero, and the states $\langle j|$ and $\langle j'|$ are degenerate for zero flux. We than have

$$f_n(\omega)=\chi_0^{(m)}(\omega+2m\phi)-\chi_0^{(m)}(\omega-2m\phi)\,, \tag{22}$$

with $\chi_0^{(m)}(\omega)$ being the spectral function of the $\phi=0$ case, given by

$$\chi_0^{(m)}(\omega)=\frac{1}{4\pi m}[\Theta(\omega-\omega_-)-\Theta(\omega-\omega_+)]\,,$$

with $\omega_\pm=2m_F m\pm m^2$, m_F being the Fermi angular momentum, and $\Theta(\omega)$ is the Heaviside step function. We see from this example that, in this order of perturbation, the energy difference between $\Delta E_{\rm FM}$ and $\Delta E_{\rm AFM}$ results essentially from the different energies of the virtual states (this can be clearly seen in the case of a delta function interaction where the matrix elements are constants and equal for both configurations). These intermediate states constitute the same set for both configurations, a fact that should be contrasted with exchange mechanisms, where two configurations differ in energy because of the difference in availability of intermediate states. A simple example is the strong interaction limit of the Hubbard model, where virtual transitions to states with two (antiparallel-spin) electrons in a single atomic site lower the energy of configurations with antiparallel spins in nearest-neighbor atoms. These intermediate states are not available if the spins are parallel, and therefore the ferromagnetic configuration is not corrected in second order. As a result of this "intermediate-state exclusion" the

antiferromagnetic configuration is favored. Our mechanism is of different origin since we are considering two distinguishable nonoverlapping systems and therefore there is no exchange.

In summary, we showed that whenever exchange between two T-violating subsystems could be neglected, second-order perturbation theory in a Coulomb-type interaction implies that the antiferromagnetic configuration is favored. We also discussed the examples of two rings enclosing fluxes that can be either parallel or antiparallel. When translated to the anyon theory of high-T_c superconductivity, our results imply that the antiferromagnetic ordering of chirality among the planes is favored, the bias being not extensive but proportional to the perimeter of the (two-dimensional) sample. There are, however, other mechanisms that could favor the FM arrangement, like the "classical" magnetic energy, or the Josephson coupling between planes. To get an order of magnitude estimate, we assume that the "asymmetry" in χ is of order 1 ($\chi_{\mathbf{k}}-\chi_{-\mathbf{k}}\sim\chi_{\mathbf{k}}$) corrected by an "edge effect factor" d/R, where d is the interparticle distance and R is a typical domain size perimeter. Using the fact that the main weight of $\chi_{\mathbf{k}}(\omega)$ is the plasmon pole, and that d is of order of the interplane distance D, we get ΔE/particle $\sim(D/R)\omega_P$, with ω_P the three-dimensional plasma frequency. Typical twin domain widths are [14] $R\sim5000$ Å. If we identify the "domains" corresponding to coherent T violations with the twin domains then we estimate ΔE/particle $\sim10^{-3}$ eV. An estimate of the Josephson-induced bias is the Josephson energy $\Delta E_{\mathrm{Jos}}\simeq\phi_0 J_c/2\pi$, with J_c the c-axis critical current. This is arguably a competing interaction favoring the "ferromagnetic" alignment [15]. If we take [16] $J_c\sim250$ A/cm^2, we get ΔE_{Jos}/particle $\sim10^{-9}$ eV. The unpaired magnetic energy is also proportional to the perimeter of the sample. An estimate of this interaction relative to the Coulomb effect gives $|\Delta E_{\mathrm{magn}}/\Delta E|\sim10^{-4}\log(R/D)$, which again for the domain sizes mentioned above is a small quantity.

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