Monte Carlo simulations of quantum systems with global updates

Alejandro Muramatsu
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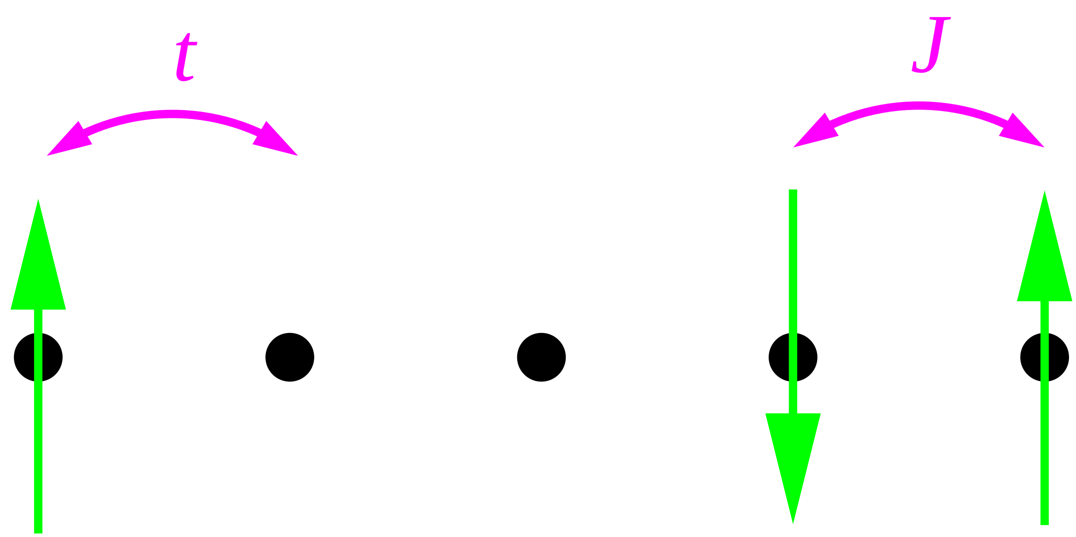
Fermionic systems with strong correlations

The t-J model



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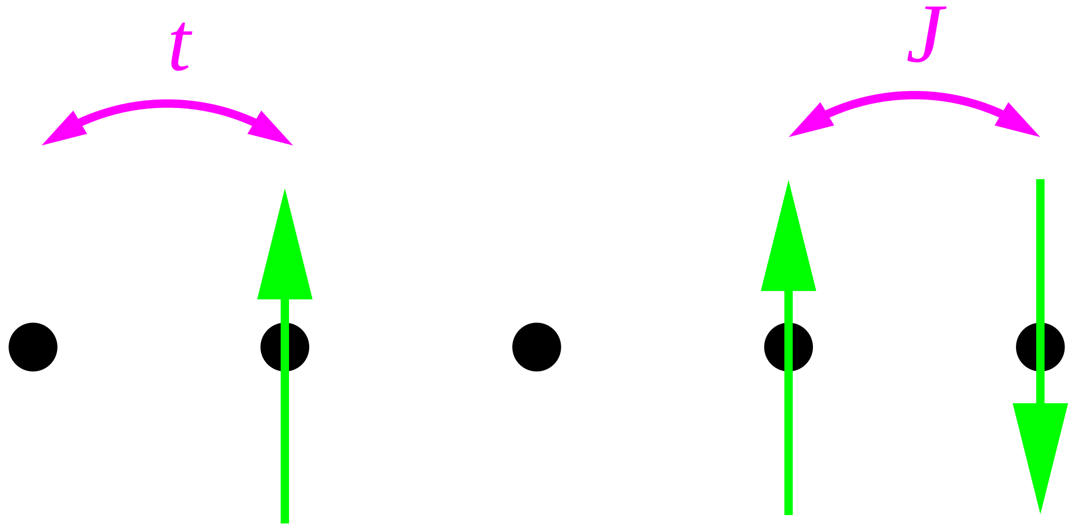

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Start with the general Hamiltonian for electrons with Coulomb interaction

$$H = \sum_{\substack{i,j \\ \sigma}} c^\dagger_{i,\sigma} < i \mid T \mid j > c_{j,\sigma} + \frac{1}{2} \sum_{\substack{i,j,k,\ell \\ \sigma,\sigma'}} c^\dagger_{i,\sigma} c^\dagger_{j,\sigma'} < i,j \mid V \mid k,\ell > c_{k,\sigma'} c_{\ell,\sigma}$$

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Matrix element for the Coulomb interaction

$$< i,j \mid V \mid k,\ell > = \int \mathrm{d}^3x\, \mathrm{d}^3x' \, \frac{\varphi^*_{\sigma}(\boldsymbol{x}-\boldsymbol{R}_i)\, \varphi^*_{\sigma'}(\boldsymbol{x}'-\boldsymbol{R}_j)\, \varphi_{\sigma'}(\boldsymbol{x}'-\boldsymbol{R}_k)\, \varphi_{\sigma}(\boldsymbol{x}-\boldsymbol{R}_\ell)}{\mid \boldsymbol{x}-\boldsymbol{x}' \mid}$$

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where $\hat{n}_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ **and** $U \equiv < i,i \mid V \mid i,i >$.

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Model for itinerant magnetism, antiferromagnetism, high temperature superconductivity and degenerate quantum gases on optical lattices

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Perturbation

$$T = -t \sum_{\substack{<i,j> \\ \sigma}} c^{\dagger}_{i,\sigma}\, c_{j,\sigma}$$

Projectors

P **to the subspace of singly occupied sites** $\longrightarrow \{|\, 0 >, |\!\uparrow>, |\!\downarrow>\}$

Q **to the complementary subspace** $\longrightarrow |\!\uparrow\downarrow>$

First order

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$$\hookrightarrow PTP \quad = \quad -t \sum_{\substack{<i,j> \\ \sigma}} \tilde{c}^{\dagger}_{i,\sigma}\, \tilde{c}_{j,\sigma} \ , \qquad \textbf{where } \tilde{c}_{j,\sigma} = c_{j,\sigma} P$$

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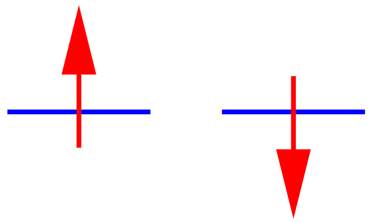

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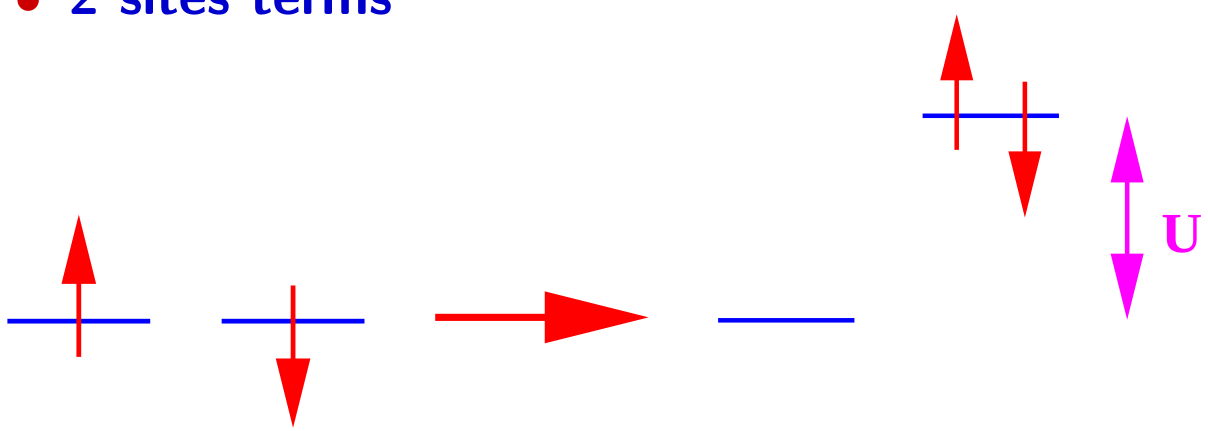

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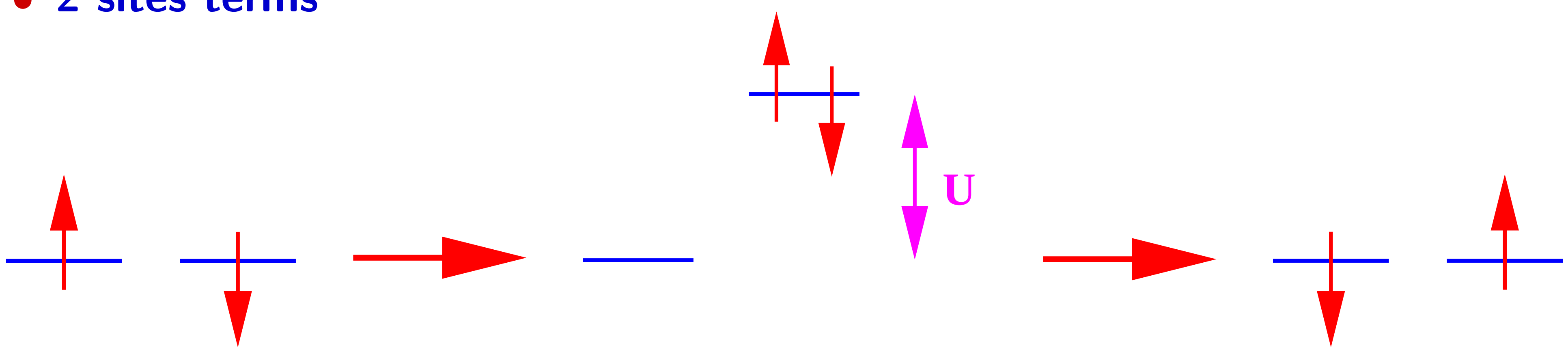

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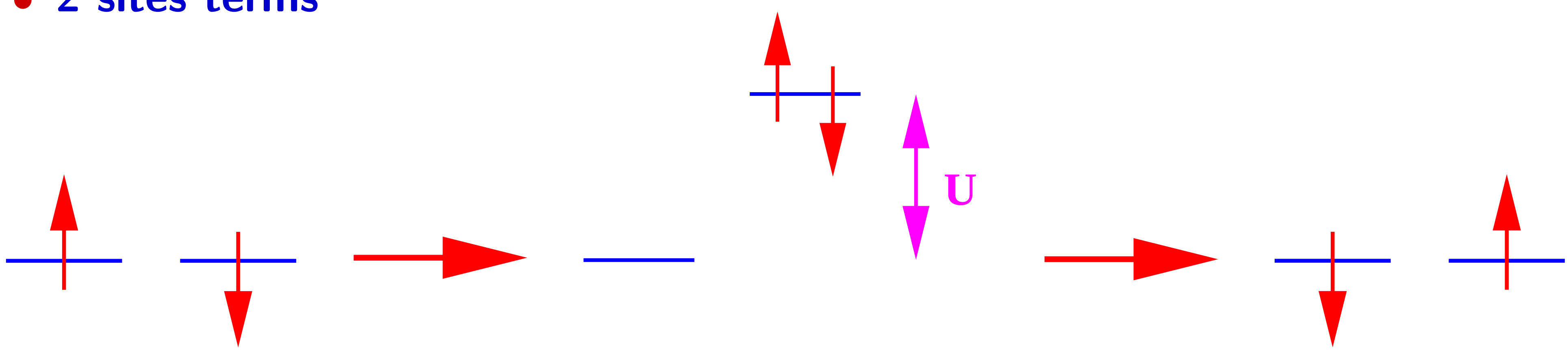

$$\hookrightarrow J \sum_{<i,j>} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4} \tilde{n}_i \tilde{n}_j \right) \quad \textbf{with} \quad J = \frac{4t^2}{U}$$

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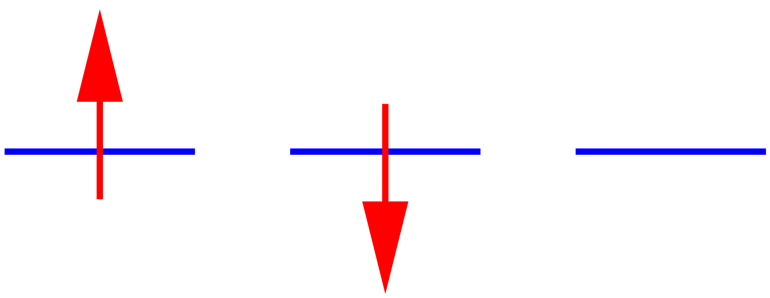

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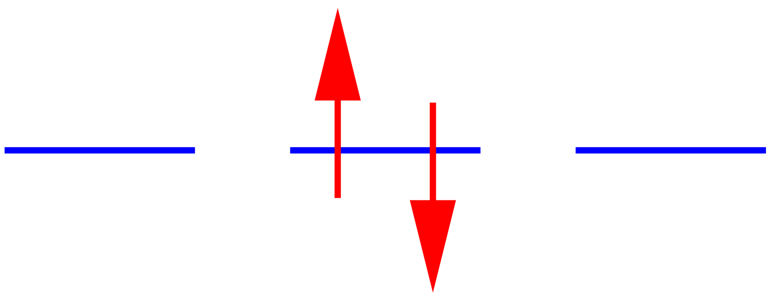

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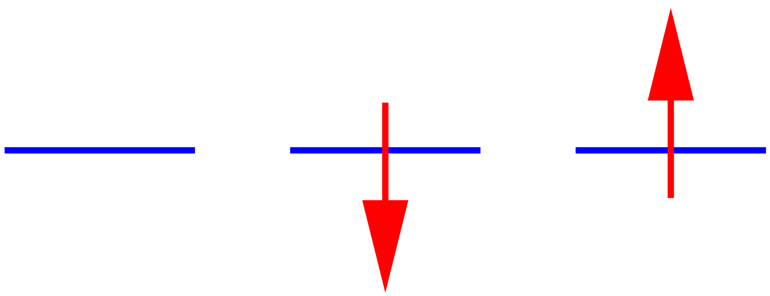

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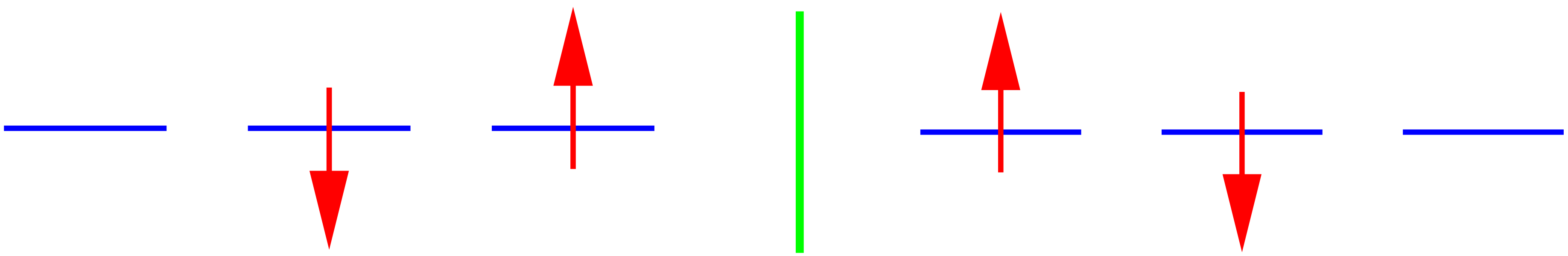

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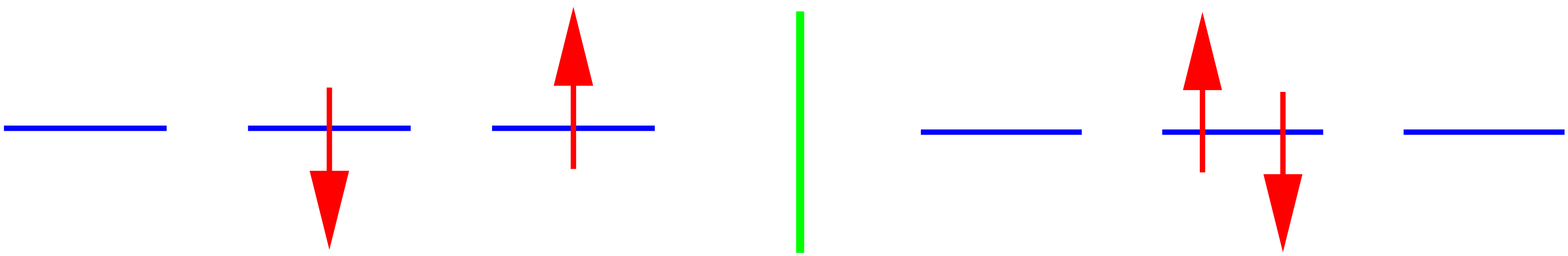

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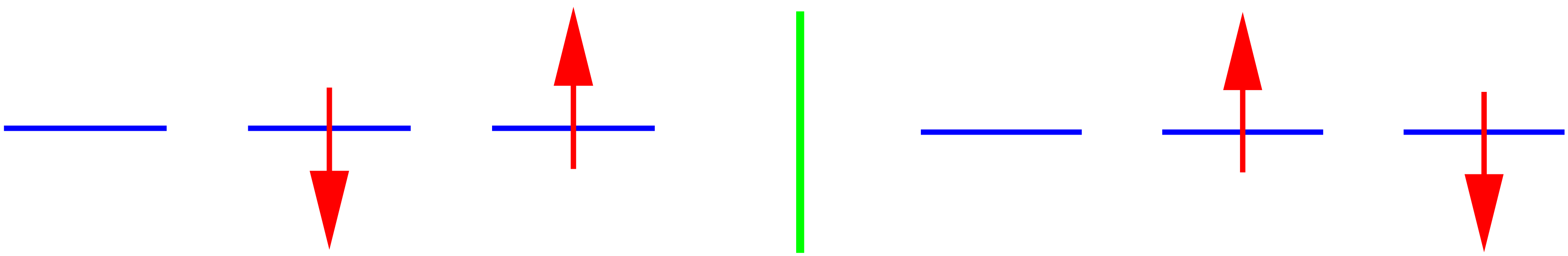

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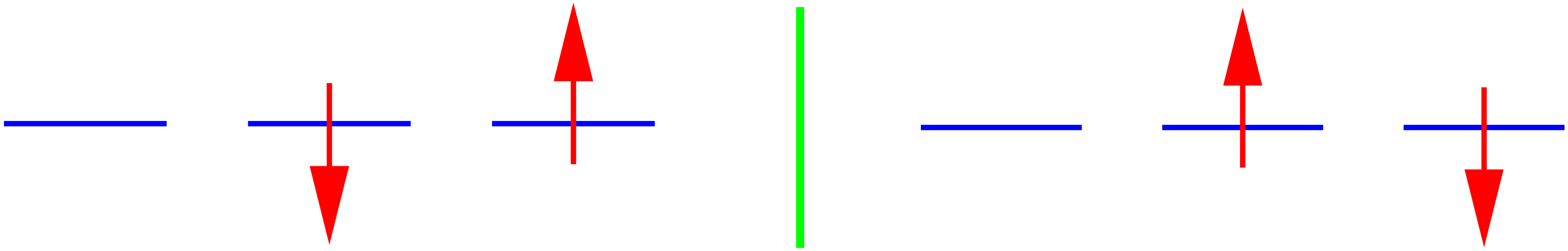

$$\hookrightarrow -\frac{J}{4}\sum_{\substack{<i,j,k>\\ \sigma}}\left(\tilde{c}^{\dagger}_{i,\sigma}\tilde{n}_{j,-\sigma}\tilde{c}_{k,\sigma}-\tilde{c}^{\dagger}_{i,\sigma}\tilde{c}^{\dagger}_{j,-\sigma}\tilde{c}_{j,\sigma}\tilde{c}_{k,-\sigma}\right)$$

assisted and pair hopping.

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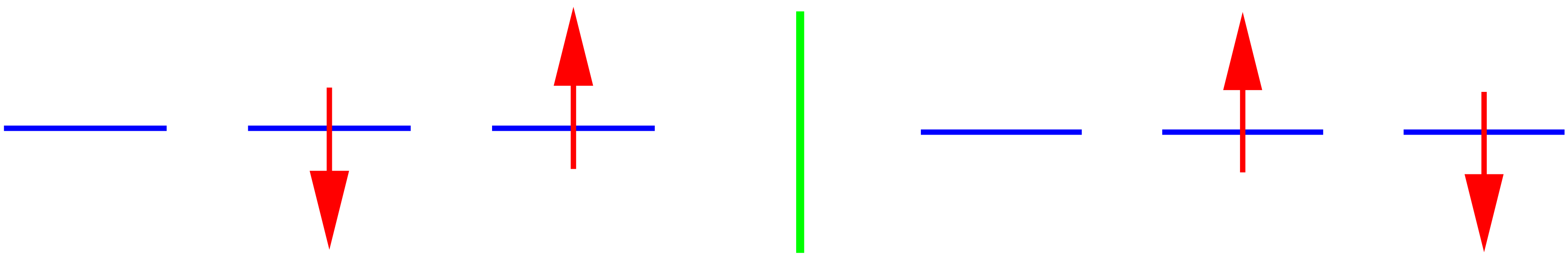

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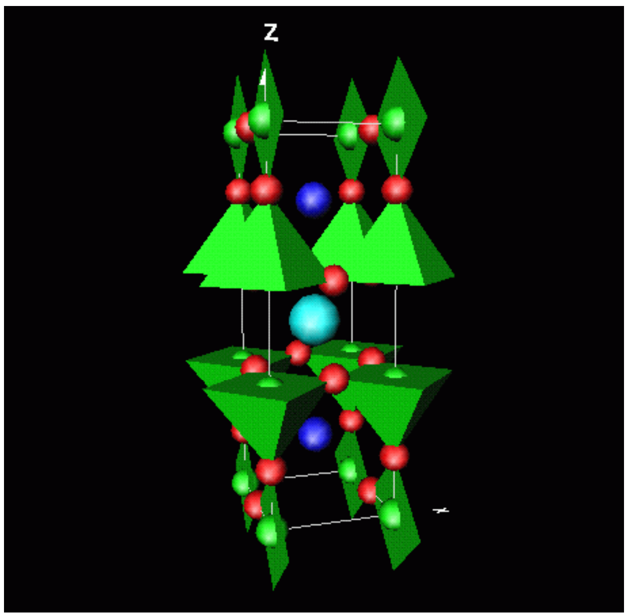

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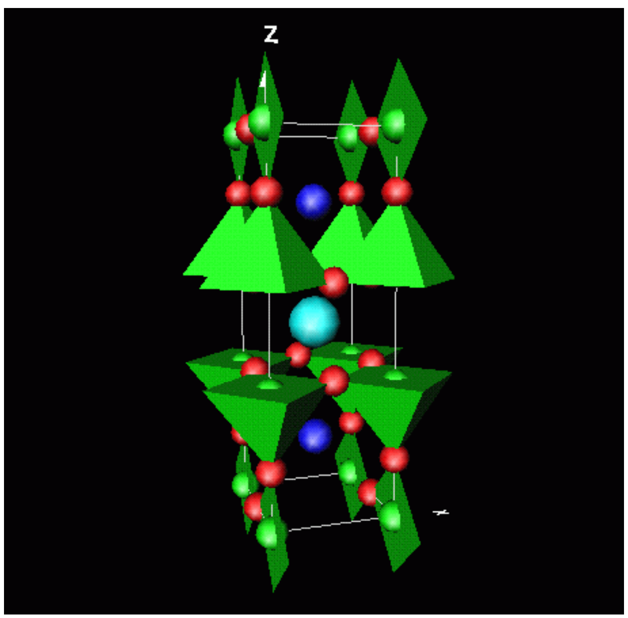

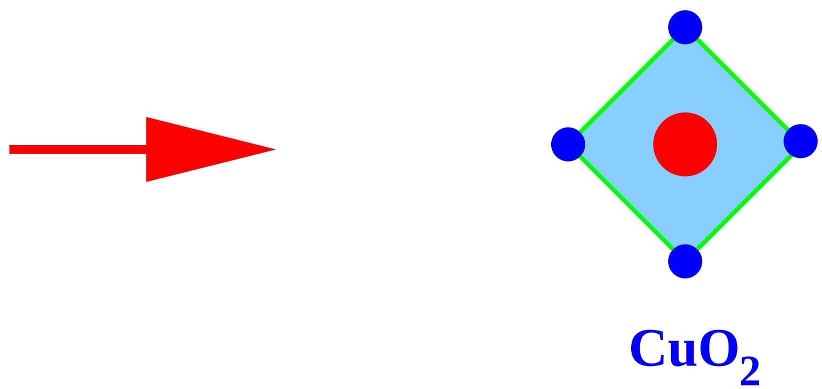

Physical value $J \sim 0.3 - 0.5t$

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- **QMC simulations**

  M. Calandra and S. Sorella, Phys. Rev. B **61**, R11894 (2000)

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Mapping to S-1/2 pseudospins and spinless fermions.

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$$\begin{array}{rcrcl} c^{\dagger}_{i\uparrow}|0>_i & \rightarrow & |v>_i & \leftrightarrow & |0,\Uparrow>_i \ , \\ |0>_i & \rightarrow & f^{\dagger}_i|v>_i & \leftrightarrow & |1,\Uparrow>_i \ , \\ c^{\dagger}_{i\downarrow}|0>_i & \rightarrow & \sigma^{-}_i|v>_i & \leftrightarrow & |0,\Downarrow>_i \ , \\ c^{\dagger}_{i\downarrow}c^{\dagger}_{i\uparrow}|0>_i & \rightarrow & f^{\dagger}_i\sigma^{-}_i|v>_i & \leftrightarrow & |1,\Downarrow>_i \ , \end{array}$$

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c^{\dagger}_{i\downarrow}c^{\dagger}_{i\uparrow}|0>_i &\rightarrow & f^{\dagger}_i\sigma^{-}_i|v>_i &\leftrightarrow |1,\Downarrow>_i \ ,
\end{aligned}$$

$$\Longrightarrow \qquad \boxed{c^{\dagger}_{i\uparrow} = \gamma_{i+}f_i - \gamma_{i-}f^{\dagger}_i\,, \quad c^{\dagger}_{i\downarrow} = \sigma_{i-}(f_i + f^{\dagger}_i)}$$

where $\gamma_{i\pm} = (1 \pm \sigma^z_i)/2$ **and** $\sigma^{\pm}_i = (\sigma^x_i \pm i\sigma^y_i)/2$

t-J model in the new representation

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where $P_{ij} = (1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)/2$**,** $\Delta_{ij} = (1 - n_i - n_j)$ **and** $n_i = f_i^\dagger f_i$**.**

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- **Holonomic constraint:** $\mathcal{Q} \equiv \sum_i (1 - \sigma_{iz}) f_i^\dagger f_i = 0$
- $\left[\mathcal{Q}, \tilde{H}_{t-J}\right] = 0 \Longrightarrow$ **States evolve in the physical subspace**

3.3 Single hole dynamics and loop-algorithm

M. Brunner, F.F. Assaad, and A. Muramatsu, Phys. Rev. B **62**, 15480 (2000)

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$$G_\uparrow(i-j,\tau) = \langle T \tilde{c}_{i\uparrow}(\tau)\tilde{c}^\dagger_{j\uparrow}\rangle = \langle T f^\dagger_i(\tau) f_j\rangle$$

Inserting complete sets of spin states $\longrightarrow$

$$\begin{aligned} - \quad G(i-j,-\tau) &= \frac{\sum_{\sigma_1}\langle v| \otimes \langle \sigma_1| e^{-(\beta-\tau)\tilde{H}_{t-J}} f_j e^{-\tau \tilde{H}_{t-J}} f^\dagger_i |\sigma_1\rangle \otimes |v\rangle}{\sum_{\sigma_1}\langle \sigma_1| e^{-\beta \tilde{H}_{t-J}} |\sigma_1\rangle} \\ &= \sum_{\boldsymbol{\sigma}} P(\boldsymbol{\sigma}) \frac{\langle v| f_j e^{-\Delta\tau \tilde{H}(\sigma_n,\sigma_{n-1})} e^{-\Delta\tau \tilde{H}(\sigma_{n-1},\sigma_{n-2})} \dots e^{-\Delta\tau \tilde{H}(\sigma_2,\sigma_1)} f^\dagger_i |v\rangle}{\langle \sigma_n| e^{-\Delta\tau \tilde{H}_{t-J}} |\sigma_{n-1}\rangle \dots \langle \sigma_2 e^{-\Delta\tau \tilde{H}_{t-J}} |\sigma_1\rangle} \\ &= \sum_{\boldsymbol{\sigma}} P(\boldsymbol{\sigma}) G(i,j,\tau,\boldsymbol{\sigma}) + \mathcal{O}(\Delta\tau^2) \end{aligned}$$

- $P(\boldsymbol{\sigma})$: **probability distribution of a Heisenberg antiferromagnet.**
  $\Longrightarrow$ **Sum over spins** $\longrightarrow$ **world-line loop-algorithm.**

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- Accurate determination of the quasiparticle weight

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One-particle spectral function and the Green's function in imaginary time

$$G(\boldsymbol{k}, \tau) = \int_{-\infty}^{\infty} d\omega \, \frac{\mathrm{e}^{-\omega\tau}}{1 + \mathrm{e}^{-\beta\omega}} \, A(\boldsymbol{k}, \omega)$$

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Need very accurate data and consistency checks

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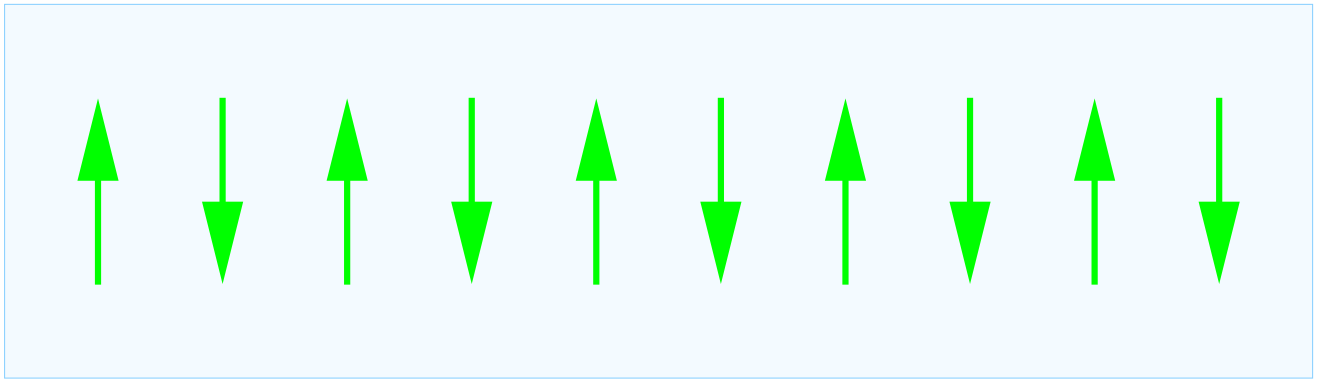

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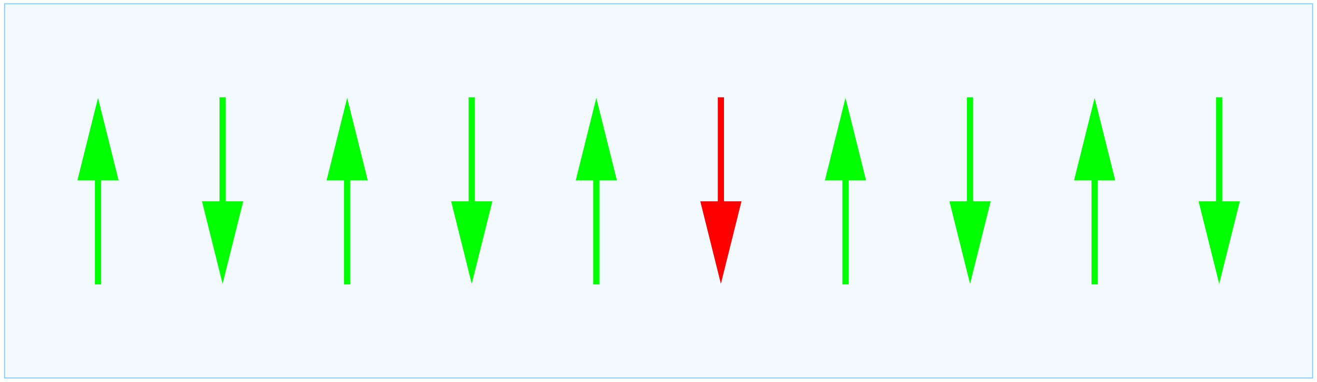

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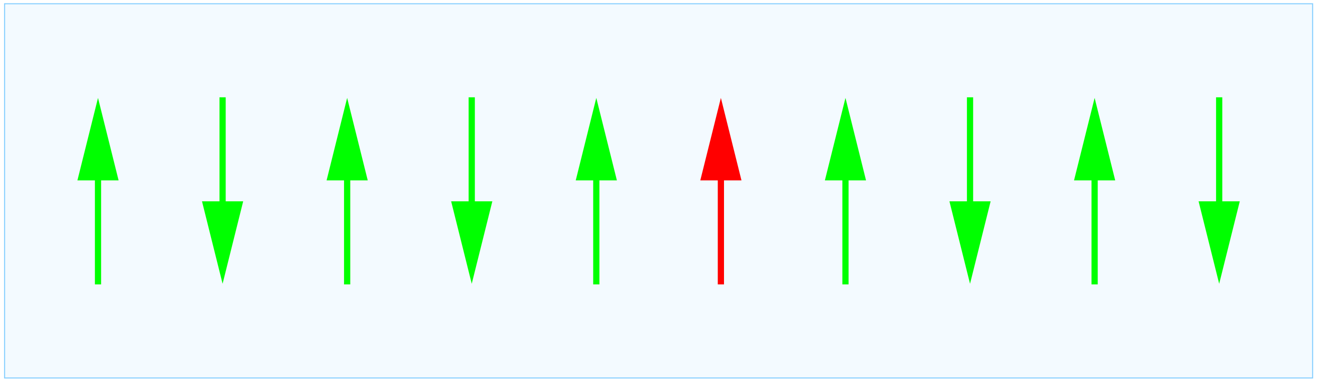

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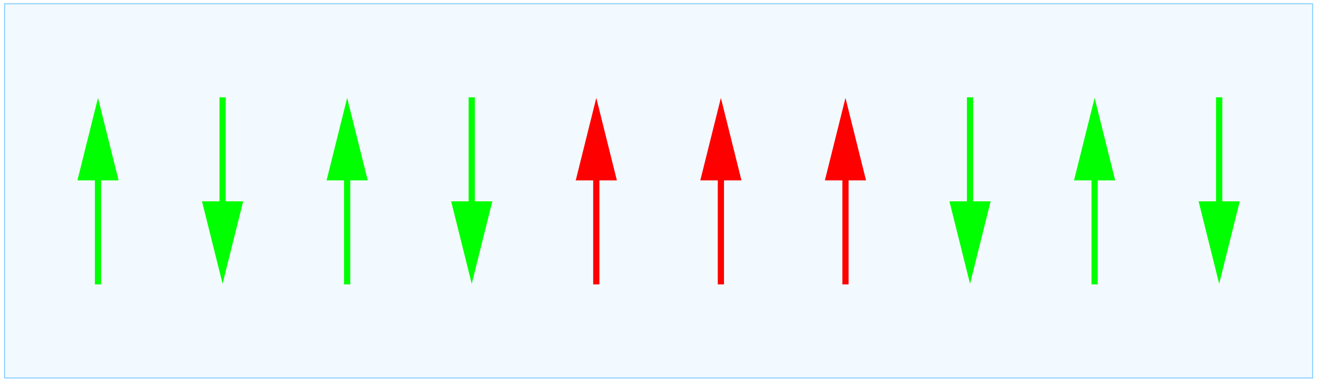

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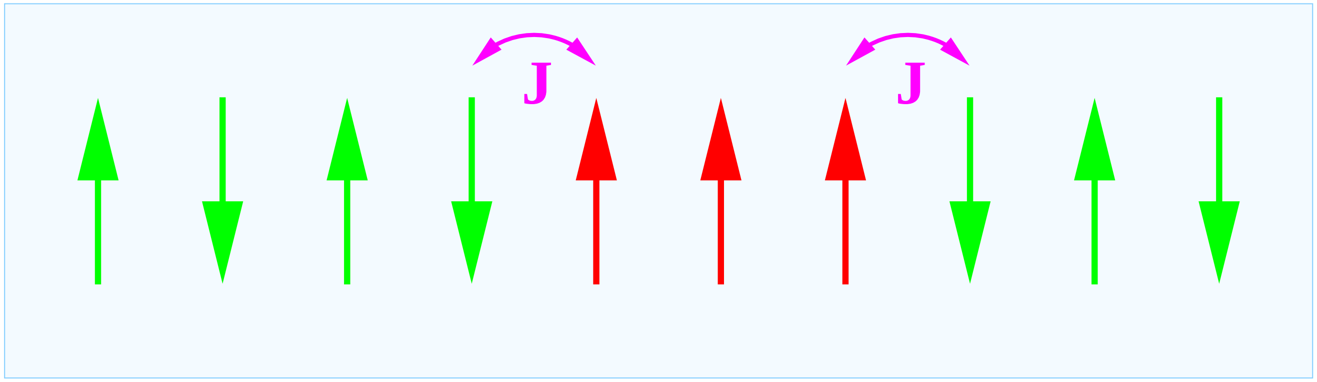

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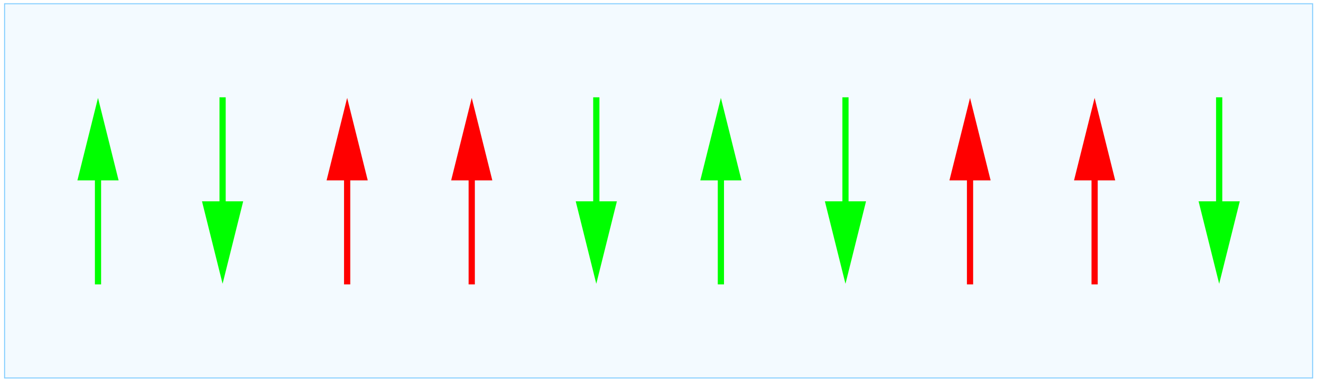

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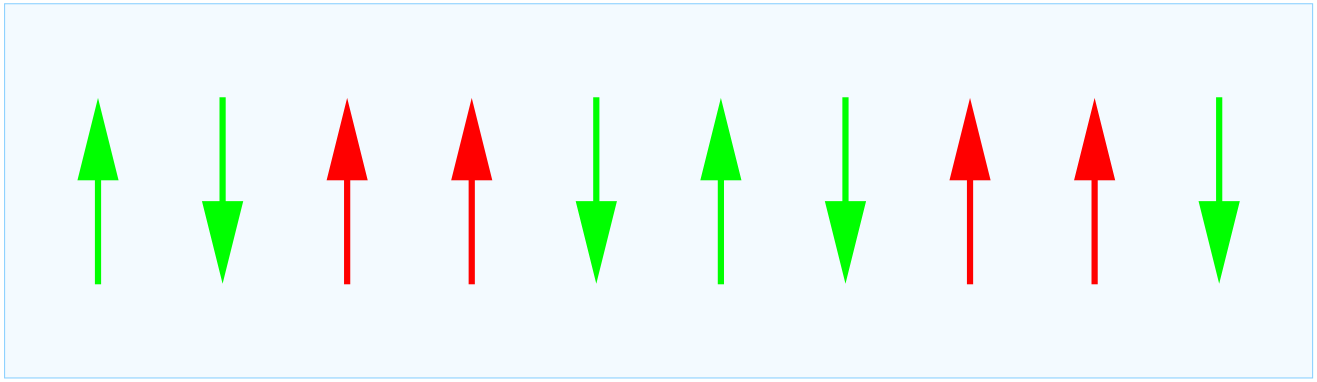

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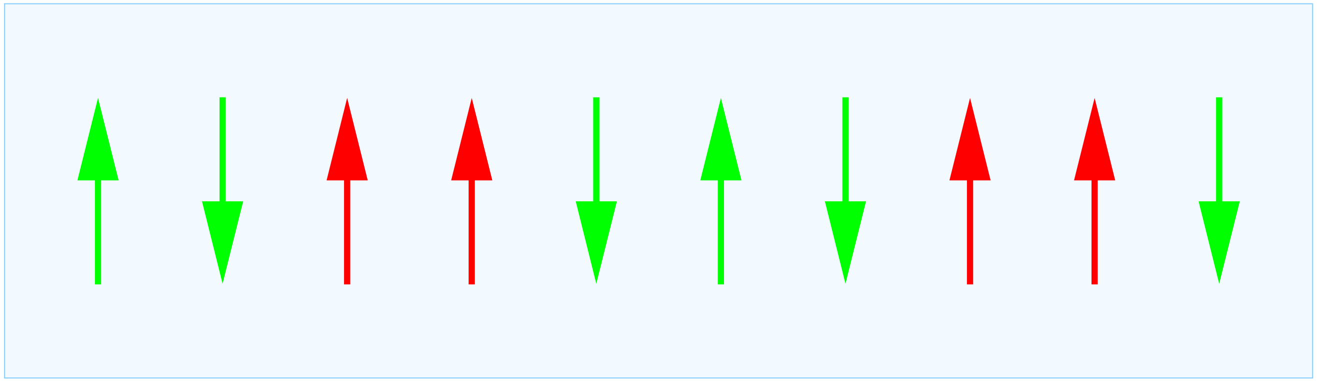

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Spinons as free excitations

$$H_H = J \sum_{<i,j>} \boldsymbol{S}_i \cdot \boldsymbol{S}_j = -\frac{J}{2} \sum_{\substack{<i,j> \\ \alpha,\beta}} c^\dagger_{i\alpha} c_{j\alpha} c^\dagger_{i\beta} c_{j\beta}$$

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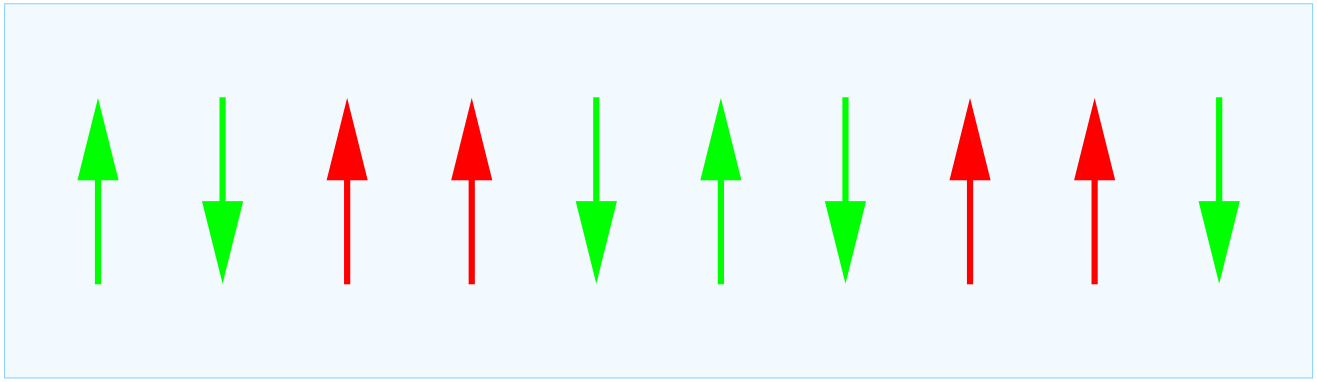

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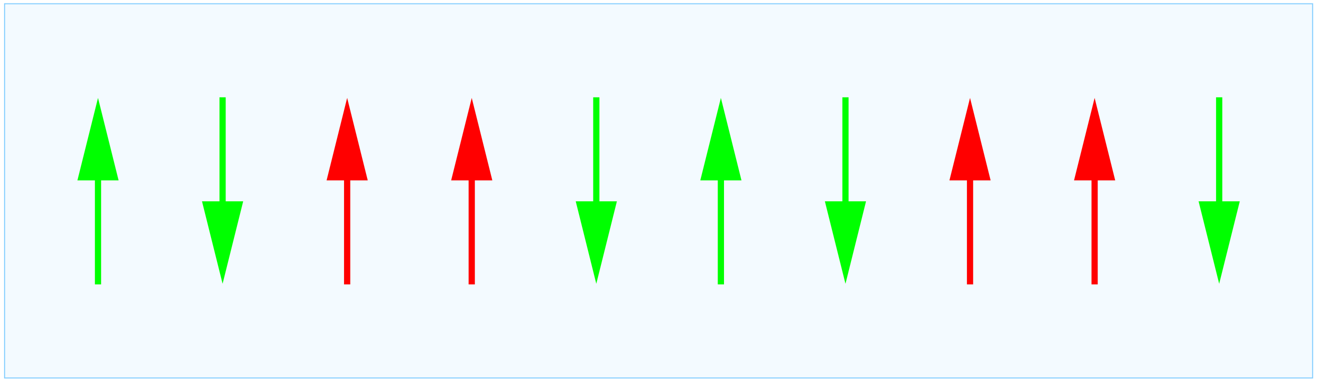

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$$= \sum_k \epsilon_s(k)\, c^\dagger_{k\alpha} c_{k\alpha} \qquad \text{with} \quad \epsilon_s(k) = -J < c^\dagger_i c_j > \cos ka$$

Two-spinon excitations in the one-dimensional Heisenberg model

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Magnon as a composite excitation

$$E_M(Q_M) = \epsilon_s(q_1) + \epsilon_s(q_2) \; , \qquad Q_M = q_1 + q_2 + \pi$$

with

$$\epsilon_s(q) = J \cos qa \; , \qquad -\frac{\pi}{2} \leq q \leq \frac{\pi}{2}$$

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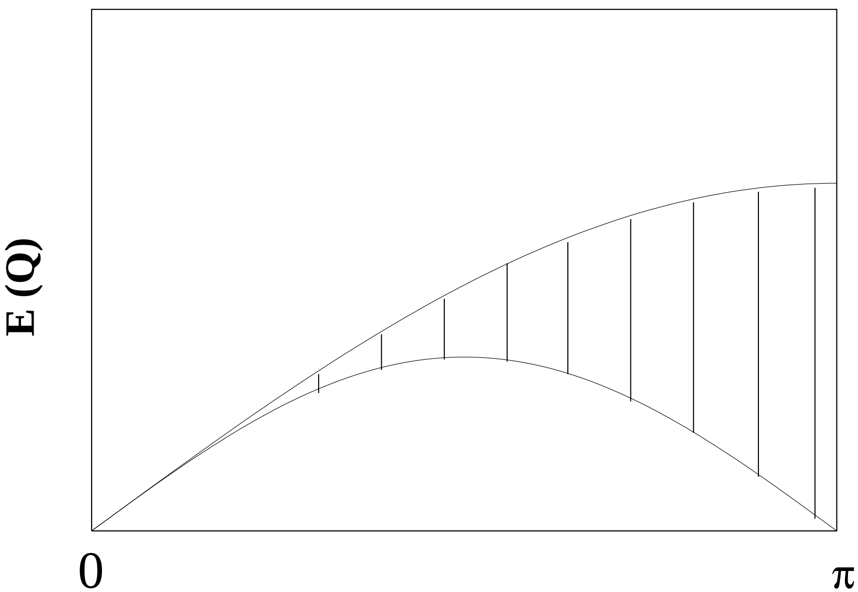

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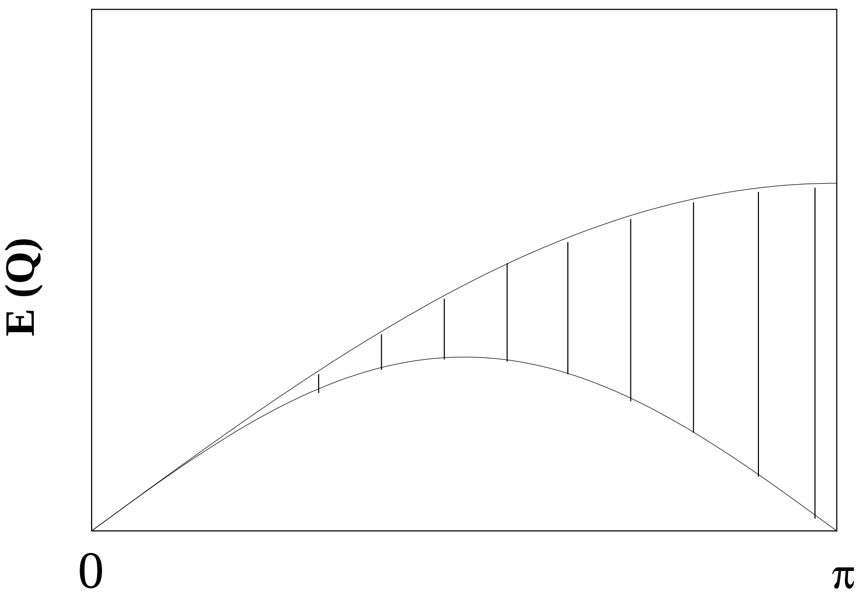

$$E_M^{max} = J\sqrt{2\,(1-\cos Q)}$$

$$E_M^{min} = J \sin Q$$

3.4.2 Charge-spin separation in a doped AF chain: spinons + holons

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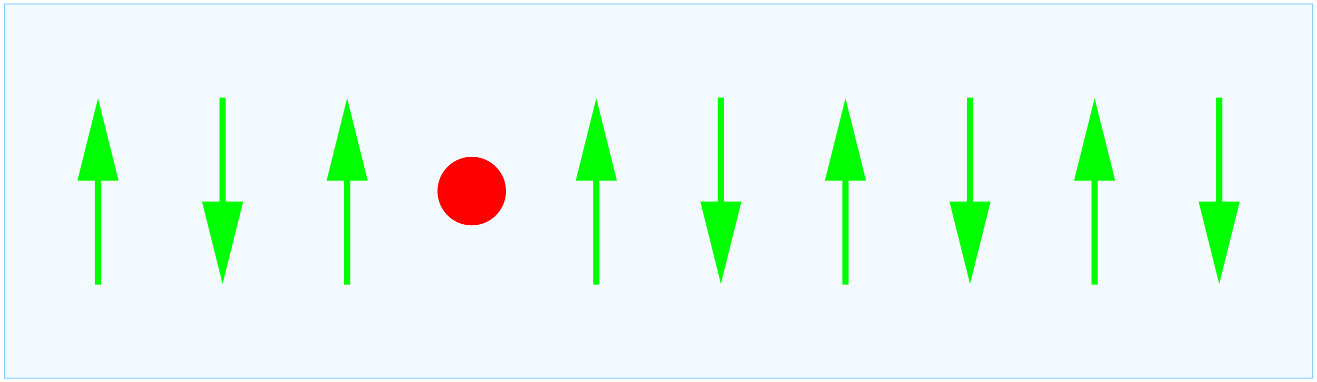

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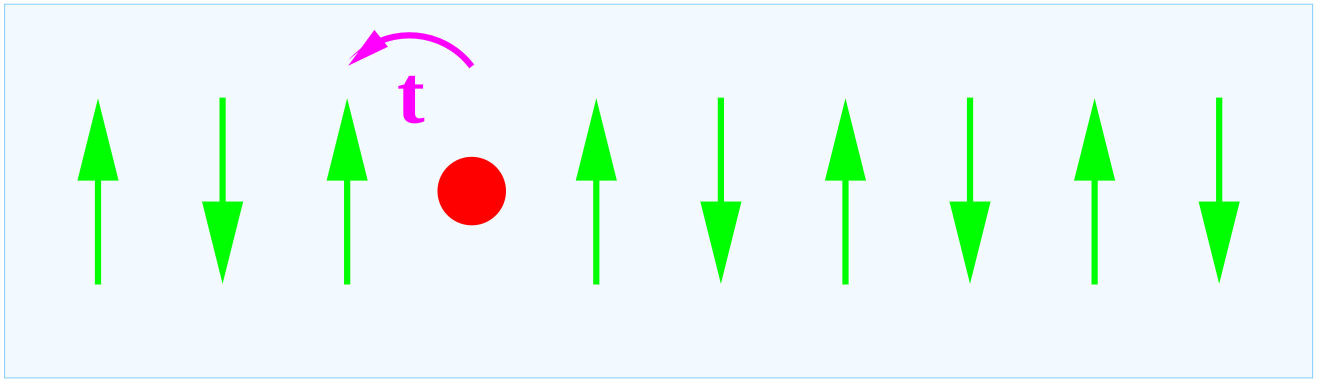

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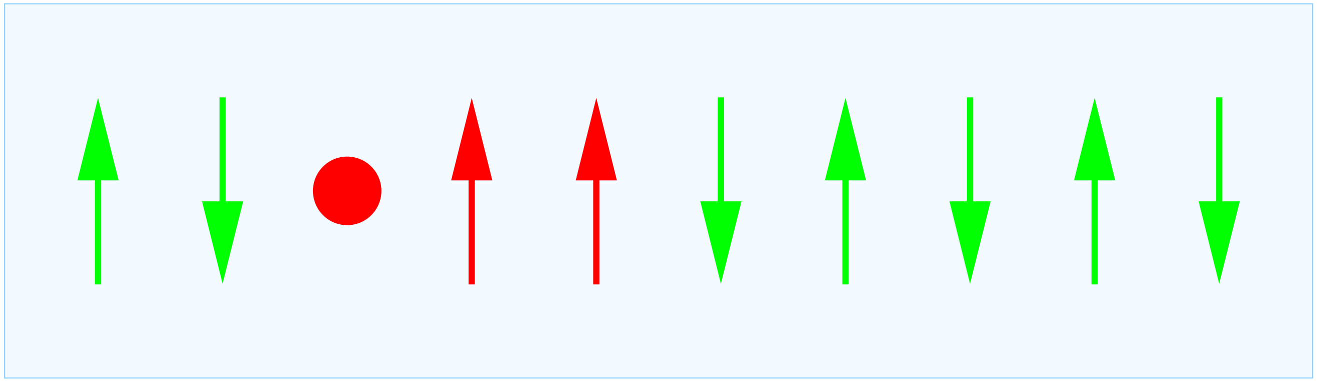

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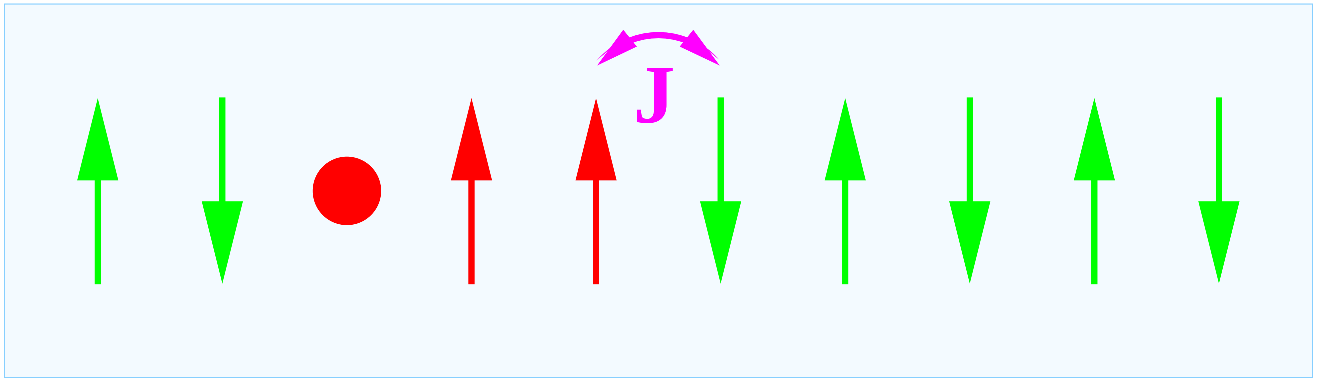

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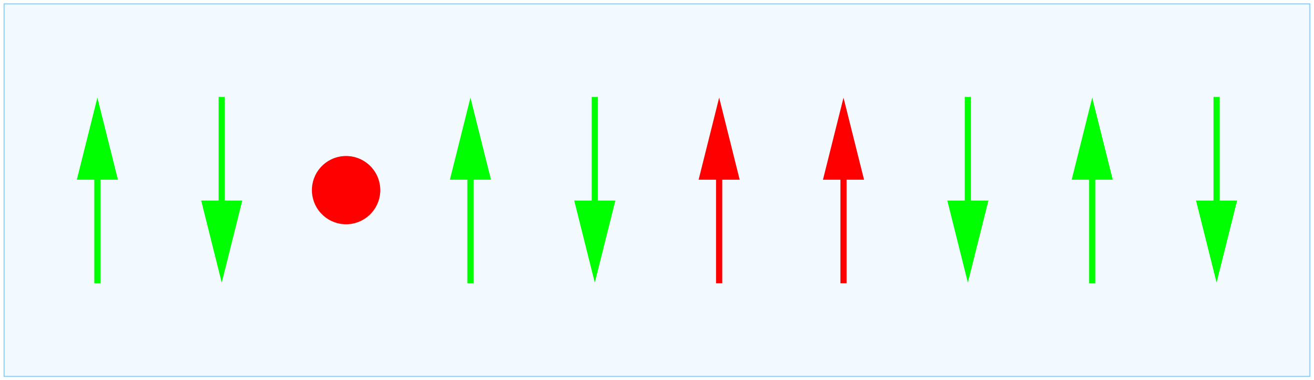

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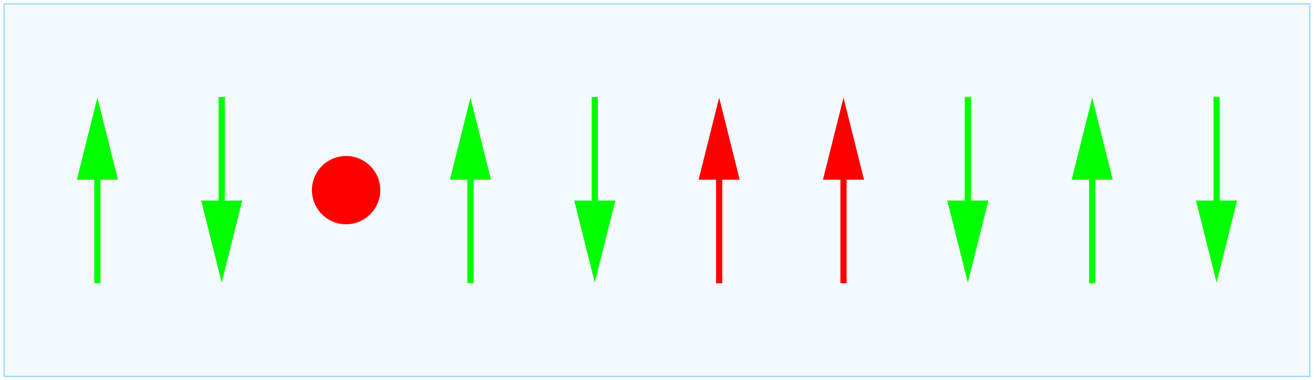

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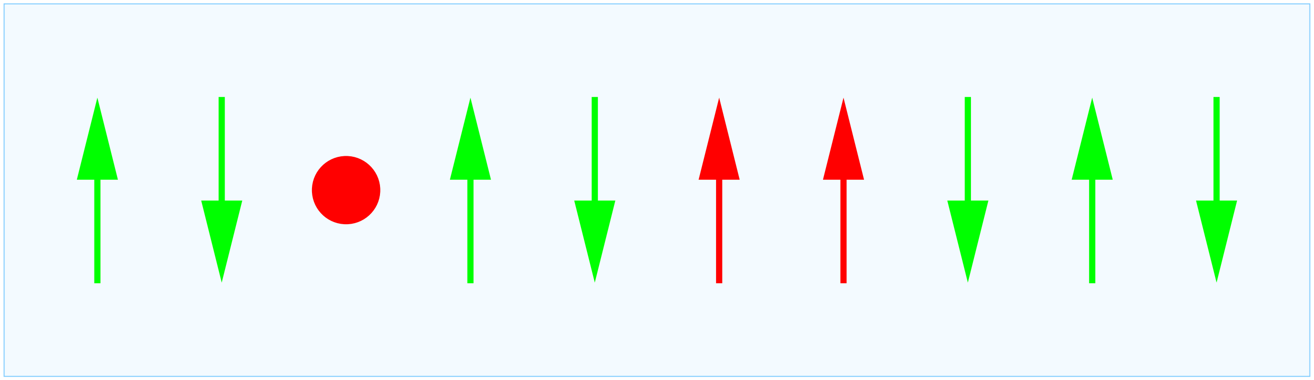

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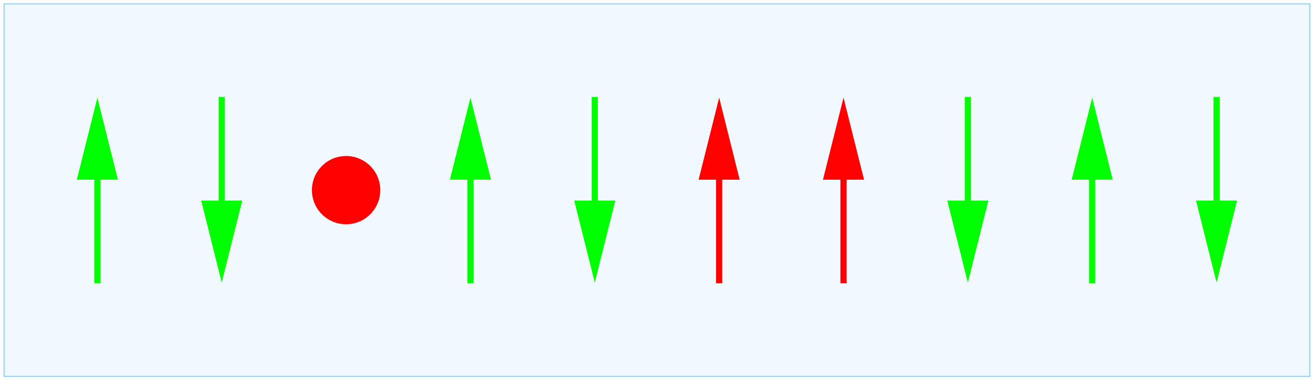

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holon: $\epsilon_h = -2t \cos q_h$

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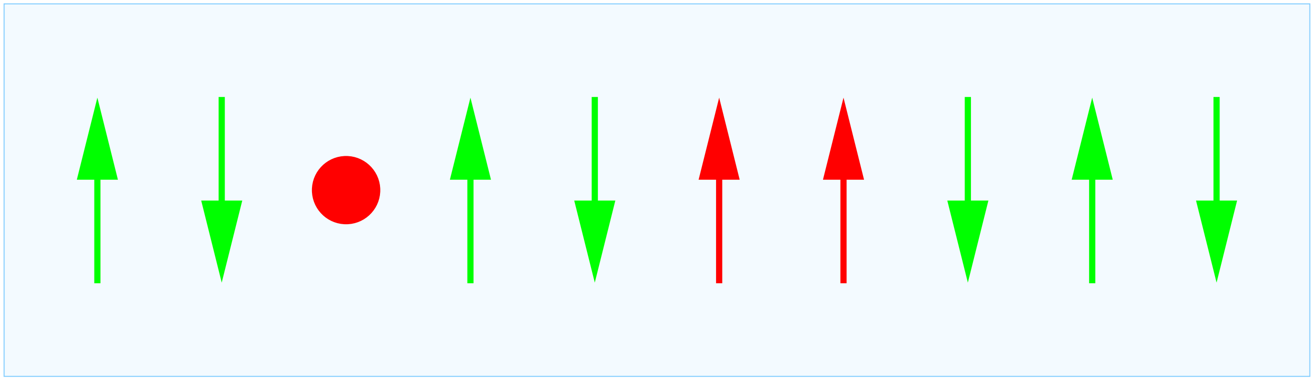

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Energy and momenta of a hole

$$E(k) = \epsilon_h(q_h) - \epsilon_s(q_s) \ , \quad \textbf{with} \quad k = q_h - q_s$$

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Spectral function from QMC simulations

M. Brunner, F.F. Assaad, and A. Muramatsu, Eur. Phys. J. B **16**, 209 (2000)

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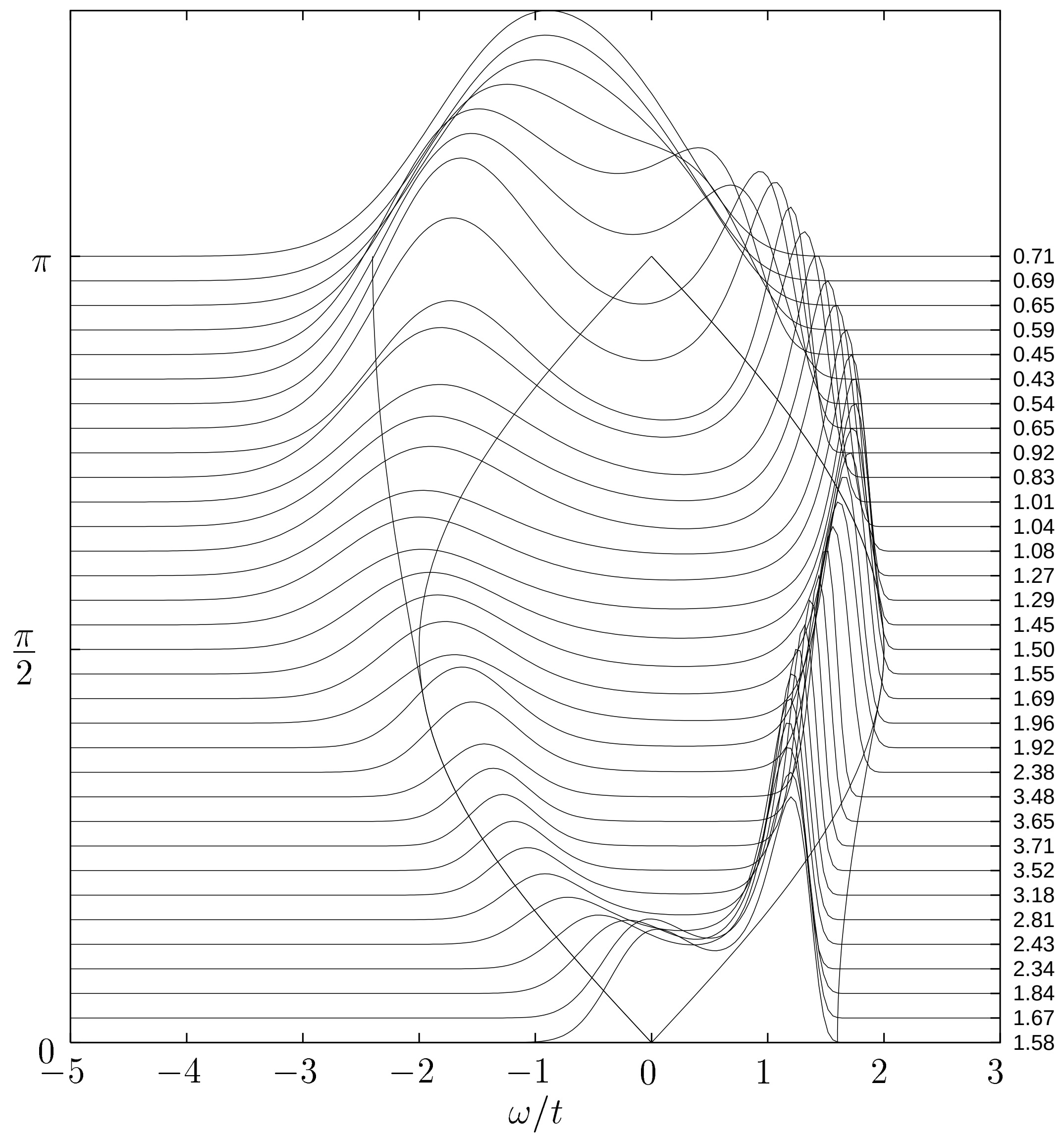
N = 64 **J = 0.4 t**



Full lines: compact support

At the supersymmetric point

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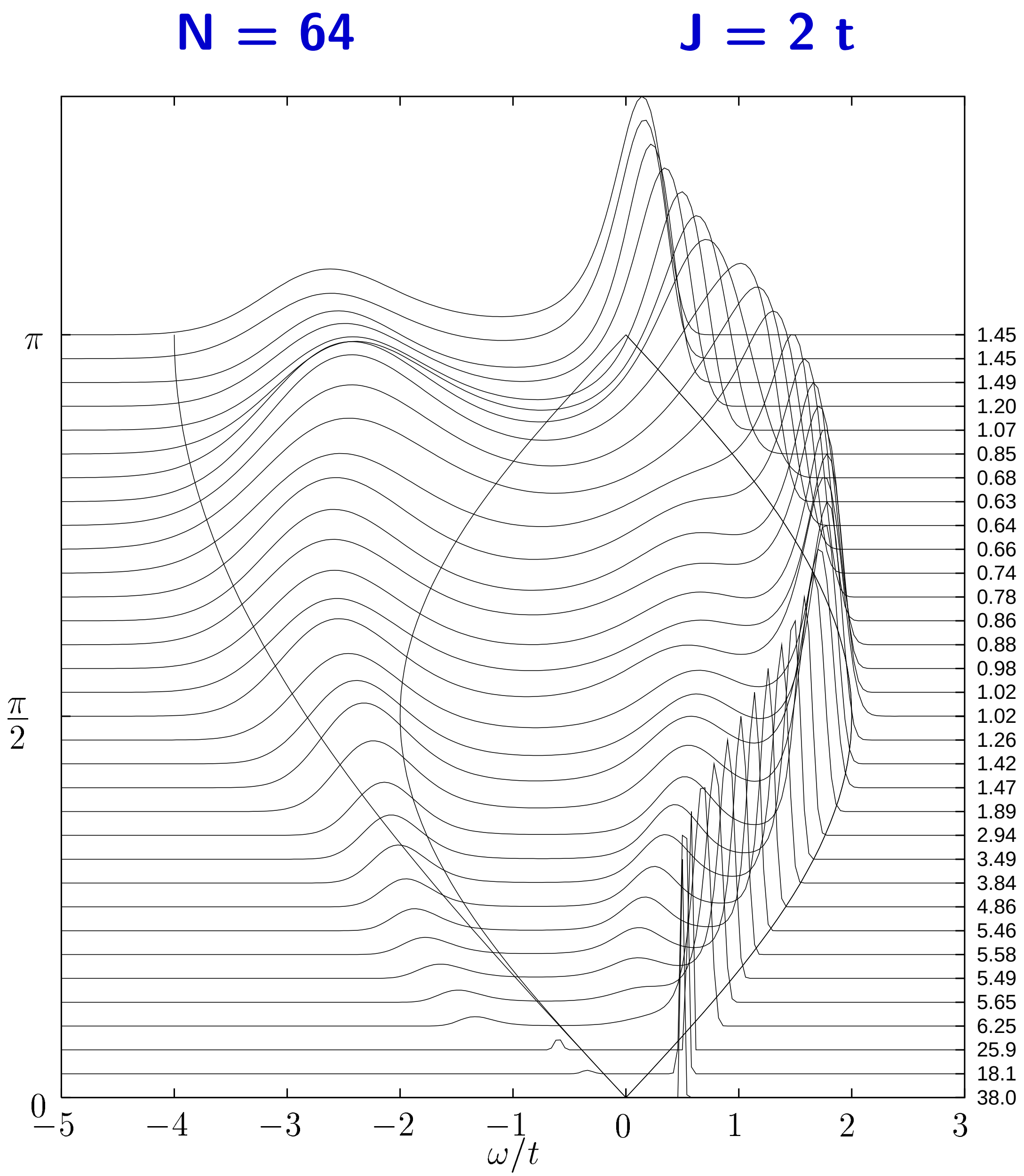

At $k = 0$ all the weight is concentrated on one point

Quasiparticle weight

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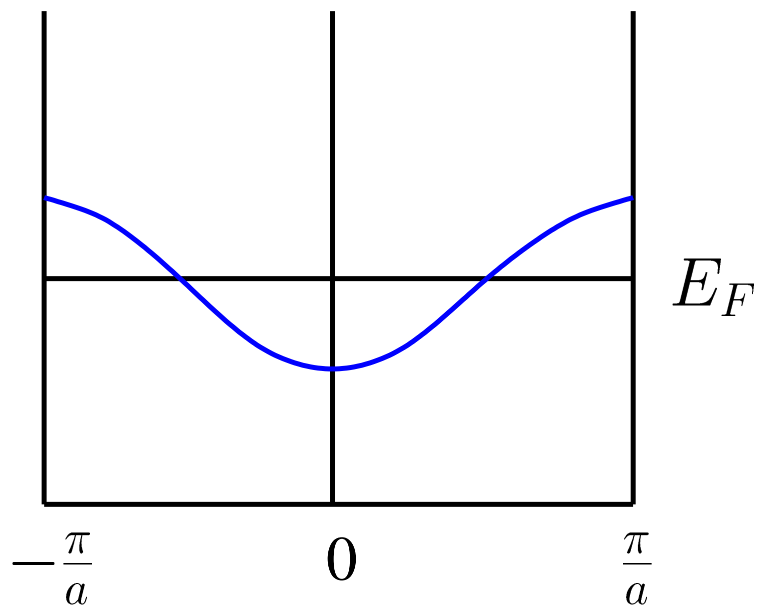
Non-interacting fermions



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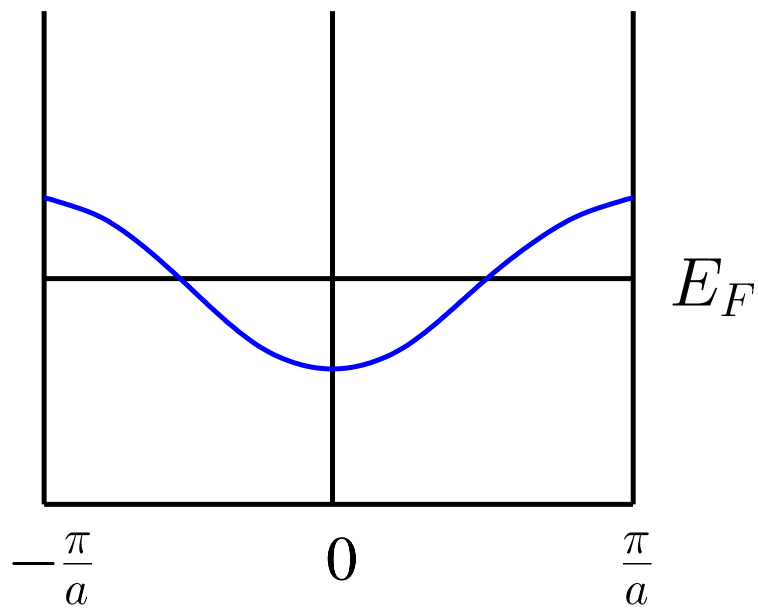
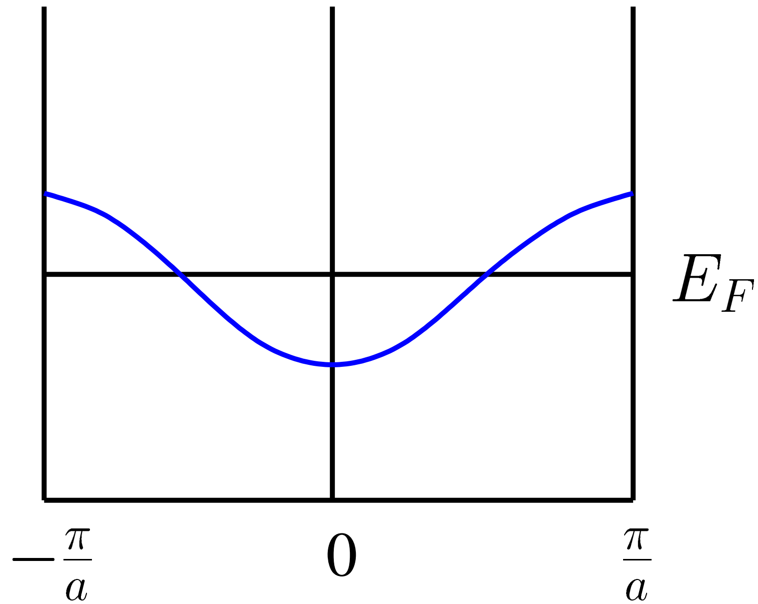


Green's function

$$G(\boldsymbol{k},\omega) \quad = \quad \left[\frac{\theta(k-k_F)}{\omega-\mu-\epsilon_{\boldsymbol{k}}+i\eta}+\frac{\theta(k_F-k)}{\omega-\mu+\epsilon_{\boldsymbol{k}}-i\eta}\right]$$

Quasiparticle weight

Non-interacting fermions



Green's function

$$G(\boldsymbol{k},\omega) = \left[\frac{\theta(k-k_F)}{\omega-\mu-\epsilon_{\boldsymbol{k}}+i\eta}+\frac{\theta(k_F-k)}{\omega-\mu+\epsilon_{\boldsymbol{k}}-i\eta}\right]$$

Quasiparticle weight $z(\boldsymbol{k}) = 1$

Interacting fermions

Interacting fermions

Formal solution

$$G = \left[G^{(0)^{-1}} - \Sigma^* \right]^{-1}$$

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For a homogeneous system or a lattice model

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Renormalized energies due to interaction

$$\epsilon_{\boldsymbol{k}} = \epsilon^0_{\boldsymbol{k}} + \mathrm{Re}\tilde{\Sigma}(\boldsymbol{k}, \omega)$$

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Lifetime due to interaction

$$G(\boldsymbol{k}, \omega) = \frac{z(\boldsymbol{k})}{\hbar\omega - \mu - \epsilon_{\boldsymbol{k}} + i\Gamma} + G_{inc}$$

Coherent and incoherent parts of the propagator

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$$G_c(\boldsymbol{k}, \omega) = \frac{z(\boldsymbol{k})}{\omega - \mu - \epsilon_{\boldsymbol{k}} + i\Gamma}$$

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Coherently propagating particle for times $t < 1/\Gamma$

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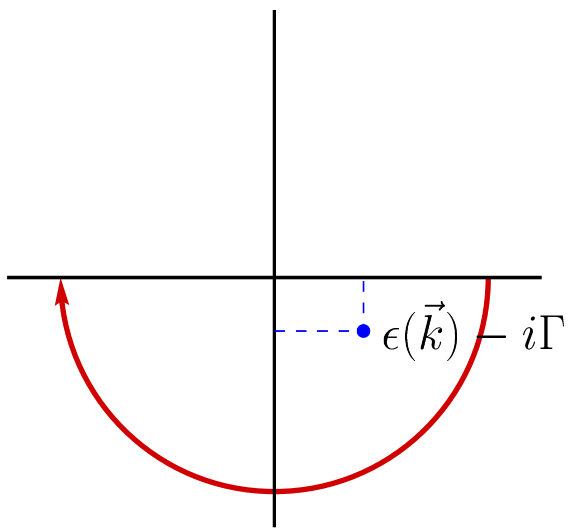

Quasiparticle weight from QMC simulations

Quasiparticle weight from QMC simulations

In imaginary time

$$\lim_{\tau \to \infty} G(k,\tau) \propto z(k) \exp\left[\tau\left(E_0^N - E_0^{N-1}(k)\right)\right]$$

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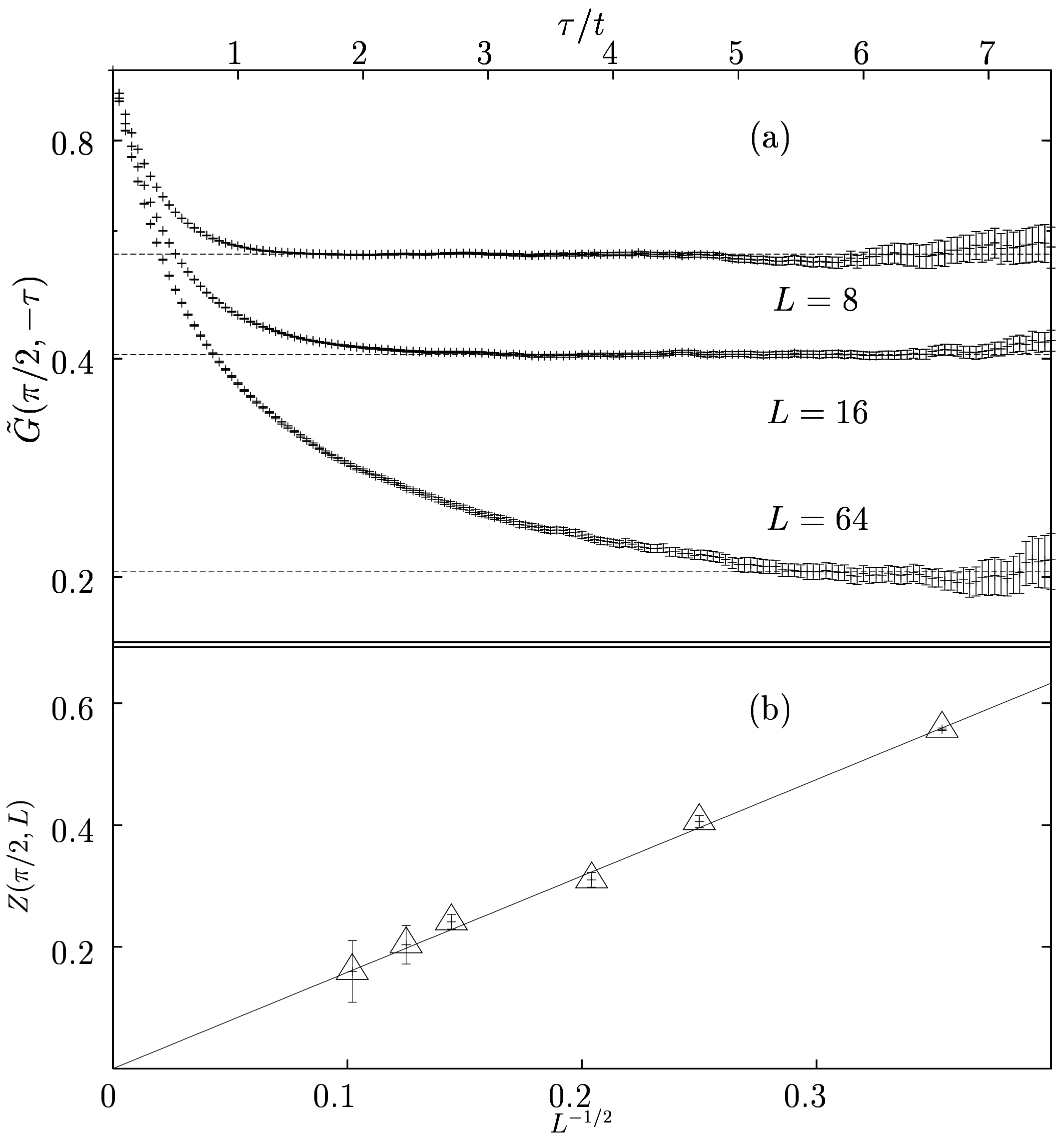


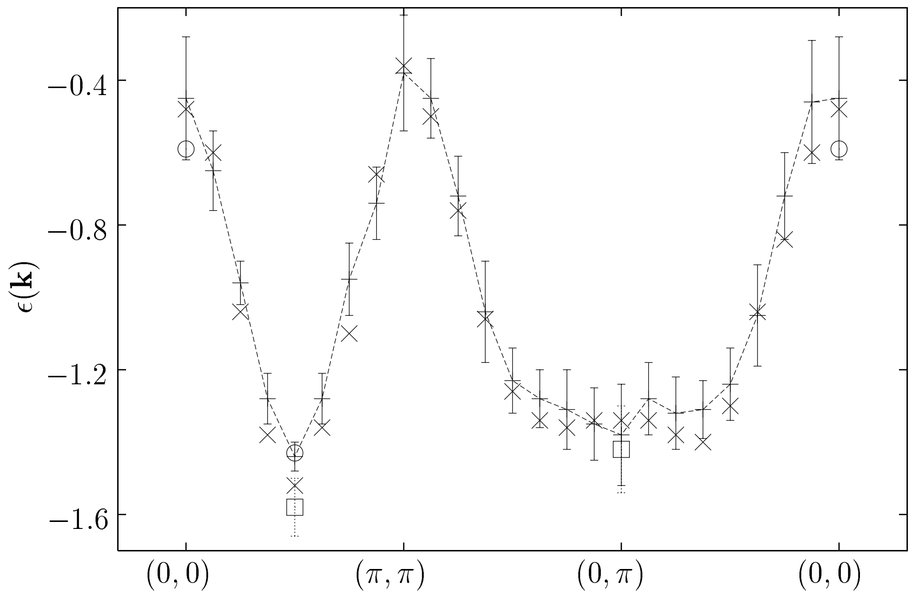
3.5 Single hole dynamics in 2-D

M. Brunner, F.F. Assaad, and A. Muramatsu, Phys. Rev. B **62**, 15480 (2000)

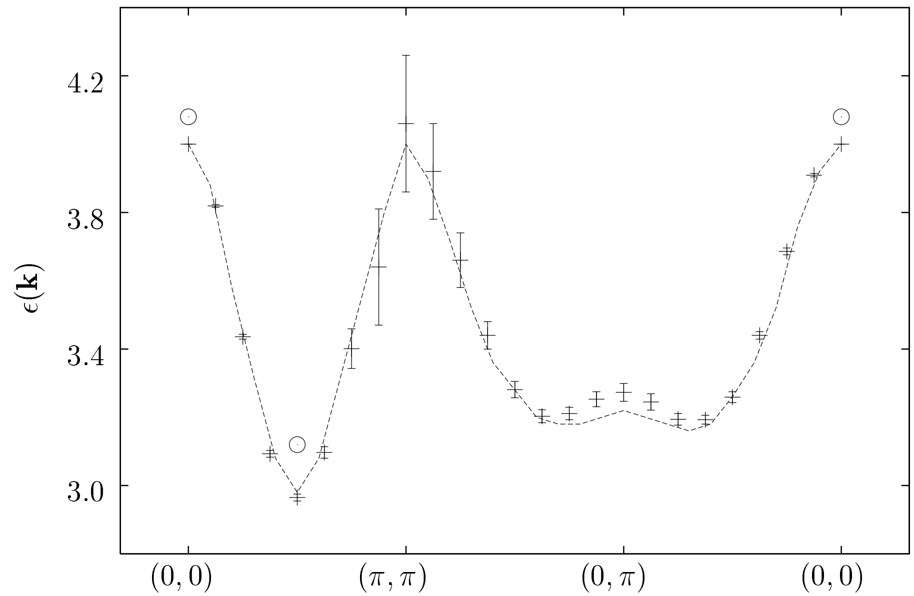
Quasiparticle dispersion for the square lattice

$$\lim_{\tau \to \infty} G(\boldsymbol{k}, \tau) \propto z(\boldsymbol{k}) \exp\left[\tau \left(E_0^N - E_0^{N-1}(\boldsymbol{k})\right)\right]$$

N = 16 × 16



J = 0.4 t

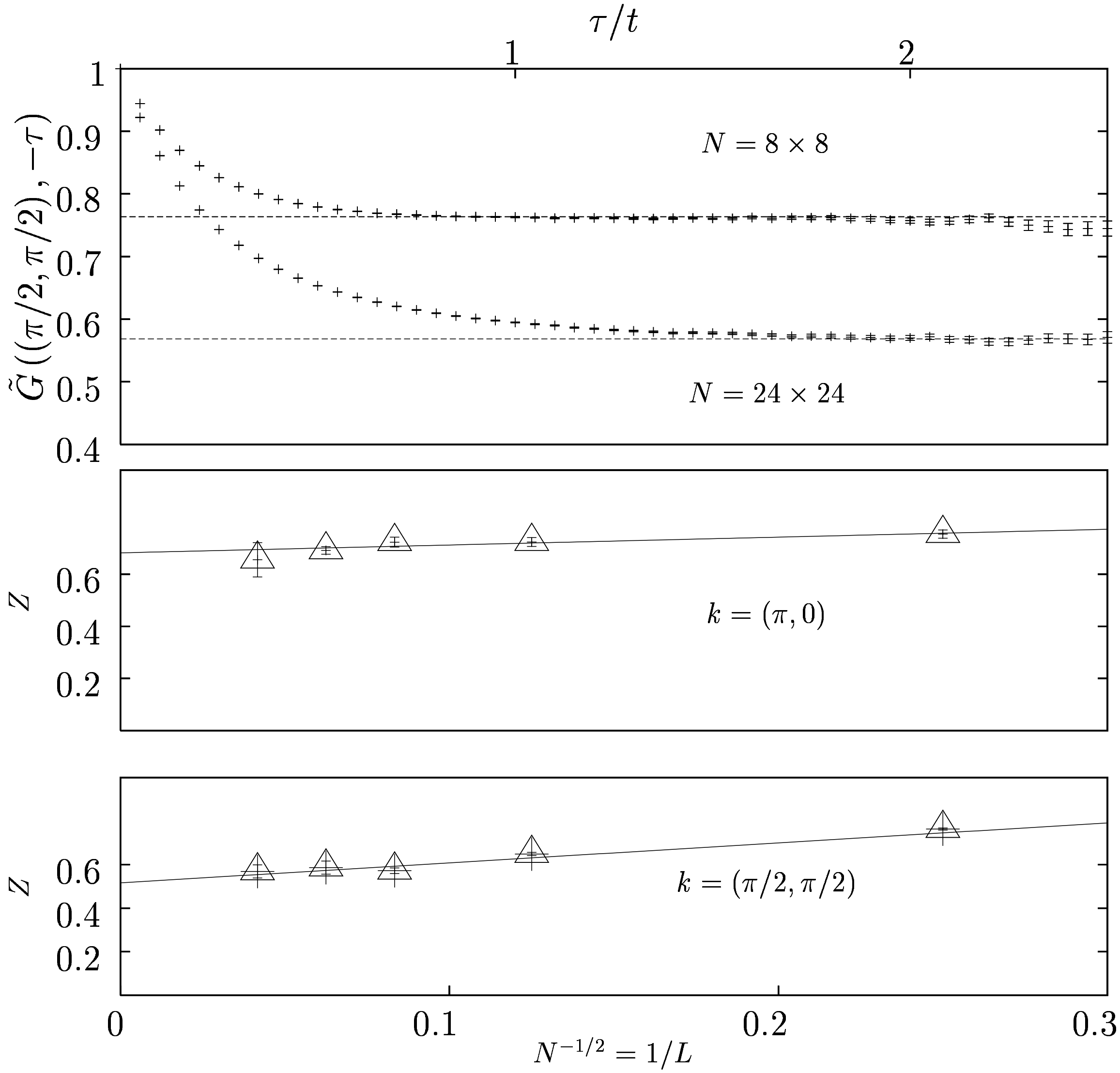


J = 2 t

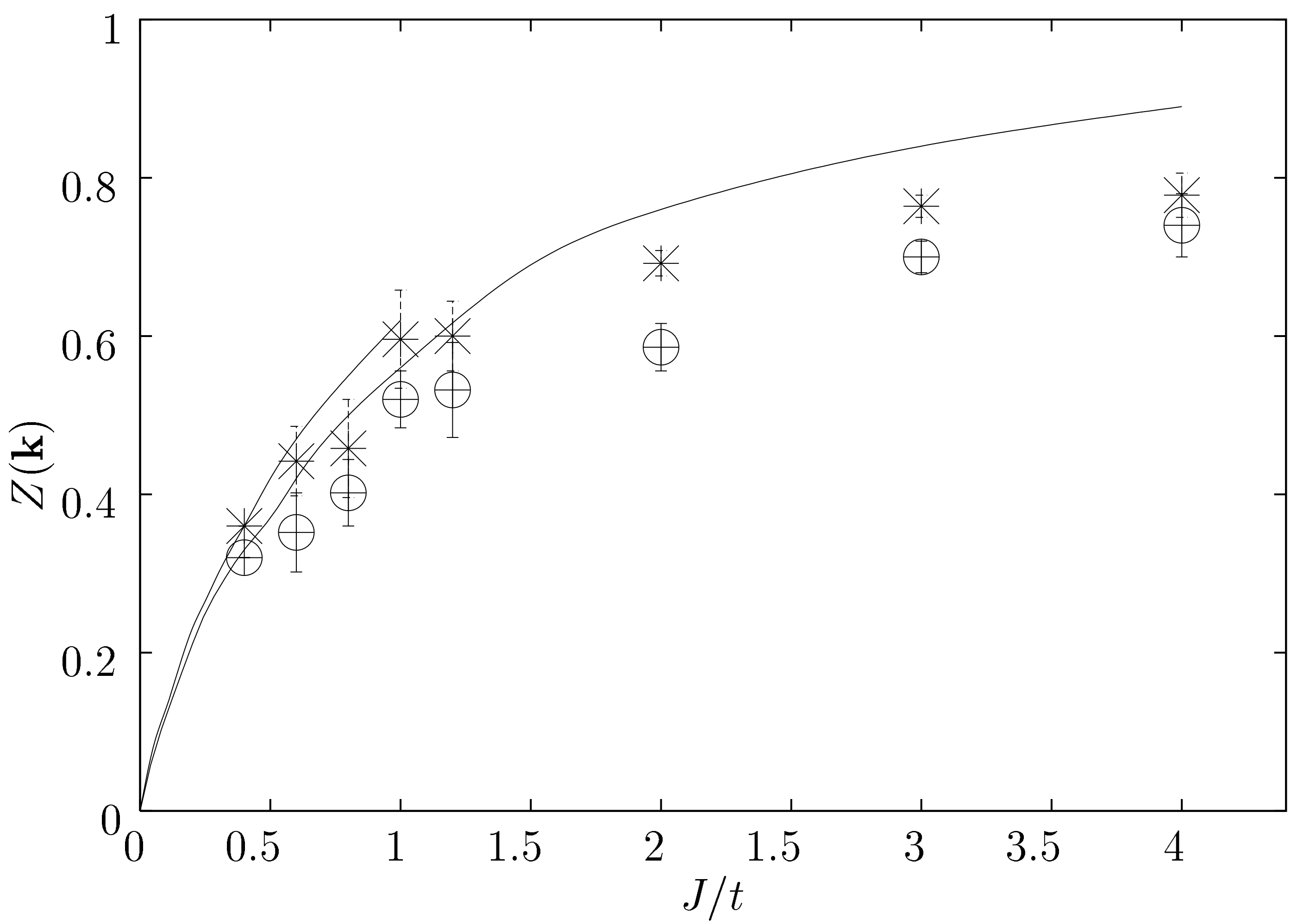
Quasiparticle weight for a hole in the square lattice

Finite quasiparticle weight in 2-dimensions

J = 2t



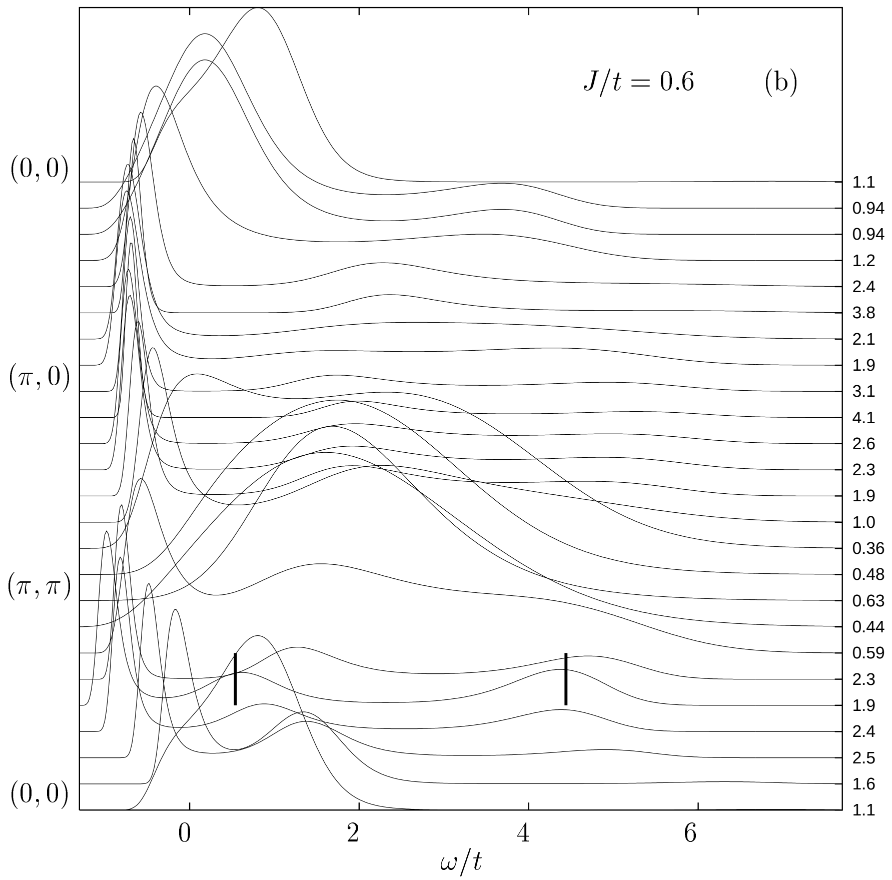
Quasiparticle weight vs. J in the thermodynamic limit



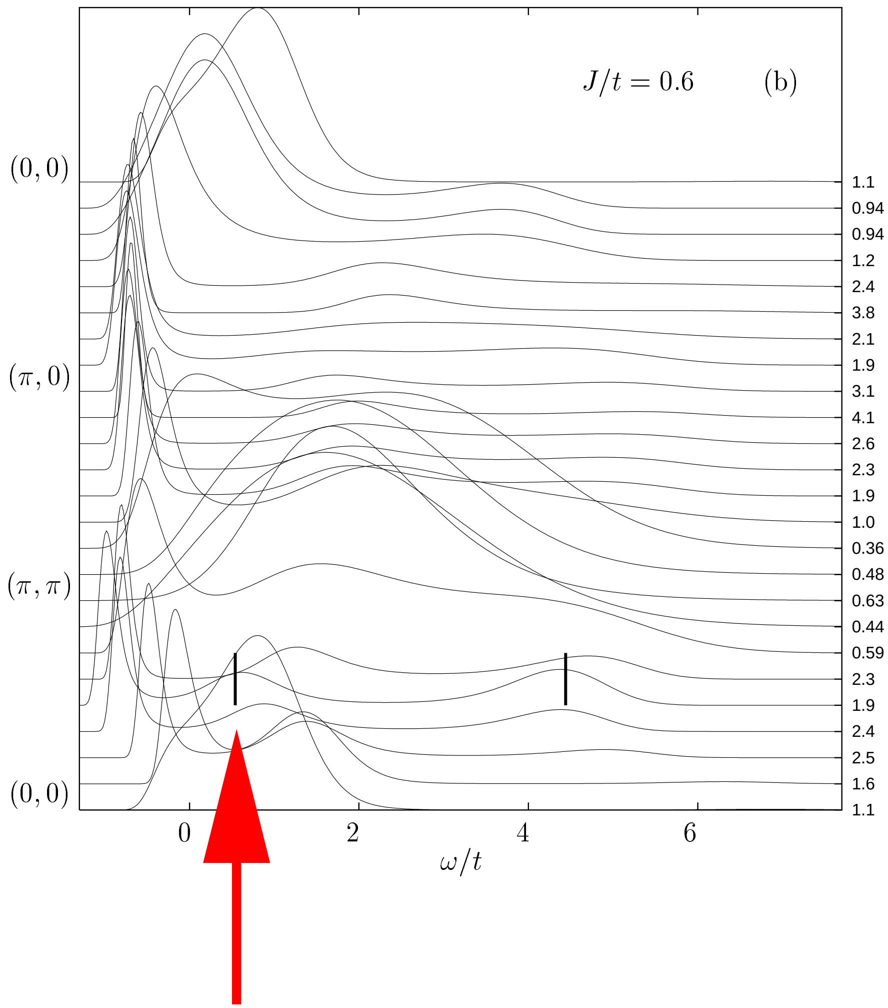
Full lines: **Self-consistent Born approximation**

G. Martínez and P. Horsch, Phys. Rev. **44**, 317 (1991)

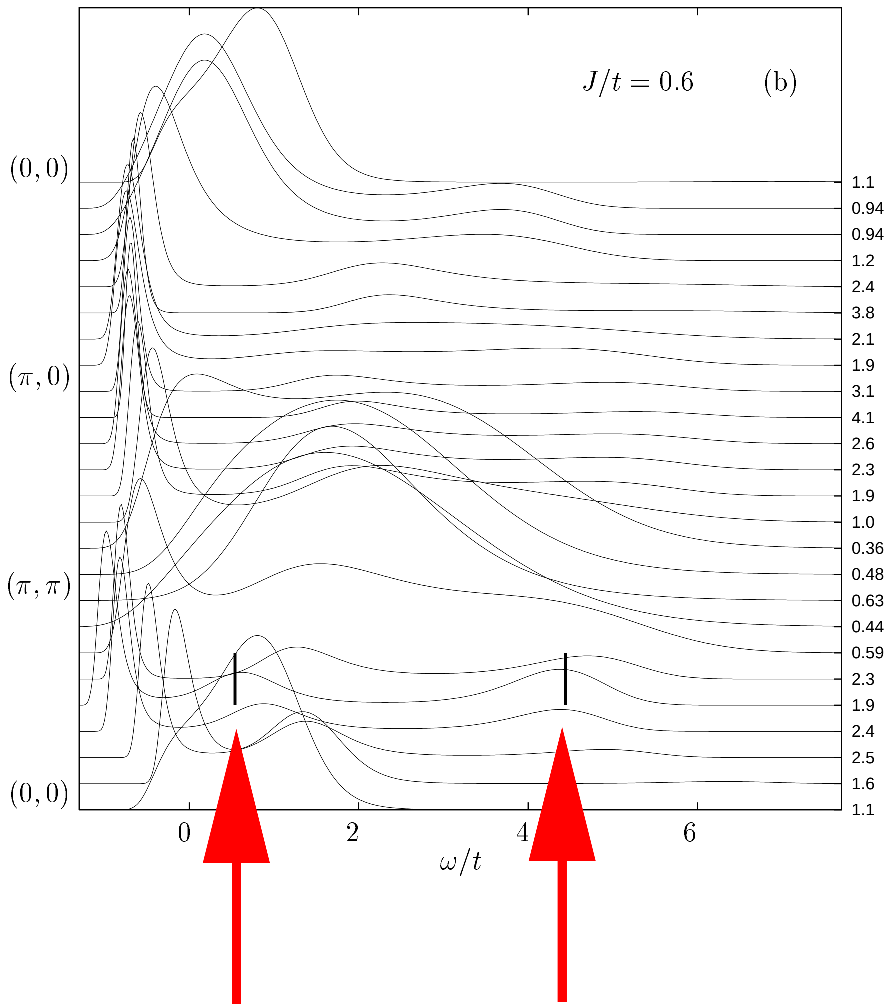
Resonances in the spectrum



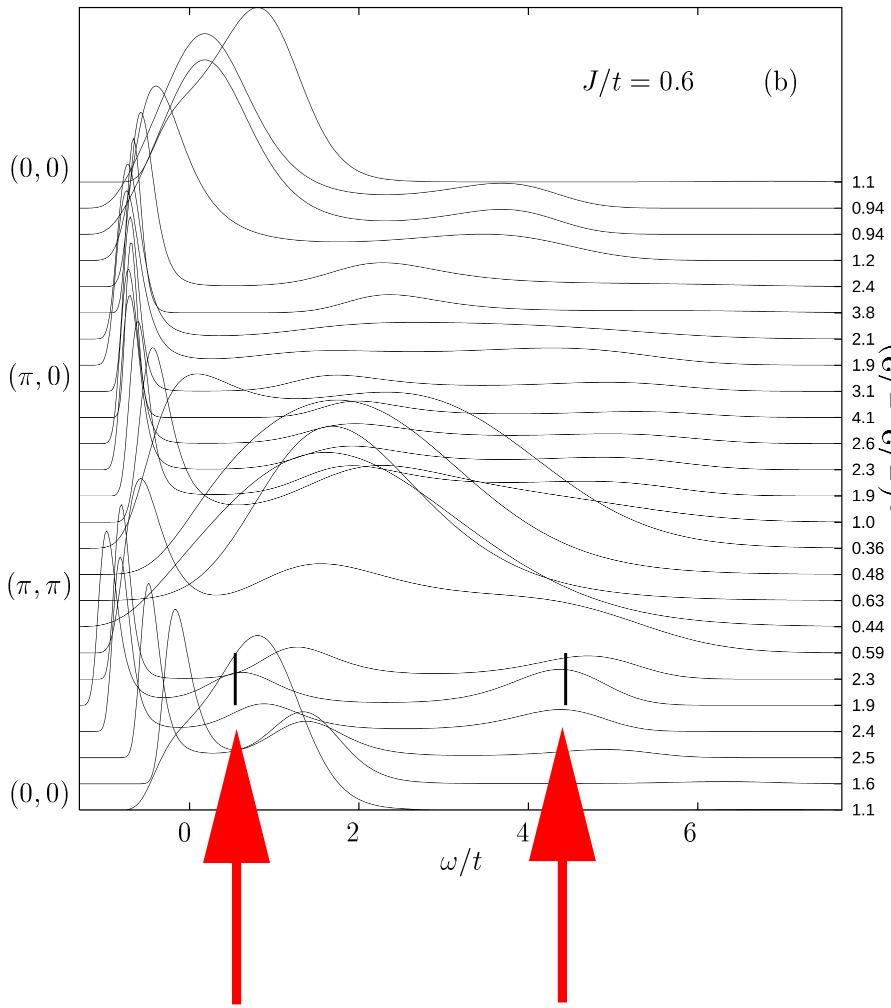
Resonances in the spectrum

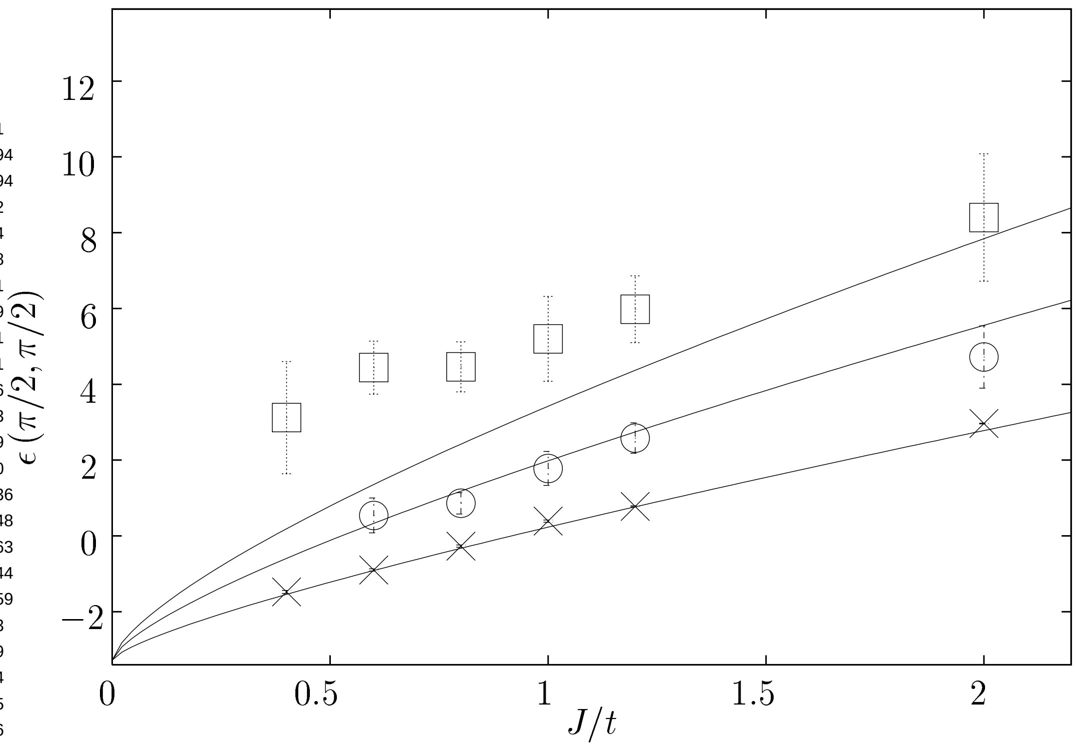


Resonances in the spectrum



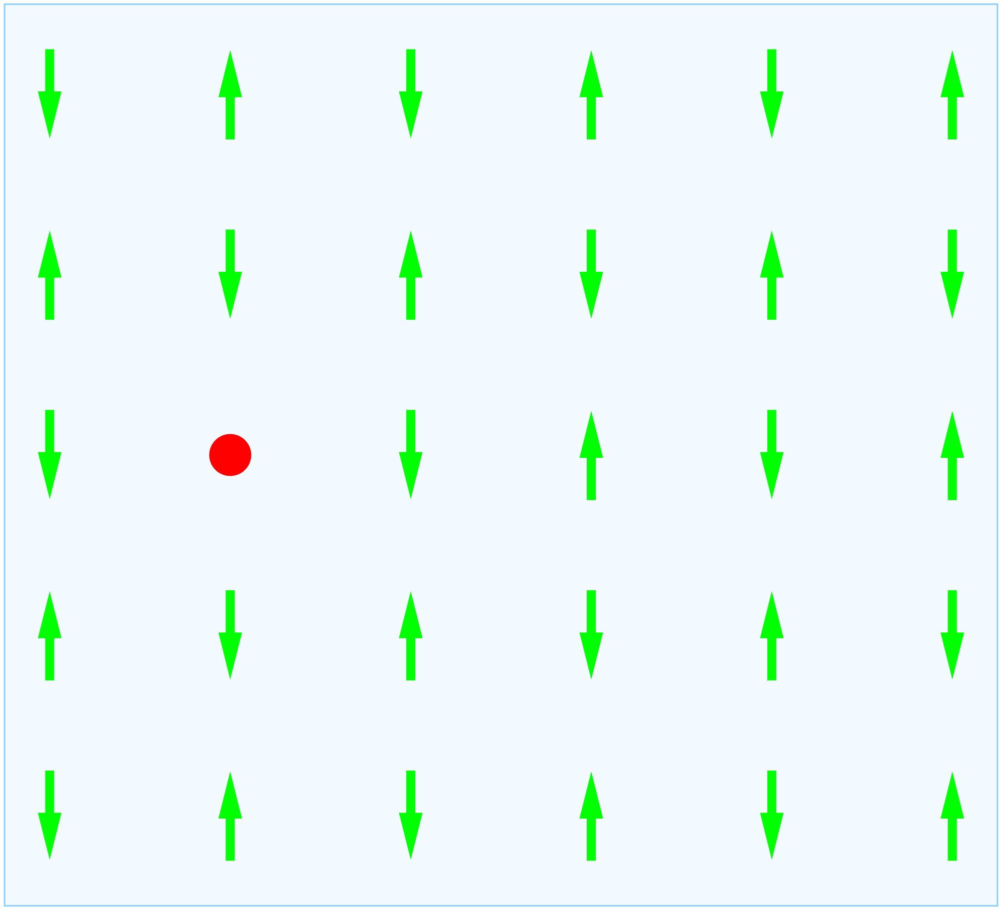
Resonances in the spectrum



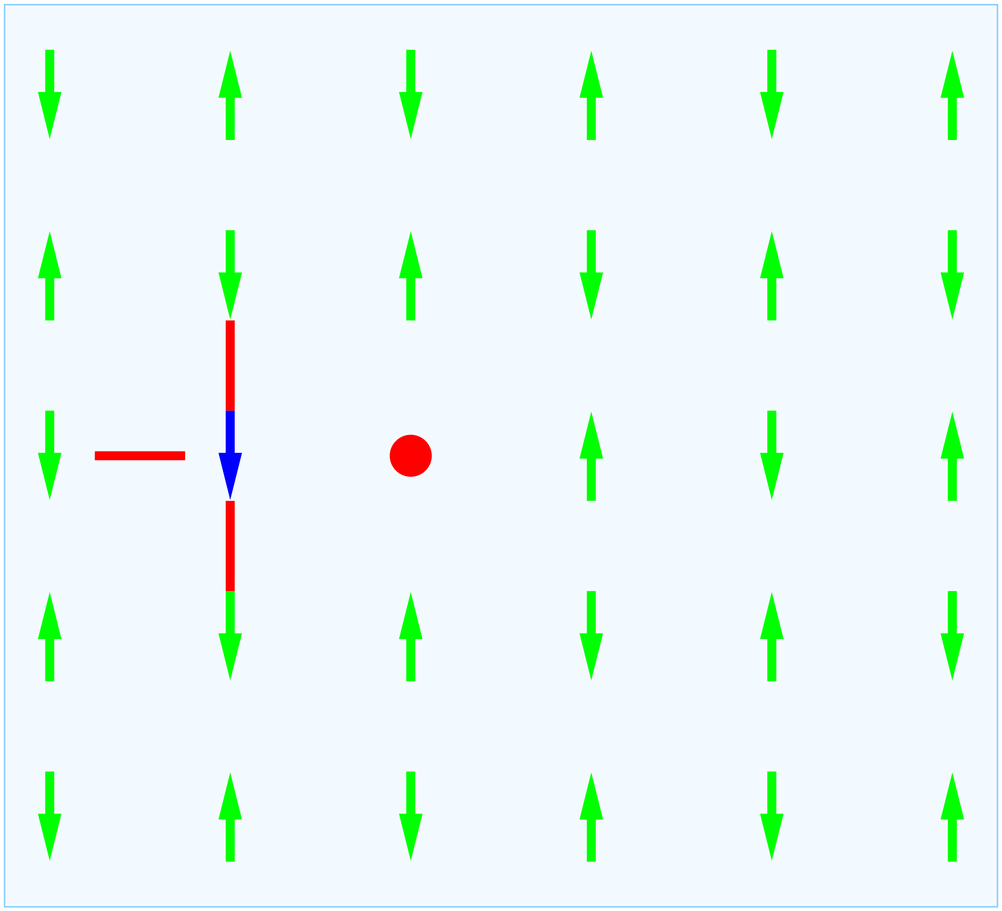


solid lines $\sim a_i \left(\frac{J}{t}\right)^{\frac{2}{3}}$

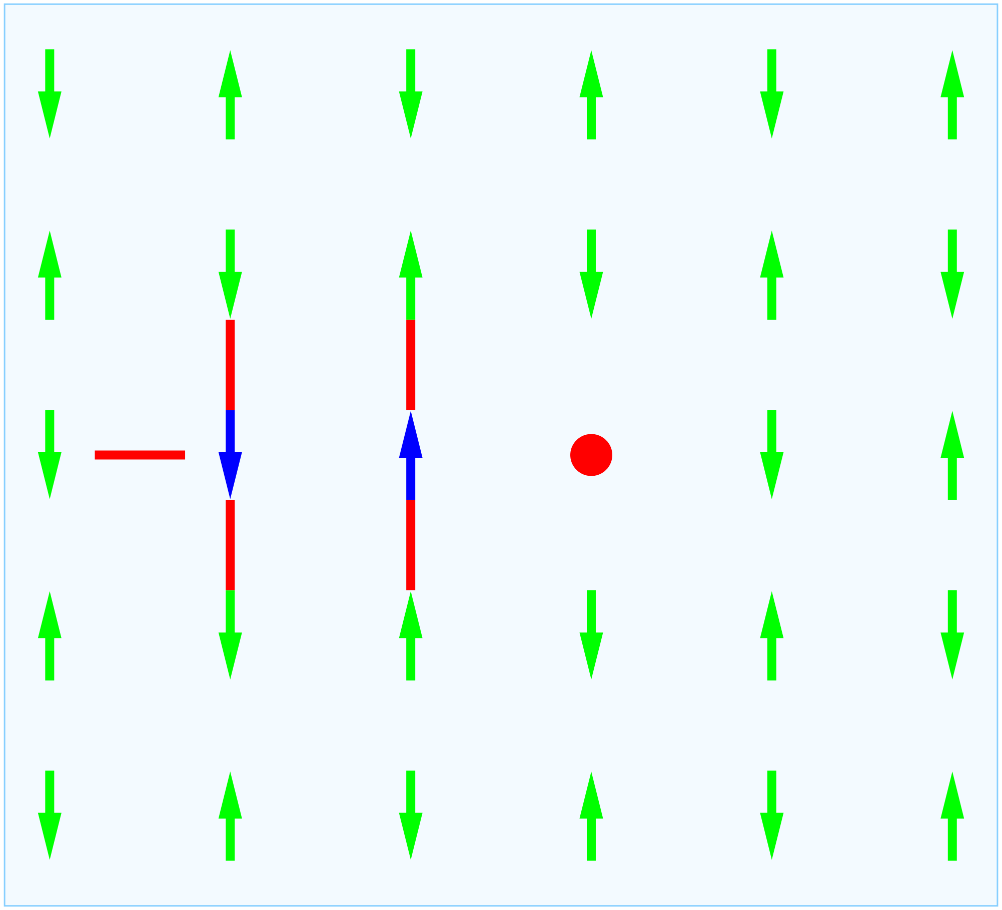
String excitations



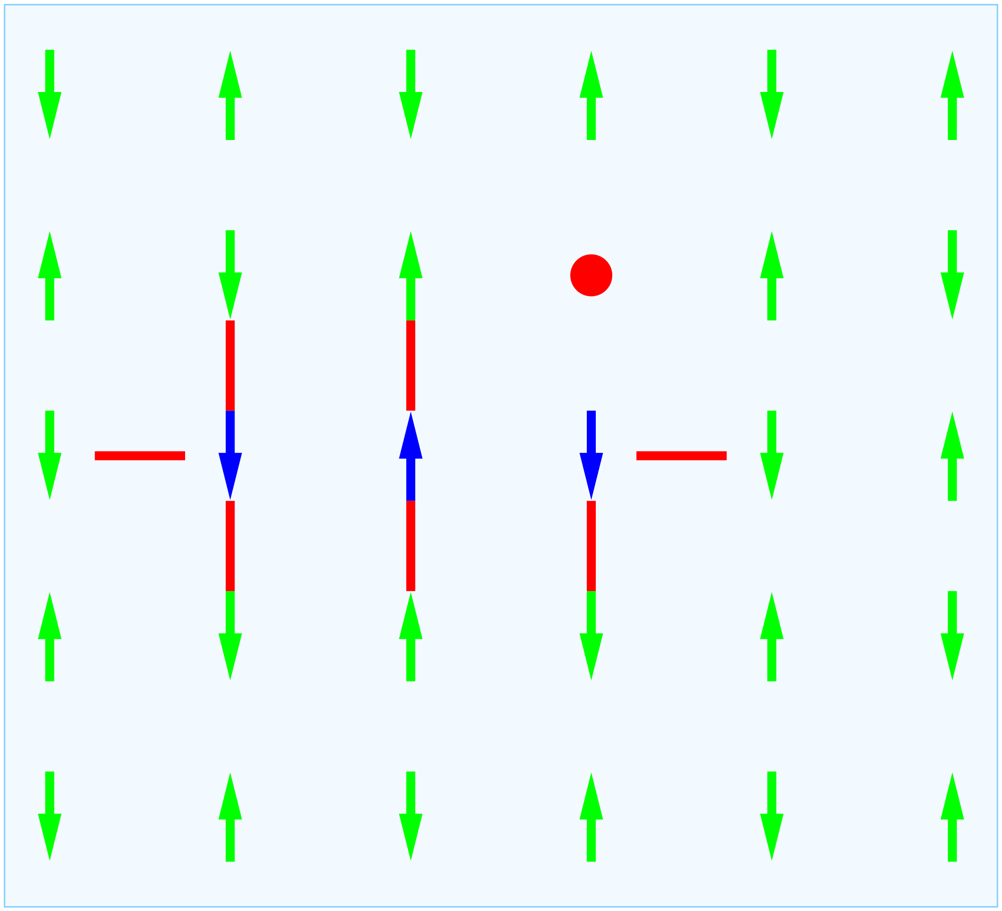
String excitations



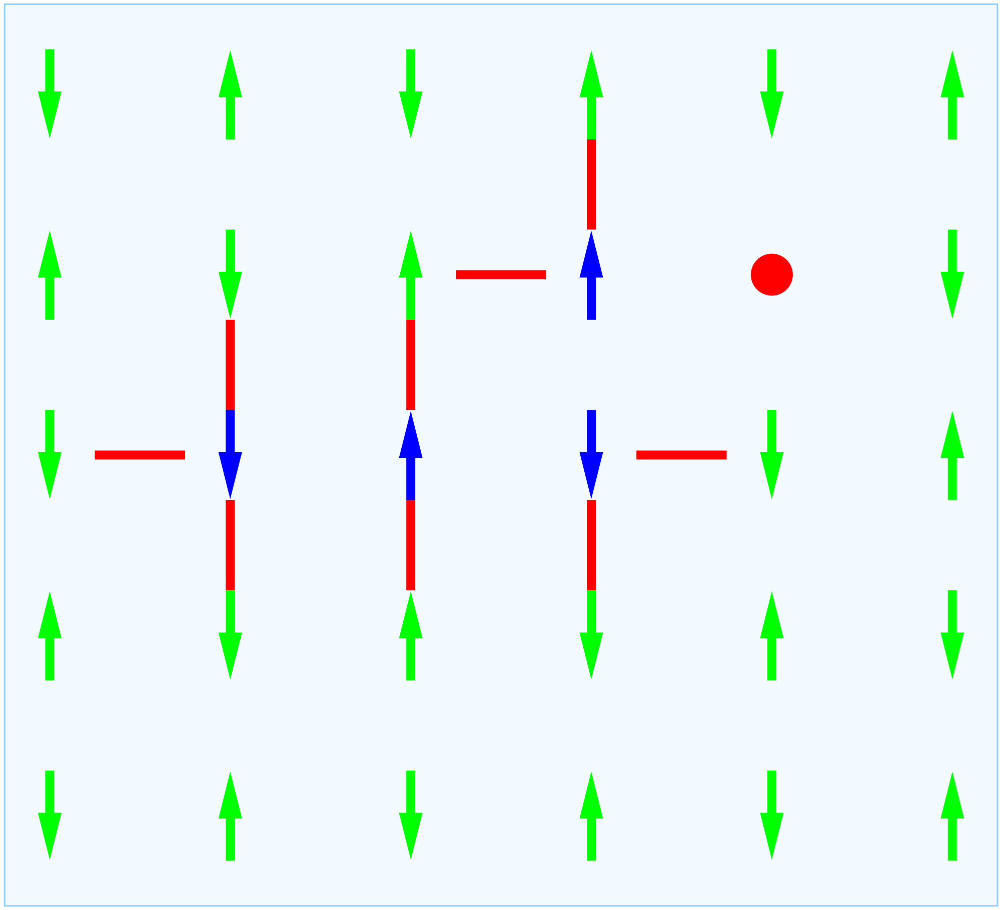
String excitations



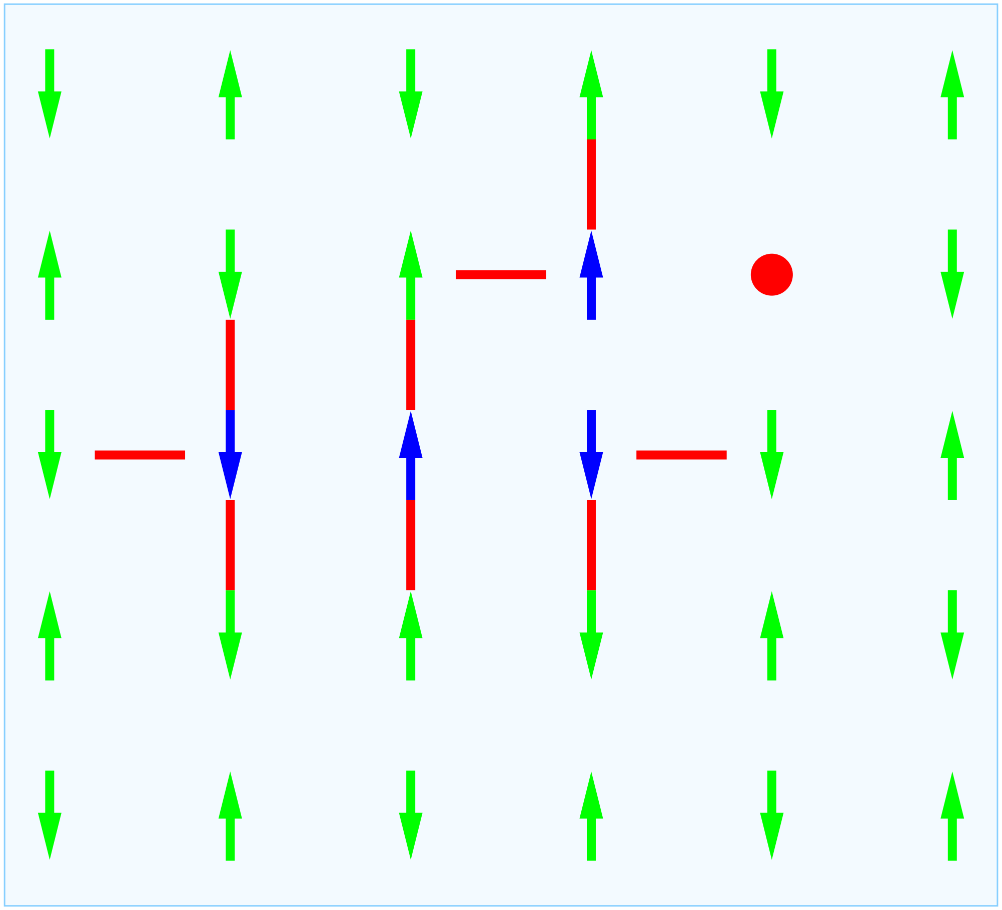
String excitations



String excitations



String excitations



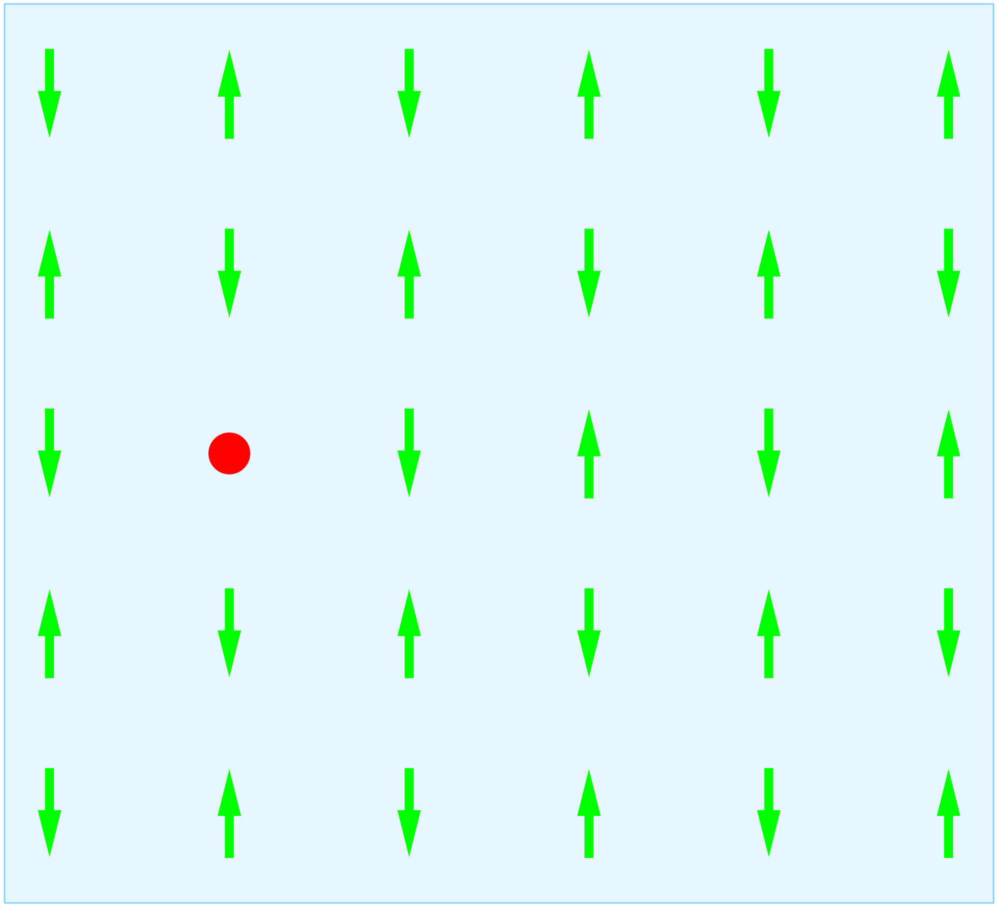
In the continuum limit

$$H_{string} = -t\frac{\partial^2}{\partial x^2} + Jx - 2\sqrt{3}t$$

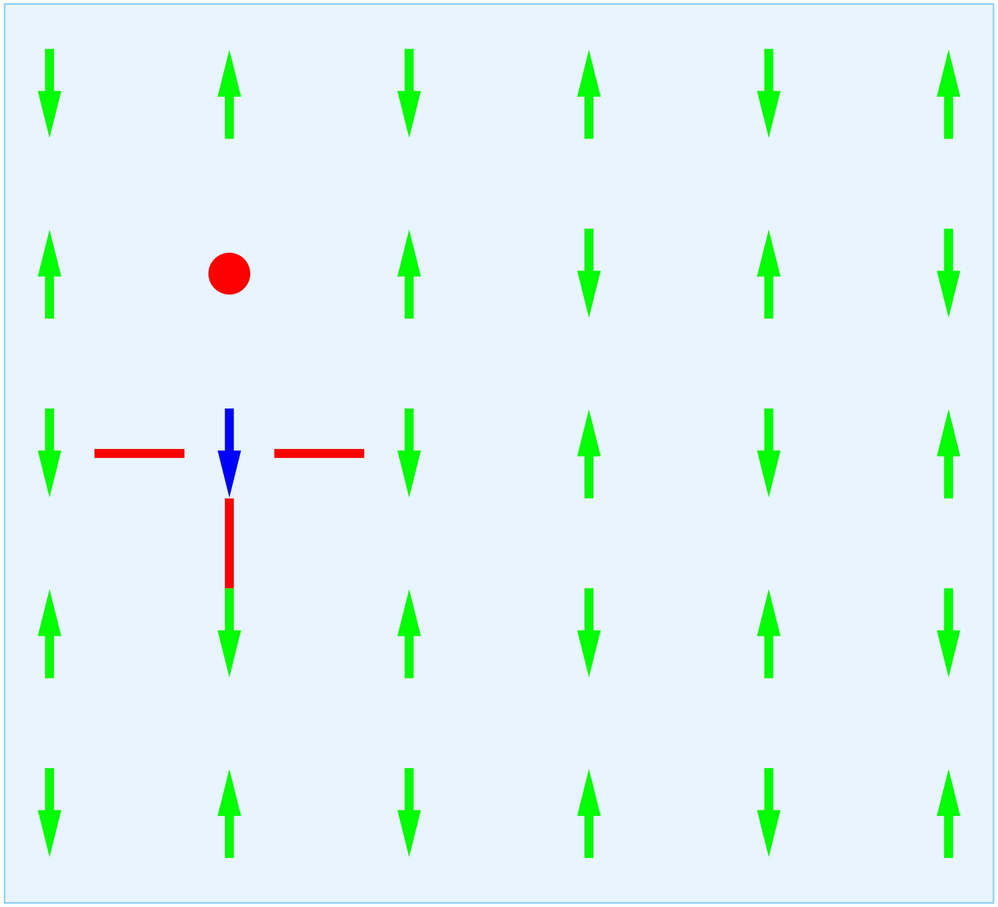
Eigenvalues

$$E_i = a_i \left(\frac{J}{t}\right)^{\frac{2}{3}} t \qquad \left\{ \begin{array}{lcl} a_1 & = & 2.33 \\ a_2 & = & 4.09 \\ a_3 & = & 5.52 \end{array} \right.$$

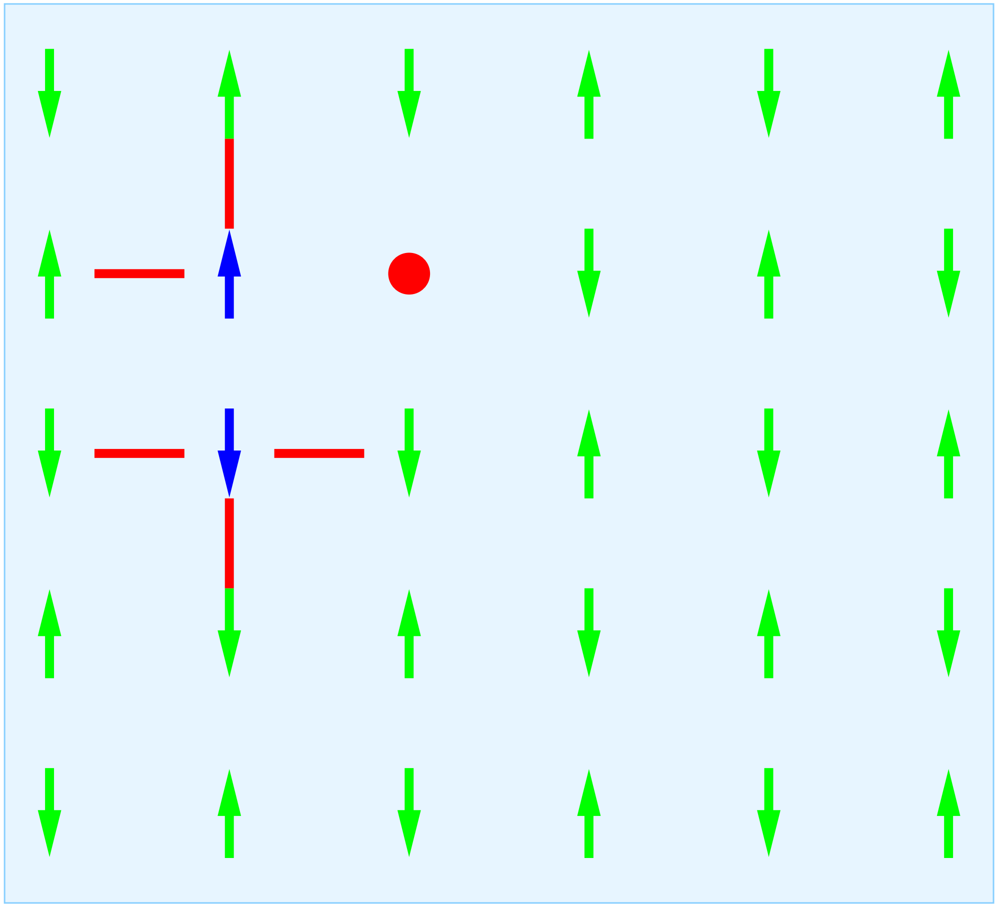
Quasiparticle as a composite fermion



Quasiparticle as a composite fermion



Quasiparticle as a composite fermion



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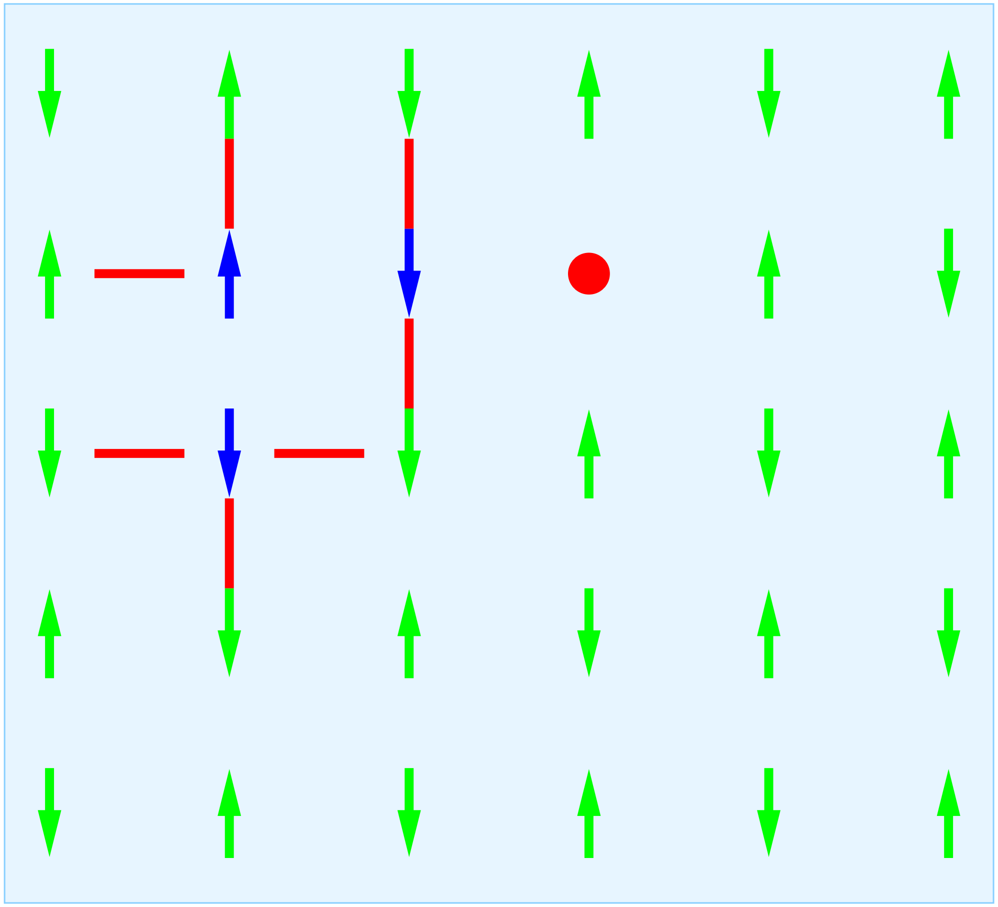

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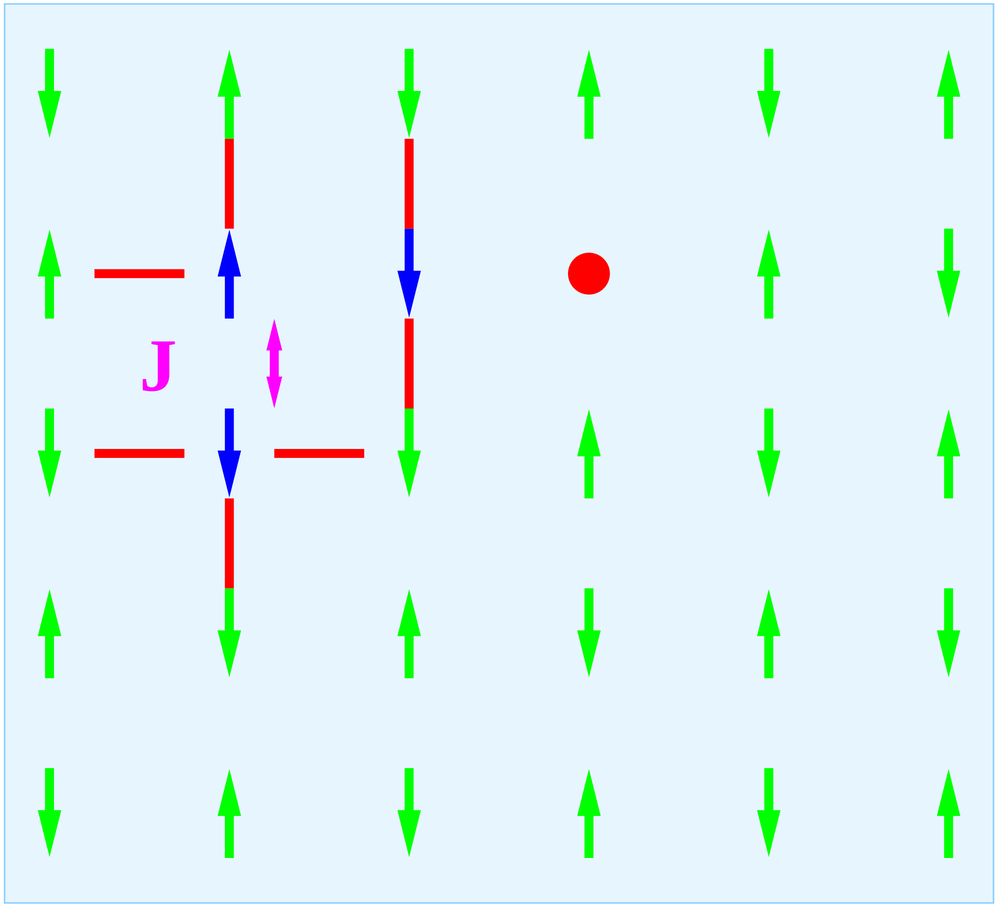
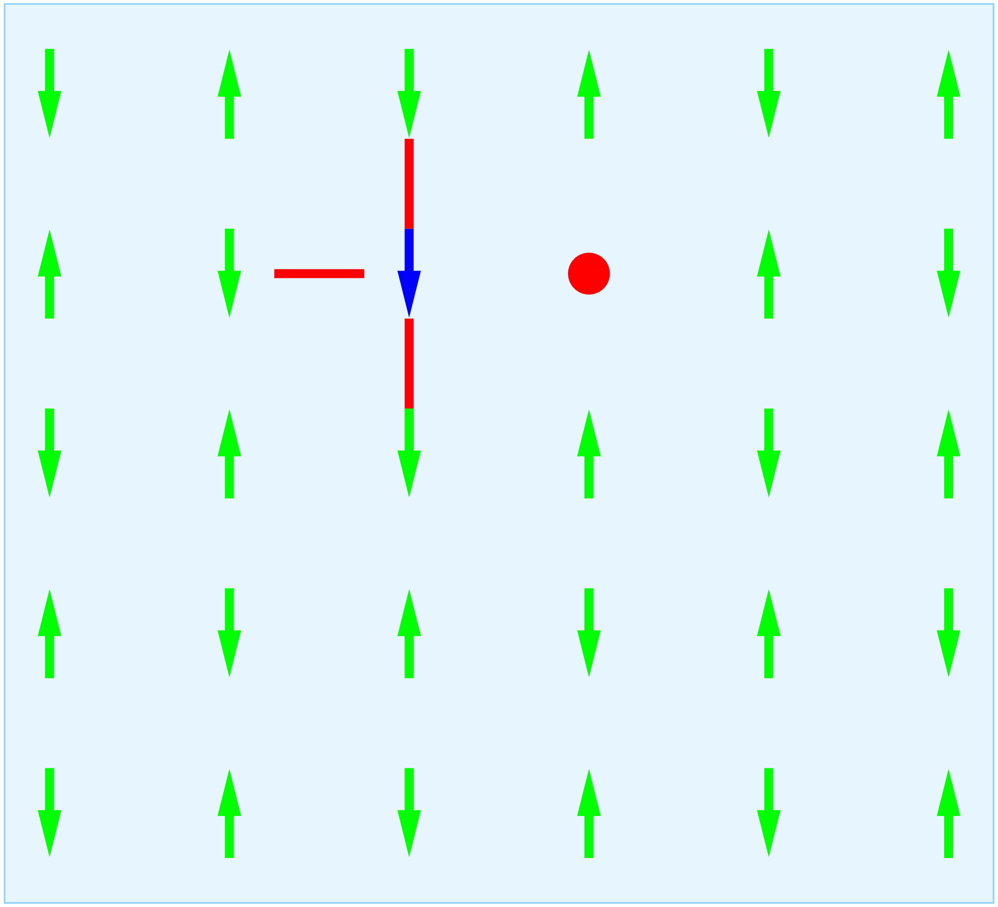
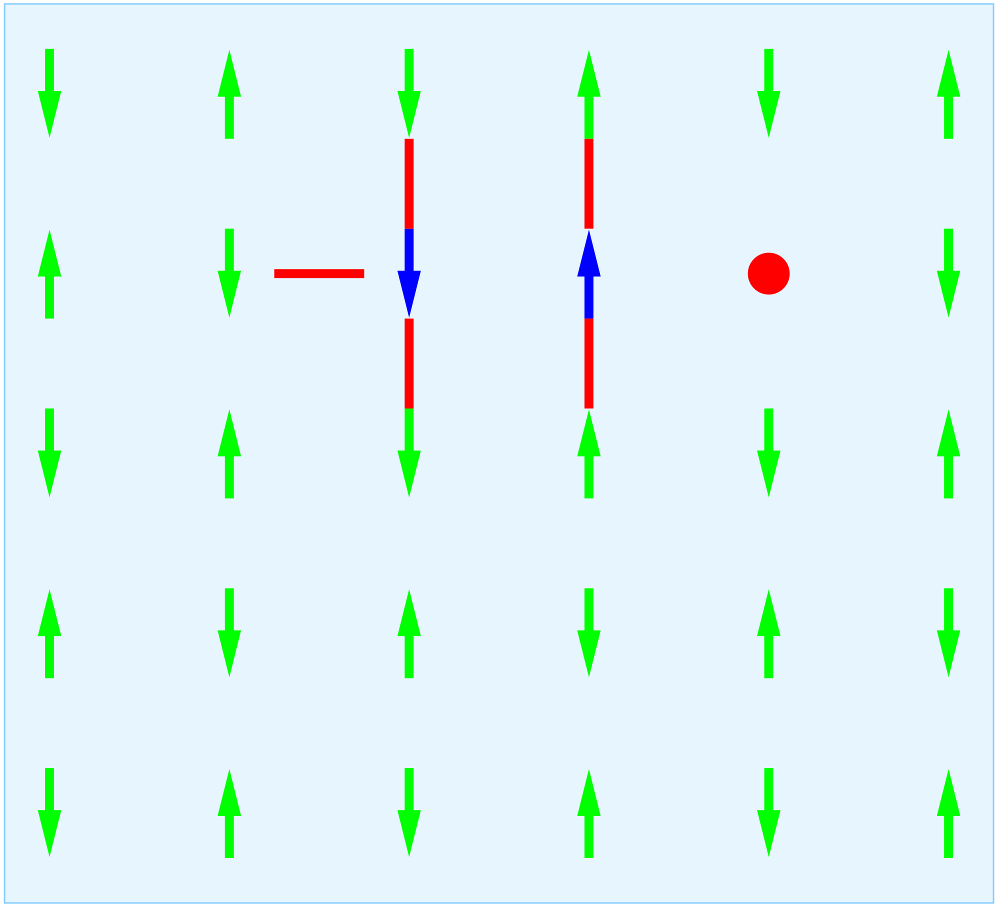


Quasiparticle as a composite fermion



Quasiparticle as a composite fermion



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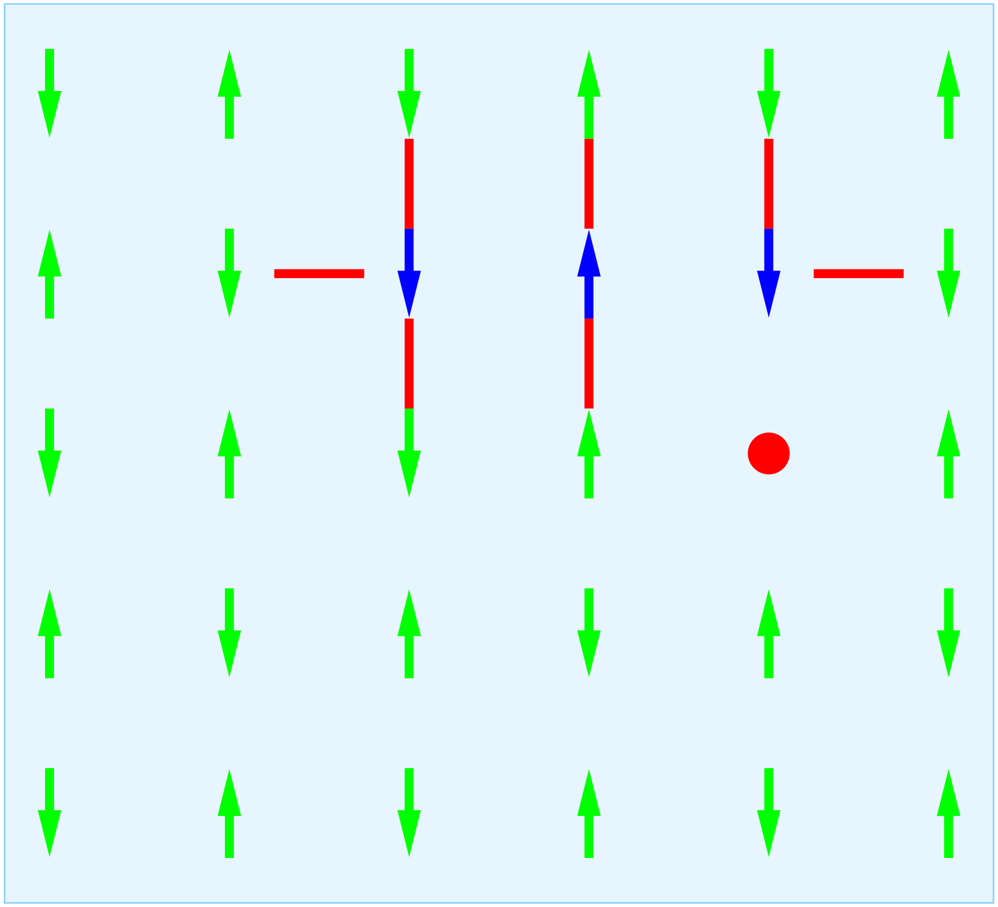

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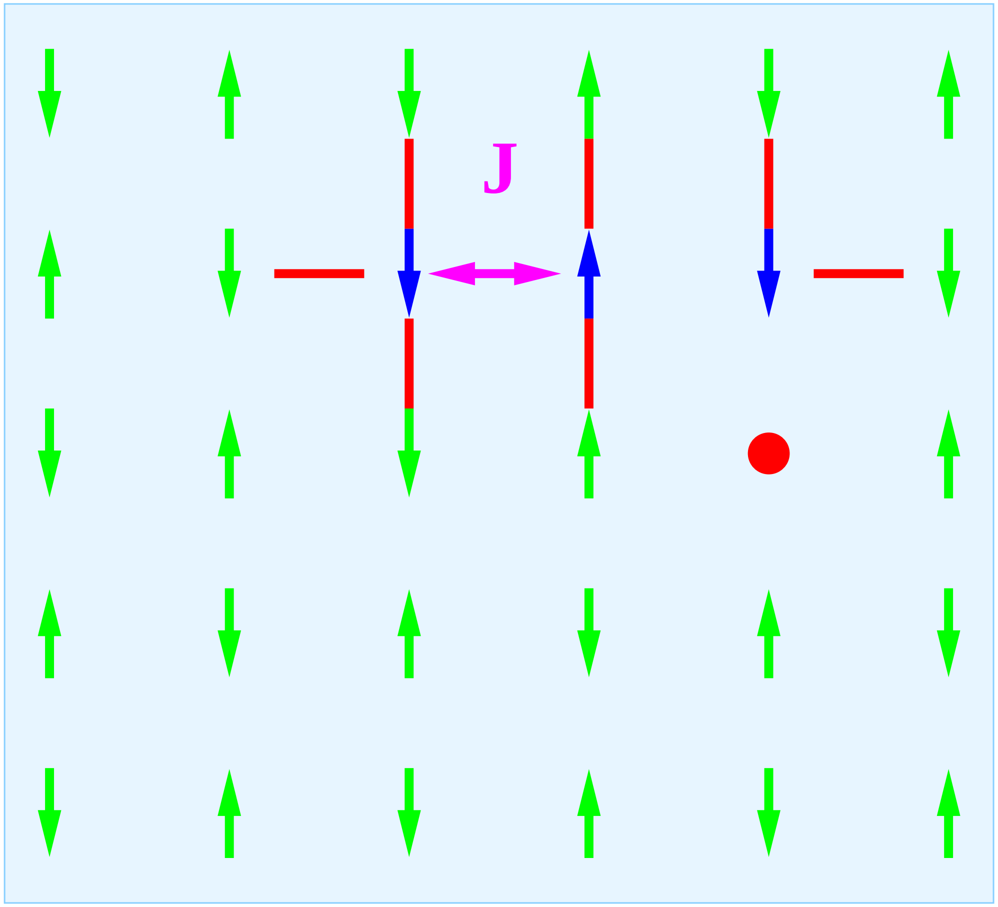

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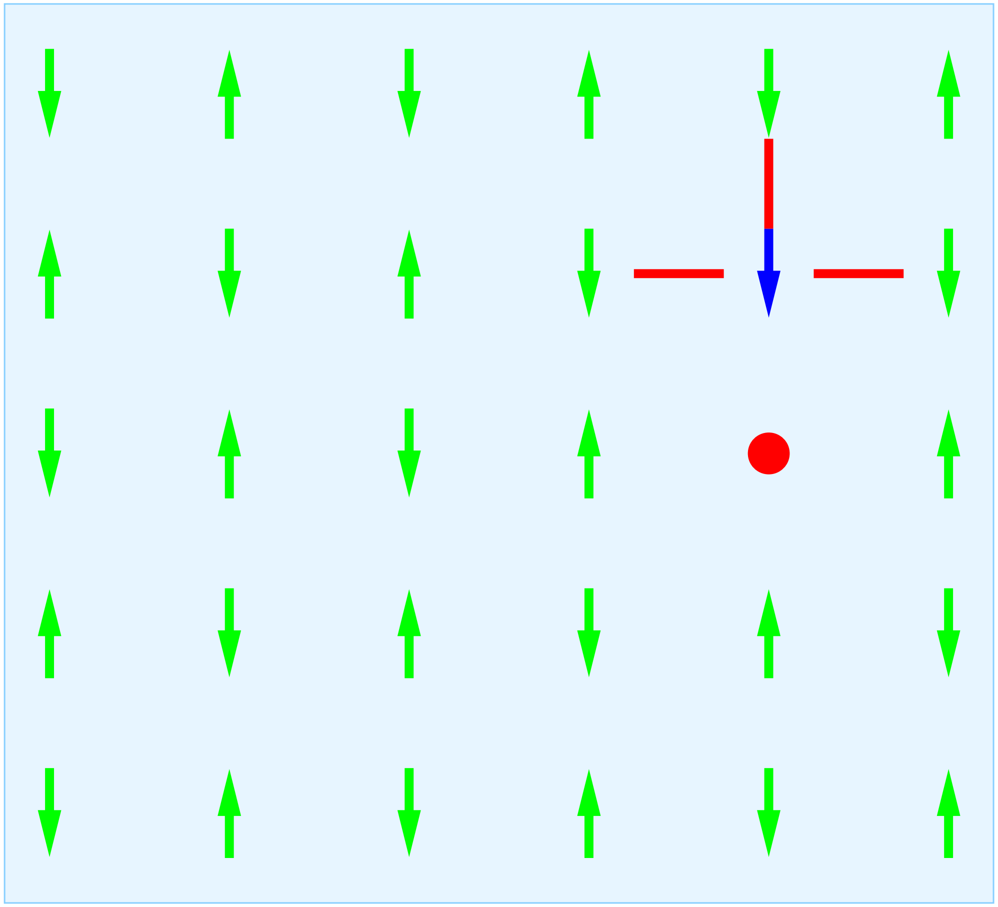

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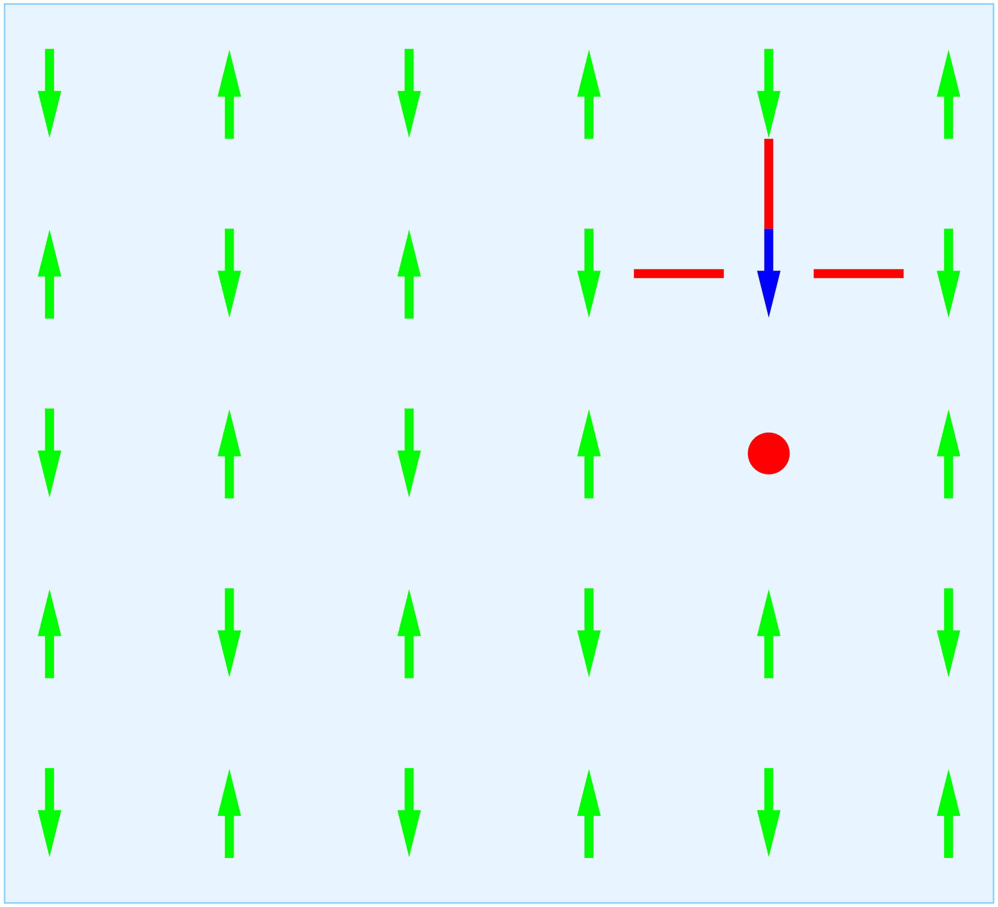

Confinement of holon-spinon pair