Hermaphrodite Orbitals with and without Time-Reversal Symmetry

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The localization tensor, alias second cumulant moment $\langle r_\alpha r_\beta \rangle_{\rm c}$ of the electron distribution, is an intensive quantity characterizing the ground-state wavefunction, and is finite in any insulator [1]. In absence of time-reversal (TR) symmetry, this same tensor acquires an off-diagonal imaginary part [2], proportional to the Chern number C_1 (in 2d).
I specialize here to the case of noninteracting electrons (either HF or KS). Within either periodic or "open" (cluster-like) boundary conditions we have

$$\mathrm{Re}\, \langle r_\alpha r_\beta \rangle_{\rm c} = \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta |\rho(\mathbf{r}, \mathbf{r}')|^2, \tag{1}$$

where ρ is the one-body density matrix, and single orbital occupancy is assumed. When performing a localization transformation upon the occupied orbitals, the real part of $\langle r_\alpha r_\beta \rangle_{\rm c}$ sets a minimum for the quadratic spread in any given direction, averaged over all the orbitals; this statement holds, again, within both kinds of boundary conditions [3].
From now on, I further specialize to the crystalline case. Then the trace of $\langle r_\alpha r_\beta \rangle_{\rm c}$ equals the Marzari-Vanderbilt $\Omega_{\rm I}$ (divided by the number of occupied bands) while the orbitals which actually minimize the quadratic spread in a given direction have been called "hermaphrodite orbitals" (Wannier-like in one direction, Bloch-like in the orthogonal ones); they decay faster than any polynomial [4].
As for the cases where TR symmetry is broken, we have some experience only in 2d, for either the quantum-Hall (noninteracting) fluid, or the Haldane model Hamiltonian [5].
In a quantum-Hall fluid the dc longitudinal conductance vanishes, hence the system is effectively an insulator. Then $\mathrm{Re}\, \langle r_\alpha r_\beta \rangle_{\rm c}$ is finite, while $\mathrm{Im}\, \langle r_\alpha r_\beta \rangle_{\rm c}$ is proportional to C_1 (hence to the Hall conductivity). Despite the finiteness of $\mathrm{Re}\, \langle r_\alpha r_\beta \rangle_{\rm c}$, two-dimensional localization of the orbitals *cannot* be achieved. Instead, the hermaphrodite orbitals do exist. All can be worked out analytically in the case of a flat substrate potential, where the density matrix appearing in Eq. (1) has a Gaussian decay and the trace of $\langle r_\alpha r_\beta \rangle_{\rm c}$ equals precisely the squared magnetic length (at filling one). The hermaphrodite orbitals happen to coincide with the Landau-gauge orbitals [2]; notice that ρ is *not* gauge-invariant by a change of the magnetic gauge (although its modulus is such).
Depending on its parameters, the Haldane model may represent either a normal insulator ($C_1 = 0$) or a Chern insulator ($C_1 = \pm 1$). While the normal case is such by all counts, the Chern case is like the quantum-Hall case: $\mathrm{Re}\, \langle r_\alpha r_\beta \rangle_{\rm c}$ is finite, $\mathrm{Im}\, \langle r_\alpha r_\beta \rangle_{\rm c}$ is proportional to C_1, and two-dimensional localization of the orbitals *cannot* be achieved [6]. I conjecture that hermaphrodite orbitals still exist.
Other issues, related to macroscopic orbital magnetization, will be possibly discussed.

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