Quantum phase transitions

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Quantum Phase Transitions Cambridge University Press





What is a quantum phase transition ?

Non-analyticity in ground state properties as a function of some control parameter g



True level crossing: Usually a *first*-order transition

Avoided level crossing which becomes sharp in the infinite volume limit:

second-order transition







- Theory for a quantum system with strong correlations: describe phases on either side of g_c by expanding in deviation from the quantum critical point.
- Critical point is a novel state of matter without quasiparticle excitations
- Critical excitations control dynamics in the wide *quantum-critical* region at non-zero temperatures.

Important property of ground state at $g=g_c$: temporal and spatial <u>scale invariance</u>; characteristic energy scale at other values of $g: \Delta \sim |g - g_c|^{zv}$

Outline

- I. Quantum Ising Chain
- II. Landau-Ginzburg-Wilson theory Mean field theory and the evolution of the excitation spectrum.
- III. Superfluid-insulator transition Boson Hubbard model at integer filling.
- IV. Tilting the Mott insulator Density wave order at an Ising transition.
- V. Bosons at fractional filling Beyond the Landau-Ginzburg-Wilson paradigm.

I. Quantum Ising Chain

I. Quantum Ising Chain

Degrees of freedom: j = 1...N qubits, N "large" $|\uparrow\rangle_{j}, |\downarrow\rangle_{j}$ or $|\rightarrow\rangle_{j} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{j} + |\downarrow\rangle_{j}), \ |\leftarrow\rangle_{j} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{j} - |\downarrow\rangle_{j})$

Hamiltonian of decoupled qubits:

$$H_0 = -Jg\sum_j \sigma_j^x$$



Coupling between qubits:

$$H_{1} = -J \sum_{j} \sigma_{j}^{z} \sigma_{j+1}^{z}$$

$$(| \rightarrow \rangle_{j} \langle \leftarrow | + | \leftarrow \rangle_{j} \langle \rightarrow |) (| \rightarrow \rangle_{j+1} \langle \leftarrow | + | \leftarrow \rangle_{j+1} \langle \rightarrow |)$$

Prefers neighboring qubits are *either* $|\uparrow\rangle_{j}|\uparrow\rangle_{j+1}$ or $|\downarrow\rangle_{j}|\downarrow\rangle_{j+1}$ (not entangled)

Full Hamiltonian

$$H = H_0 + H_1 = -J\sum_j \left(g\sigma_j^x + \sigma_j^z\sigma_{j+1}^z\right)$$

leads to entangled states at g of order unity





LiHoF₄

Lowest excited states:

$$\left|\ell_{j}\right\rangle = \left|\cdots \rightarrow \rightarrow \rightarrow \leftarrow_{j} \rightarrow \rightarrow \rightarrow \rightarrow \cdots\right\rangle + \cdots$$

Coupling between qubits creates "flipped-spin" *quasiparticle* states at momentum p

$$|p\rangle = \sum_{j} e^{ipx_{j}/\hbar} |\ell_{j}\rangle$$

Excitation energy $\varepsilon(p) = \Delta + 4J \sin^{2}\left(\frac{pa}{2\hbar}\right) + O(g^{-1})$
Excitation gap $\Delta = 2gJ - 2J + O(g^{-1})$
 $-\frac{\hbar\pi}{a}$
 p
 $\frac{\hbar\pi}{a}$

Entire spectrum can be constructed out of multi-quasiparticle states



At T > 0, collisions between quasiparticles broaden pole to a Lorentzian of width $1/\tau_{\varphi}$ where the *phase coherence time* τ_{φ}

is given by
$$\frac{1}{\tau_{\varphi}} = \frac{2k_{B}T}{\pi\hbar}e^{-\Delta/k_{B}T}$$

S. Sachdev and A.P. Young, Phys. Rev. Lett. 78, 2220 (1997)

Strongly-coupled qubits $(g \ll 1)$

Ground states:

 $|G\uparrow\rangle = |\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\rangle$

 $-\frac{g}{2} | \cdots \uparrow \cdots \rangle - \cdots$

Ferromagnetic moment $N_0 = \langle G | \sigma^z | G \rangle \neq 0$

Second state $|G\downarrow\rangle$ obtained by $\uparrow \Leftrightarrow \downarrow$ $|G\downarrow\rangle$ and $|G\uparrow\rangle$ mix only at order g^N

Lowest excited states: domain walls

$$\left| d_{j} \right\rangle = \left| \cdots \uparrow \uparrow \uparrow \uparrow \uparrow_{j} \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \rangle + \cdots \right\rangle$$

Coupling between qubits creates new "domainwall" *quasiparticle* states at momentum *p*

$$\left| p \right\rangle = \sum_{j} e^{ipx_{j}/\hbar} \left| d_{j} \right\rangle$$

Excitation energy $\varepsilon(p) = \Delta + 4Jg \sin^{2}\left(\frac{pa}{2\hbar}\right) + O\left(g^{2}\right)$

Excitation gap $\Delta = 2J - 2gJ + O(g^2)$



Dynamic Structure Factor $S(p, \omega)$: Strongly-coupled qubits $(g \ll 1)$ Cross-section to flip a $|\rightarrow\rangle$ to a $|\leftarrow\rangle$ (or vice versa) while transferring energy $\hbar \omega$ and momentum *p*



At T > 0, motion of domain walls leads to a finite *phase coherence time* τ_{φ} , and broadens coherent peak to a width $1/\tau_{\varphi}$ where $\frac{1}{\tau_{\varphi}} = \frac{2k_B T}{\pi \hbar} e^{-\Delta/k_B T}$

S. Sachdev and A.P. Young, Phys. Rev. Lett. 78, 2220 (1997)





No quasiparticles --- dissipative critical continuum



S. Sachdev and J. Ye, Phys. Rev. Lett. **69**, 2411 (1992). S. Sachdev and A.P. Young, Phys. Rev. Lett. **78**, 2220 (1997).

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II. Landau-Ginzburg-Wilson theory

Mean field theory and the evolution of the excitation spectrum

- Identify order parameter $\phi(x,\tau) \sim \sigma_j^z$
- Symmetries:

Spin inversion:	$\phi ightarrow -\phi$
Time reversal	au ightarrow - au
Spatial inversion	$x \rightarrow -x$

• Write down most general Lagrangian consistent with symmetries

$$\mathcal{Z} = \int \mathcal{D}\phi(x,\tau) \exp\left(-\int d^d x \int d\tau \mathcal{L}\left[\phi\right]\right)$$
$$\mathcal{L}\left[\phi\right] = \frac{1}{2} \left(\partial_\tau \phi\right)^2 + \frac{c^2}{2} \left(\nabla_x \phi\right)^2 + \frac{r}{2} \phi^2 + \frac{u}{4} \phi^4 + \dots$$

• Identify phases at $r \gg 0$ and $r \ll 0$ with the paramagnet and the ferromagnet respectively.

Quantum field theory formally resembles the classical statistical mechanics of an Ising model in d+1 dimensions. Theory of second-order classical phase transitions implies that at the critical point the susceptibility depends on the d+1 dimensional momentum k as

$$\chi(k) \sim \frac{1}{k^{2-\eta}}$$

After analytic continuation, and using the "Lorentz invariance" of the critical theory, the quantum critical point therefore has the following dynamic susceptibility at T = 0.

$$\chi(p,\omega) \sim \frac{1}{(c^2 p^2 - \omega^2)^{1-\eta/2}}$$

At T > 0, we have to consider a classical statistical mechanics problem in finite geometry with a 'temporal' direction of extent $L_{\tau} = \hbar/(k_B T)$. Finite size scaling now implies that the susceptibility at the critical point obeys

$$\chi(k) \sim L_{\tau}^{2-\eta} F\left(kL_{\tau}\right)$$

After analytic continuation, the quantum system has the dynamic response (note: can no longer use "Lorentz invariance")

$$\chi''(0,\omega) \sim \frac{1}{T^{2-\eta}} \Phi\left(\frac{\hbar\omega}{k_B T}\right)$$

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III. Superfluid-insulator transition

Boson Hubbard model at integer filling



LGW theory: continuous quantum transitions between these states

M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).

I. The Superfluid-Insulator transition

Boson Hubbard model

Degrees of freedom: Bosons, b_j^{\dagger} , hopping between the sites, *j*, of a lattice, with short-range repulsive interactions.

$$H = -t \sum_{\langle ij \rangle} b_i^{\dagger} b_j - \mu \sum_j n_j + \frac{U}{2} \sum_j n_j (n_j - 1) + \cdots$$
M.PA. Fisher, P.

 $n_i \equiv b_i b_i$

M.PA. Fisher, P.B. Weichmann,G. Grinstein, and D.S. Fisher*Phys. Rev. B* 40, 546 (1989).

For small U/t, ground state is a superfluid BEC with superfluid density \approx density of bosons

What is the ground state for large U/t?

Typically, the ground state remains a superfluid, but with

superfluid density \ll density of bosons



The superfluid density evolves smoothly from large values at small U/t, to small values at large U/t, and there is no quantum phase transition at any intermediate value of U/t.

(In systems with Galilean invariance and at zero temperature, superfluid density=density of bosons always, independent of the strength of the interactions)

What is the ground state for large U/t?

<u>Incompressible, insulating ground states</u>, with zero superfluid density, appear at special commensurate densities





Excitations of the insulator: infinitely long-lived, finite energy *quasiparticles* and *quasiholes*



Energy of quasi-particles/holes:
$$\varepsilon_{p,h}(p) = \Delta_{p,h} + \frac{p^2}{2m_{p,h}^*}$$



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Excitations of the insulator: infinitely long-lived, finite energy *quasiparticles* and *quasiholes*



Energy of quasi-particles/holes:
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LGW theory of the superfluid insulator transition

- Identify order parameter $\Psi(x,\tau) \sim b_j^{\dagger}$
- Symmetries:

Gauge invariance: $\Psi \to \Psi e^{i\theta}$ Time reversal $\tau \to -\tau$; $\Psi \to \Psi^*$ Spatial inversion

• Write down most general Lagrangian consistent with symmetries

$$\mathcal{Z} = \int \mathcal{D}\Psi(x,\tau) \exp\left(-\int d^d x \int d\tau \mathcal{L}\left[\Psi\right]\right)$$
$$\mathcal{L}\left[\Psi\right] = K\Psi^* \frac{\partial \Psi}{\partial \tau} + |\partial_\tau \Psi|^2 + c^2 |\nabla_x \Psi|^2 + r|\Psi|^2 + \frac{u}{2}|\Psi|^4 + \dots$$

- Identify phases at $r \gg 0$ and $r \ll 0$ with the insulator and the superfluid respectively.
- For $K \neq 0$, the particle and hole excitations have different energies.

• Gauge-invariance of the underlying boson Hamiltonian shows that

$$K = -\frac{\partial r}{\partial \mu}$$

• In mean-field theory, the ground state energy, E, across the superfluidinsulator transition has the non-analytic term

$$E = E_0 - \frac{r^2}{2u}\theta(-r)$$

(Beyond mean-field theory, the non-analytic term is $E \sim r^{(d+z)\nu}$).

- Because the density of bosons $= -\partial E/\partial \mu$, this implies a change in the boson density across the transition unless $\partial r/\partial \mu = 0$
- A superfluid-insulator transition at fixed boson density must have.

$$K = 0$$

Boson Green's function $G(p, \omega)$:

Insulating ground state

Cross-section to add a boson

while transferring energy $\hbar\omega$ and momentum p



Similar result for quasi-hole excitations obtained by removing a boson





M.P.A. Fisher, G. Girvin, and G. Grinstein, *Phys. Rev. Lett.* 64, 587 (1990).
K. Damle and S. Sachdev *Phys. Rev.* B 56, 8714 (1997).

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IV. Tilting the Mott insulator

Density wave order at an Ising transition

Applying an "electric" field to the Mott insulator а \$ U Ш b Ш U



 $V_0 = 16 E_{recoil} \tau_{perturb} = 9 ms$

 $V_0 = 20 E_{recoil} \tau_{perturb} = 20 ms$



$$H = -t \sum_{\langle ij \rangle} \left(b_i^{\dagger} b_j + b_j^{\dagger} b_i \right) + \frac{U}{2} \sum_i n_i \left(n_i - 1 \right) - \sum_i \mathbf{E} \cdot \mathbf{r}_i n_i$$
$$n_i = b_i^{\dagger} b_i$$

$$|U-E|, t \ll E, U$$

Describe spectrum in subspace of states resonantly coupled to the Mott insulator

S. Sachdev, K. Sengupta, and S.M. Girvin, *Physical Review B* 66, 075128 (2002)





Nearest neighbor dipole



Creating dipoles on nearest neighbor links creates a state with relative energy U-2E; such states are *not* part of the resonant manifold



Nearest neighbor dipole



Nearest-neighbor dipoles

Dipoles can appear resonantly on non-nearest-neighbor links. Within resonant manifold, dipoles have infinite on-link and nearest-link repulsion

Charged excitations (in one dimension)



Effective Hamiltonian for a quasiparticle in one dimension (similar for a quasihole):

$$H_{\text{eff}} = -\sum_{j} \left[3t \left(b_{j}^{\dagger} b_{j+1} + b_{j+1}^{\dagger} b_{j} \right) + Ej b_{j}^{\dagger} b_{j} \right]$$

Exact eigenvalues $\varepsilon_m = Em$; $m = -\infty \cdots \infty$ Exact eigenvectors $\psi_m(j) = J_{j-m}(6t/E)$

All charged excitations are strongly localized in the plane perpendicular electric field. Wavefunction is periodic in time, with period h/E (Bloch oscillations) Quasiparticles and quasiholes are not accelerated out to infinity

A non-dipole state



State has energy 3(U-E) but is connected to resonant state by a matrix element smaller than t^2/U

State is not part of resonant manifold

Hamiltonian for resonant dipole states (in one dimension)

$$d_{\ell}^{\dagger} \Rightarrow \text{Creates dipole on link } \ell$$
$$H_{d} = -\sqrt{6t} \sum_{\ell} \left(d_{\ell}^{\dagger} + d_{\ell} \right) + (U - E) \sum_{\ell} d_{\ell}^{\dagger} d_{\ell}$$
$$\text{Constraints:} \quad d_{\ell}^{\dagger} d_{\ell} \leq 1 \quad ; \quad d_{\ell+1}^{\dagger} d_{\ell+1} d_{\ell}^{\dagger} d_{\ell} = 0$$

Determine phase diagram of H_d as a function of (U-E)/t

Note: there is <u>no explicit dipole hopping term</u>.

However, dipole hopping is generated by the interplay of terms in H_d and the constraints.

Weak electric fields: $(U-E) \gg t$

Ground state is dipole vacuum (Mott insulator) $|0\rangle$

First excited levels: single dipole states $d_{\ell}^{\dagger} \left| 0 \right\rangle$

Effective hopping between dipole states



If both processes are permitted, they exactly cancel each other. The top processes is blocked when ℓ, m are nearest neighbors

 \Rightarrow A nearest-neighbor dipole hopping term $\sim \frac{t^2}{U-E}$ is generated

Ground state has maximal dipole number.

Two-fold degeneracy associated with Ising density wave order:

 $\cdots d_{1}^{\dagger} d_{3}^{\dagger} d_{5}^{\dagger} d_{7}^{\dagger} d_{9}^{\dagger} d_{11}^{\dagger} \cdots |0\rangle \qquad or \qquad \cdots d_{2}^{\dagger} d_{4}^{\dagger} d_{6}^{\dagger} d_{8}^{\dagger} d_{10}^{\dagger} d_{12}^{\dagger} \cdots |0\rangle$





S. Sachdev, K. Sengupta, and S.M. Girvin, *Physical Review B* 66, 075128 (2002)

Non-equilibrium dynamics in one dimension

Start with the ground state at E=32 on a chain with open boundaries. Suddenly change the value of *E* and follow the evolution of the wavefunction



Critical point at E=41.85

Non-equilibrium dynamics in one dimension

Dependence on chain length





Non-equilibrium response is maximal near the Ising critical point K. Sengupta, S. Powell, and S. Sachdev, *Physical Review* A **69**, 053616 (2004)

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V. Bosons at fractional filling

Beyond the Landau-Ginzburg-Wilson paradigm



LGW theory: continuous quantum transitions between these states

M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).

Bosons at density f = 1/2

Weak interactions: superfluidity

 $\langle \Psi_{sc} \rangle \neq 0$

Strong interactions: Candidate insulating states



C. Lannert, M.P.A. Fisher, and T. Senthil, *Phys. Rev.* B **63**, 134510 (2001) S. Sachdev and K. Park, *Annals of Physics*, **298**, 58 (2002)

Predictions of LGW theory

Superconductor Charge-ordered insulator **First** $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{o} \rangle = 0$ order $\langle \Psi_{sc} \rangle = 0, \langle \rho_{o} \rangle \neq 0$ transition $r_1 - r_2$ Coexistence Superconductor Charge-ordered insulator (Supersolid) $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{Q} \rangle = 0$ $\langle \Psi_{sc} \rangle = 0, \langle \rho_0 \rangle \neq 0$ $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{o} \rangle \neq 0$ $r_1 - r_2$ "Disordered" Charge-ordered insulator Superconductor $\langle \Psi_{sc} \rangle = 0, \langle \rho_{Q} \rangle \neq 0$ $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{Q} \rangle = 0$

Superfluid insulator transition of hard core bosons at f=1/2

A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, Phys. Rev. Lett. 89, 247201 (2002)

<u>Large scale</u> (> 8000 sites) numerical study of the destruction of superfluid order at half filling with full square lattice symmetry



 $H = J \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) - K \sum_{\langle ijkl \rangle \subset \Box} \left(S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+ \right)$



C. Dasgupta and B.I. Halperin, *Phys. Rev. Lett.* **47**, 1556 (1981); D.R. Nelson, *Phys. Rev. Lett.* **60**, 1973 (1988); M.P.A. Fisher and D.-H. Lee, *Phys. Rev.* B **39**, 2756 (1989);



Strength of "magnetic" field = density of bosons = f flux quanta per plaquette

C. Dasgupta and B.I. Halperin, *Phys. Rev. Lett.* 47, 1556 (1981); D.R. Nelson, *Phys. Rev. Lett.* 60, 1973 (1988); M.P.A. Fisher and D.-H. Lee, *Phys. Rev.* B 39, 2756 (1989);

Statistical mechanics of dual superconductor is invariant under the square lattice space group:

- T_x, T_y : Translations by a lattice spacing in the x, y directions
- *R* : Rotation by 90 degrees.

Magnetic space group: $T_x T_y = e^{2\pi i f} T_y T_x$; $R^{-1}T_y R = T_x$; $R^{-1}T_x R = T_y^{-1}$; $R^4 = 1$

Strength of "magnetic" field = density of bosons = f flux quanta per plaquette

Boson-vortex duality Hofstädter spectrum of dual "superconducting" order



At density f = p / q (p, q relatively prime integers) there are q species of vortices, φ_{ℓ} (with $\ell = 1 \dots q$), associated with q gauge-equivalent regions of the Brillouin zone

Magnetic space group: $T_x T_y = e^{2\pi i f} T_y T_x$; $R^{-1}T_y R = T_x$; $R^{-1}T_x R = T_y^{-1}$; $R^4 = 1$

Boson-vortex duality Hofstäder spectrum of dual "superconducting" order



At density f = p / q (p, q relatively prime integers) there are q species of vortices, φ_{ℓ} (with $\ell = 1...q$), associated with q gauge-equivalent regions of the Brillouin zone

The q vortices form a *projective* representation of the space group

$$T_{x}: \varphi_{\ell} \to \varphi_{\ell+1} \quad ; \quad T_{y}: \varphi_{\ell} \to e^{2\pi i \ell f} \varphi_{\ell}$$
$$R: \varphi_{\ell} \to \frac{1}{\sqrt{q}} \sum_{i=1}^{q} \varphi_{m} e^{2\pi i \ell m f}$$

 $\sqrt{9} m=1$

See also X.-G. Wen, *Phys. Rev.* B 65, 165113 (2002)

The φ_{ℓ} fields characterize *both* superconducting and charge order

Superconductor/insulator :
$$\langle \varphi_{\ell} \rangle = 0 / \langle \varphi_{\ell} \rangle \neq 0$$

Charge order:

Status of space group symmetry determined by

density operators ρ_Q at wavevectors $Q_{mn} = \frac{2\pi p}{a}(m,n)$

$$\rho_{Q_{mn}} = e^{i\pi mnf} \sum_{\ell=1}^{q} \varphi_{\ell}^{*} \varphi_{\ell+n} e^{2\pi i\ell mf}$$

$$T_{x} : \rho_{Q} \to \rho_{Q} e^{iQ \cdot \hat{x}} ; \qquad T_{y} : \rho_{Q} \to \rho_{Q} e^{iQ \cdot \hat{y}}$$

$$R : \rho(Q) \to \rho(RQ)$$

The φ_{ℓ} fields characterize *both* superconducting and charge order

Competition between superconducting and charge orders: "*Extended* LGW" theory of the φ_{ℓ} fields with the action invariant under the projective transformations: $T_{x}: \varphi_{\ell} \to \varphi_{\ell+1} \quad ; \quad T_{y}: \varphi_{\ell} \to e^{2\pi i \ell f} \varphi_{\ell}$ $R: \varphi_{\ell} \to \frac{1}{\sqrt{q}} \sum_{m=1}^{q} \varphi_m e^{2\pi i \ell m f}$

Immediate benefit: There is no intermediate "disordered" phase with neither order (or without "topological" order).

Superconductor
$$\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{\varrho} \rangle = 0$$
First
order
order
($\Psi_{sc} \rangle = 0, \langle \rho_{\varrho} \rangle \neq 0$ Superconductor
 $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{\varrho} \rangle = 0$ Coexistence
(Supersolid)
 $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{\varrho} \rangle \neq 0$ Charge-ordered insulator
 $\langle \Psi_{sc} \rangle = 0, \langle \rho_{\varrho} \rangle \neq 0$ Superconductor
 $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{\varrho} \rangle = 0$ $r_1 - r_2$ Superconductor
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Superconductor
$$\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{\varrho} \rangle = 0$$
First
order
transitionCharge-ordered insulator
 $\langle \Psi_{sc} \rangle = 0, \langle \rho_{\varrho} \rangle \neq 0$ Superconductor
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 $\langle \Psi_{sc} \rangle = 0, \langle \rho_{\varrho} \rangle \neq 0$$

Superconductor $\langle \Psi_{sc} \rangle \neq 0, \langle \rho_{Q} \rangle = 0$ Second Charge-ordered insulator order transition $\langle \Psi_{sc} \rangle = 0, \langle \rho_Q \rangle \neq 0$ $r_1 - r_2$

Spatial structure of insulators for q=2 (f=1/2)



Spatial structure of insulators for q=4 (f=1/4 or 3/4)





