

Interacting spinless fermions in a diamond chain

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- 1 AB_2 chain
- 2 t-b limit
- 3 Flat bands and localized states for arrays of quantum rings
- 4 Mean-Field results for general V
- 5 The AB_2 chain in the strong coupling limit $V \rightarrow \infty$
 - Basis
- 6 Present Work
- 7 Summary

Outline

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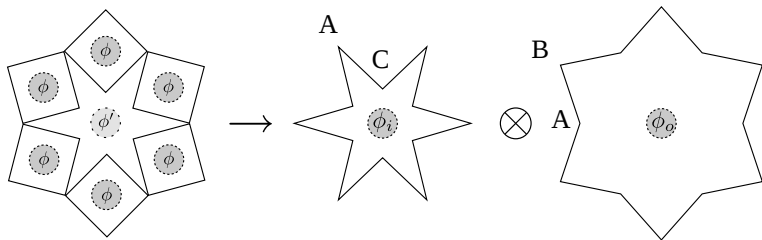


Figure 1: The diamond chain tight binding model (ϕ is a dimensionless reduced flux).

t-V Hamiltonian

$$\begin{aligned}
 H &= H_0 + V \sum_j \left(n_j^A + n_{j+1}^A \right) \left(n_j^B + n_j^C \right) \\
 H_0 &= -t \sum_{j=1}^{N_c} \left[e^{i\phi_o/2N_c} (A_j^\dagger B_j + B_j^\dagger A_{j+1}) \right. \\
 &\quad \left. + e^{-i\phi_i/2N_c} (C_j^\dagger A_j + A_{j+1}^\dagger C_j) \right] + \text{H.c.}
 \end{aligned} \tag{1}$$

Fluxes

$$\begin{aligned}
 \phi_o &= \phi' + N_c \frac{\phi}{2}, \\
 \phi_i &= \phi' - N_c \frac{\phi}{2}.
 \end{aligned} \tag{2}$$

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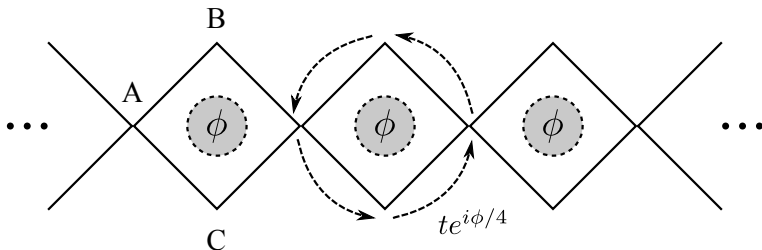


Figure 2: The diamond chain tight binding model (ϕ is a dimensionless reduced flux).

Hamiltonian

$$\begin{aligned}
 H = & -t \sum_j^{N_c} A_j^\dagger \left(e^{i\phi/4} B_j + e^{-i\phi/4} C_j \right) \\
 & + A_{j+1}^\dagger \left(e^{-i\phi/4} B_j + e^{i\phi/4} C_j \right) + \text{H.c.}
 \end{aligned} \tag{3}$$

Anderson like model

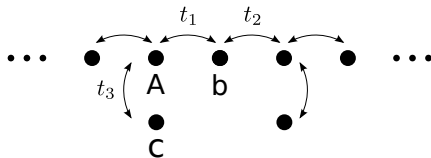


Figure 3: We can map the diamond chain into a periodic Anderson like model (non interacting) with a basis of three sites per unit cell, the hopping amplitudes being controlled by the flux.

Rotation

$$b_j^\dagger = \frac{1}{\sqrt{2}} \left(e^{-i\phi/4} B_j^\dagger + e^{i\phi/4} C_j^\dagger \right),$$

$$c_j^\dagger = \frac{1}{\sqrt{2}} \left(e^{i\phi/4} B_j^\dagger - e^{i\phi} e^{i\phi/4} C_j^\dagger \right).$$

Hopping amplitudes

$$t_1 = \sqrt{2}t,$$

$$t_2 = \sqrt{2} \cos(\phi/2)t,$$

$$t_3 = \sqrt{2} \sin(\phi/2)t.$$

Eigenstates

$$\phi = 0, \pi$$

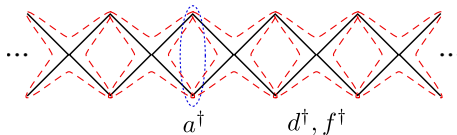


Figure 4: Eigenstates for $\phi = 0$.

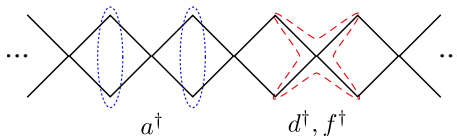


Figure 5: Localized eigenstates for $\phi = \pi$. Note that states $a_j^\dagger |0\rangle$ are only localized on B and C sites.

General ϕ

It is possible to find a two cells *non-orthogonal* localized eigenbasis for $a_j^\dagger$.

Dispersion relation

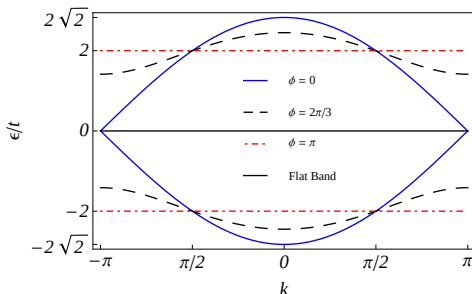


Figure 6: Dispersion relation for several values of ϕ . Gapless for $\phi = 0$ but gapped for finite ϕ achieving maximum gap for $\phi = \pi$. The bandwidth decreases with finite flux, achieving its minimum value for $\phi = \pi$.

Eigenvalues

$$\epsilon_a = 0,$$

$$\epsilon_{\pm} = \pm 2t \sqrt{1 + \cos(\phi/2) \cos(k)},$$

Dispersion relation ($\phi' \neq 0$)

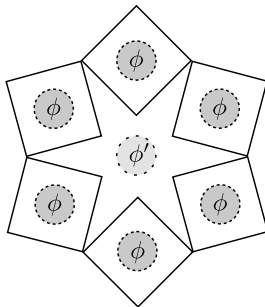


Figure 7: Dispersion relation for several values of ϕ . Gapless for $\phi = 0$ but gapped for finite ϕ achieving maximum gap for $\phi = \pi$. The bandwidth decreases with finite flux, achieving its minimum value for $\phi = \pi$.

Eigenvalues

$$\begin{aligned} \epsilon_{\text{flat}} &= 0, \\ \epsilon_{\pm} &= \pm 2t \sqrt{1 + \cos(\phi/2) \cos(\phi'/N_c + k)}. \end{aligned} \tag{4}$$

DOS

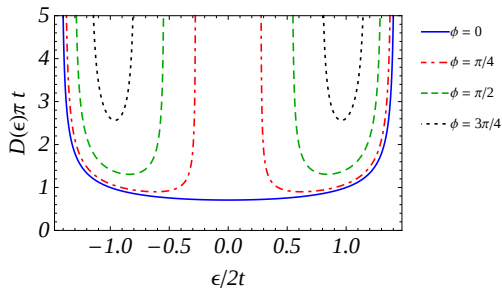


Figure 8: DOS of the diamond chain for several values of flux. Note the absence of a gap for $\phi = 0$

DOS

$$D(\epsilon') = \frac{1}{\pi t} |\epsilon'| \frac{1}{\sqrt{\cos^2(\phi/2) - (\epsilon'^2 - 1)^2}} + \delta(\epsilon'),$$

$$\epsilon' = \frac{\epsilon}{2t}.$$

GS energy

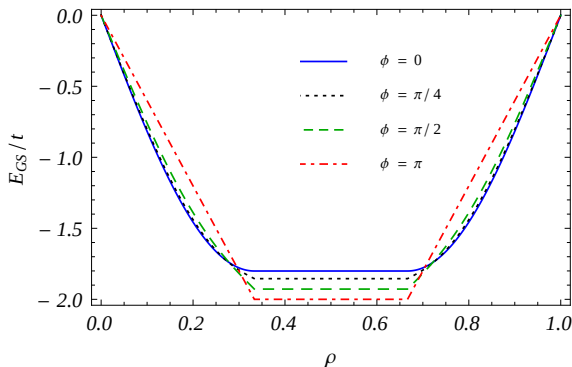


Figure 9: Ground state energy in the thermodynamic limit as a function of filling for several values of flux. E_{GS} remains constant when filling the flat band, $\rho \in [1/3, 2/3]$ achieving its minimum value on that interval for $\phi = \pi$. For $\phi = \pi$, E_{GS} has linear behavior on ρ , since all bands are flat.

GS energy

$$E_{\text{GS}} = \int_{-}^{E_F} D(\epsilon) \epsilon d\epsilon, \quad (5)$$

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t-b quantum ring

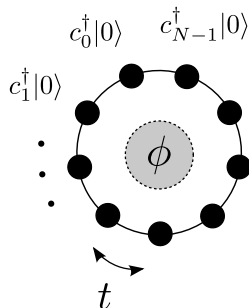


Figure 10: A tight binding quantum ring threaded by a magnetic flux ϕ .

Eigenstates and eigenenergy

$$c_k^\dagger |0\rangle = \sum_{j=0}^{N-1} e^{ikj} c_j^\dagger |0\rangle, \quad (6)$$

$$\epsilon_k = -2t \cos \left(k - \frac{\phi}{N} \right). \quad (7)$$

Standing waves

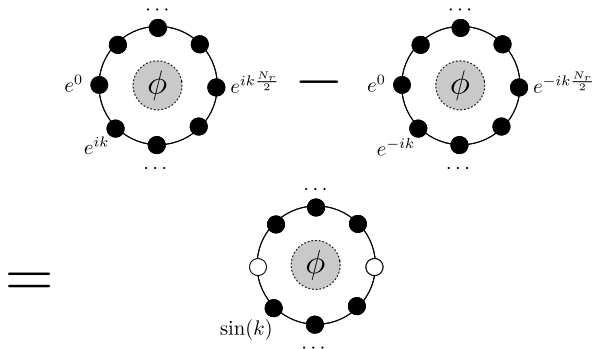


Figure 11: Summing states with opposite momenta yield a stationary wave (We assume N_r even!).

Nodes

$$j = 0, \frac{N_r}{2} \quad (8)$$

Decoupling between rings

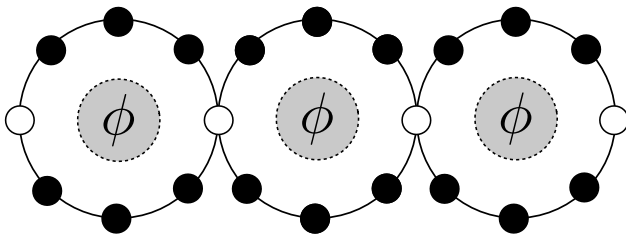


Figure 12: In a chain of rings, the rings are decoupled for our flat bands.

Flat bands

$$\epsilon_n = -2t \cos(2\pi n/N_r), \quad n = 1, \dots, N_r/2 - 1 \quad (9)$$

- There are $N_r/2 - 1$ flat bands!
- Note also that there may be more than two nodes per ring $\Rightarrow$ more complex geometries (e.g. Lieb lattice)!

$$AB_2, \phi, \phi' = 0$$

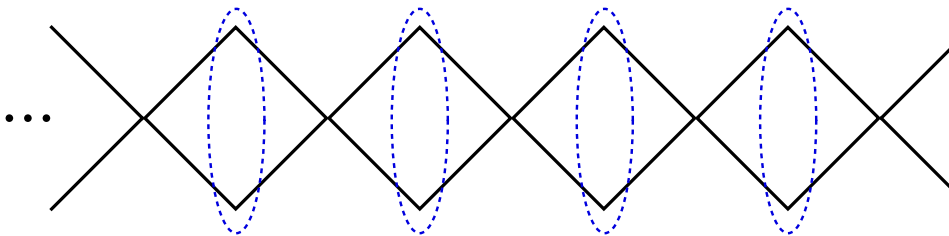
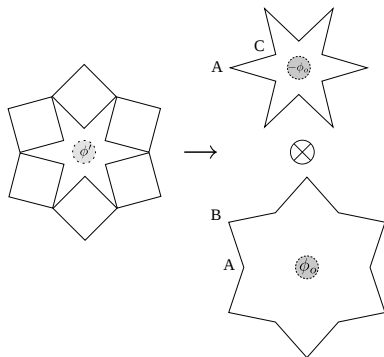


Figure 13: Flat band states in the AB_2 chain

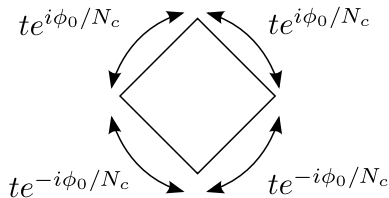
Flat bands

- $N_r = 4$
- 1 flat band
- $\epsilon_{\text{flat}} = 0$

$$\phi = 0, \phi' \neq 0$$



(a) Factorization



(b) Ring - no transl. inv.

Gauge transformation - restores transl. invariance

$$\begin{aligned} c_j^\dagger &\rightarrow e^{j \frac{\phi_0}{2N_c}} c_j^\dagger, & j = 0, \dots, \frac{N_r}{2} \\ c_j^\dagger &\rightarrow e^{j \frac{\phi_0}{2N_c} \cdot (N_r - j)} c_j^\dagger, & j = \frac{N_r}{2} + 1, \dots, N_r - 1 \end{aligned} \quad (10)$$

$$\phi \neq 0, \phi' = 0$$

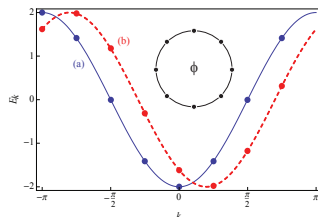


Figure 14: Dispersion relation for a quantum ring, not threaded by ϕ (blue) and threaded by ϕ (red).

Problem

- Flux breaks time reversal symmetry $\Rightarrow$ states $c_k^\dagger |0\rangle$ and $c_{-k}^\dagger |0\rangle$ not degenerate!
- $(c_k^\dagger - c_{-k}^\dagger) |0\rangle$ not an eigenstate!
- Our previous construction does not apply anymore!

$\phi = 0, \phi' \neq 0$ - fixin' it

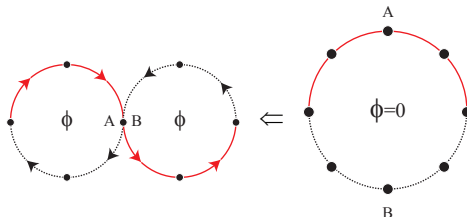


Figure 15: Obtaining a zero Peirls phase - standing waves.

The solution

- Choose two consecutive rings (“opening” them generates a larger ring)
- Peirls phase is now zero in larger ring
- Do a gauge transformation for the larger ring - states with opposite momenta are now degenerate
- Now construct standing waves for the larger ring like before

$\phi = 0, \phi' \neq 0$ - fixin' it

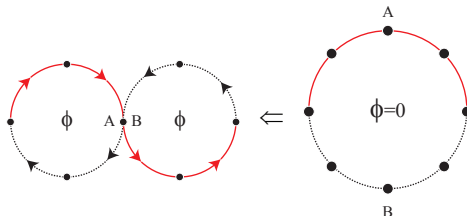


Figure 16: Obtaining a zero Peirls phase - choose a larger ring and fold it!.

Gauge transformation

$$\begin{aligned}
 c_j^\dagger &\rightarrow e^{i \frac{\phi_0}{2N_c} \cdot j} c_j^\dagger, & j = 0, \dots, \frac{N_r}{2} \\
 c_j^\dagger &\rightarrow e^{i \frac{\phi_0}{2N_c} \cdot (N_r - j)} c_j^\dagger, & j = \frac{N_r}{2} + 1, \dots, N_r \\
 c_j^\dagger &\rightarrow e^{-i \frac{\phi_0}{2N_c} \cdot (j - N_r)} c_j^\dagger, & j = N_r + 1, \dots, N_r + \frac{N_r}{2} \\
 c_j^\dagger &\rightarrow e^{-i \frac{\phi_0}{2N_c} \cdot (2N_r - j)} c_j^\dagger, & j = N_r + \frac{N_r}{2} + 1, \dots, 2N_r - 1
 \end{aligned}$$

Localized states in the Lieb lattice

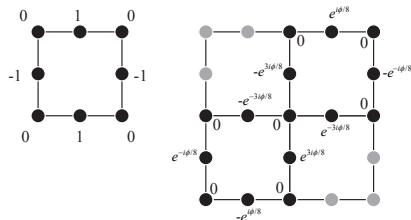


Figure 17: Localized state in a Lieb lattice, without (left) and with flux(right).

- Without flux, our solution is equal to that of H. Aoki, M. Ando, and H. Matsumura, Phys. Rev. B **54**, R17296 (Dec 1996)
- With flux our solution is much more compact than the elongated ring state of H. Aoki, M. Ando, and H. Matsumura, Phys. Rev. B **54**, R17296 (Dec 1996)

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Remarks

- Overestimation of ordered phases
- Particularly bad for 1D systems (strong quantum fluctuations)

Nearest neighbor Coulomb interaction

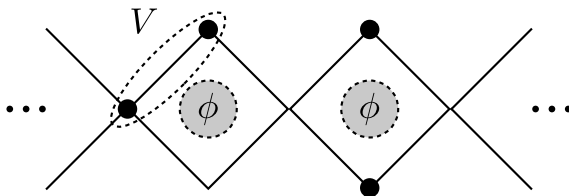


Figure 18: Nearest neighbors Coulomb interaction of strength V .

Hamiltonian

$$H = H_0 + V \sum n_j^A n_j^B + n_{j+1}^A n_j^B + n_j^A n_j^C + n_{j+1}^A n_j^C,$$

$$\phi = 0$$

Eigenvalues

Simple MF eigenvalues for $\phi = 0$:

$$\epsilon_{\sigma}^{\text{flat}} = 2V\rho_A$$

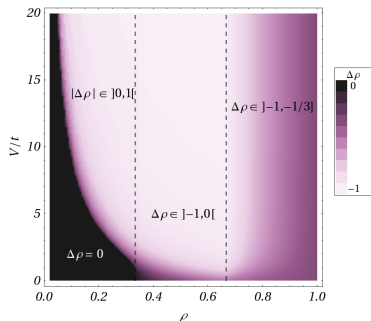
$$\epsilon_{\sigma}^{\pm} = V(\rho_A + 2\rho_B) \pm \sqrt{8t^2 \cos(k/2) + \Delta_V^2},$$

where $\Delta_V = V(\rho_A - 2\rho_B)$.

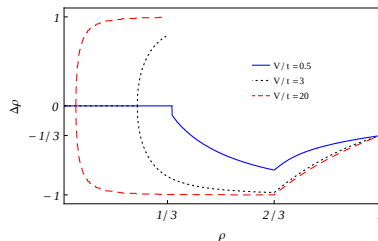
Order parameter

$$\Delta\rho = \frac{\rho_A - 2\rho_B}{\rho_A + 2\rho_B}.$$

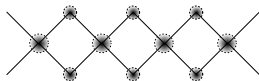
Phase diagram



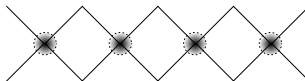
(a) Phase diagram

(b) $\Delta\rho(\rho)$ - Note the symmetry breaking

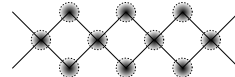
$$\Delta\rho = 0 \Rightarrow \rho_A = 2\rho_B$$



$$\Delta\rho = 1 \Rightarrow \rho_B = 0$$



$$\begin{aligned} \rho = 1 &\Rightarrow \rho_A = \rho_{B,C} = 1 \\ &\Rightarrow \Delta\rho = -1/3 \end{aligned}$$

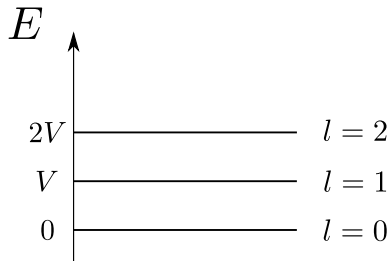


Outline

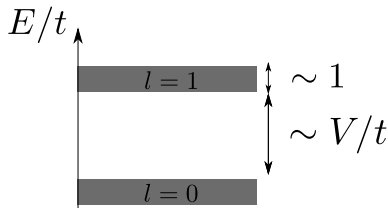
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Strong coupling

$$t = 0$$

(c) Atomic limit ($t = 0$)

$$t \neq 0$$

(d) Finite t

Strong coupling

- In the atomic limit $E = lV$, l number of double occup.
- For t finite, first order correction $\Rightarrow$ diagonalize H in each l subspace (use Gutzwiller projectors P_l)
- For $V/t \rightarrow \infty$ (strong coupling), look only at $l = 0$

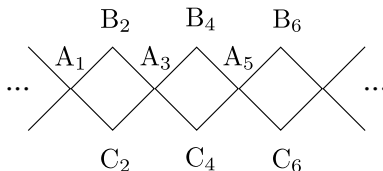
Projected Hamiltonian ($I = 0$)

Figure 19: New notation to make it easier to compare with the t-V chain.

 $I = 0$ Hamiltonian ($\phi = 0$)

$$P_0 H P_0 = -t \sum_{j \text{ odd}} e^{i\phi_0/2N_c} \left[\prod_{i \in \mathcal{P}_j} n_i^h \times A_j^\dagger (B_{j+1} + C_{j+1}) + \prod_{i \in \mathcal{P}_{j+1}} n_i^h \times (B_{j+1}^\dagger + C_{j+1}^\dagger) A_{j+2} \right] + \text{H.c.} \quad (11)$$

$$n_i^h = (1 - c_i^\dagger c_i), \quad c = A, B, C \quad (12)$$

$\mathcal{P}_j$ set of sites nearest-neighbors of the pair of sites j and $j + 1$

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Basis

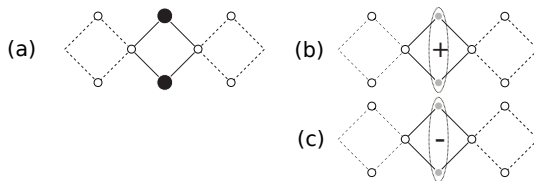


Figure 20: (a) Two particle localized states. (b) Bounding ($B_{+,i}^\dagger$) - itinerant one particle states. (c) Anti-bounding ($B_{-,i}^\dagger$) - localized one particle states

Bonding and anti-bonding

$$\begin{aligned}
 B_{+,i}^\dagger &= (B_i^\dagger + C_i^\dagger)/\sqrt{2} \\
 B_{-,i}^\dagger &= (B_i^\dagger - C_i^\dagger)/\sqrt{2}
 \end{aligned}
 \tag{13}$$

Basis

Hamiltonian

$$P_0 H P_0 = -\sqrt{2}t \sum_{j=1}^{N_c} e^{i\phi_0/2N_c} \left(\prod_{i \in \mathcal{P}_j} n_i^h \times A_j^\dagger B_{+,j+1} + \prod_{i \in \mathcal{P}_{j+1}} n_i^h \times B_{+,j+1}^\dagger A_{j+2} \right) + \text{H.c.} \quad (14)$$

Basis for $I = 0$

$$|\Psi\rangle = \prod_{i=1}^{N_{BC}} B_{\alpha_i}^\dagger C_{\alpha_i}^\dagger \prod_{j=1}^{N_{B_-}} B_{-, \beta_j}^\dagger \prod_{n=1}^{N_{B_+}} B_{+, \gamma_n}^\dagger \prod_{m=1}^{N_A} A_{\mu_m}^\dagger |0\rangle \quad (15)$$

$$\{\alpha\} \cap \{\beta\} \cap \{\gamma\} \cap \{\mu\} \cap \{\alpha \pm 1\} \cap \{\beta \pm 1\} \cap \{\gamma \pm 1\} \cap \{\mu \pm 1\} = 0 \quad (16)$$

$$2N_{BC} + N_{B_-} + N_{B_+} + N_A = N \quad (17)$$

Boundaries

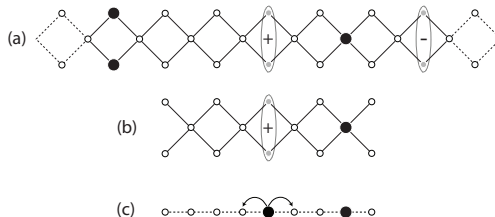


Figure 21: (a) State with localized as well as itinerant particles; (b) Open boundary region where the itinerant fermions in state given in (a) may move. Note that the open boundary regions terminate always at B and C sites. (c) Corresponding state of the linear lattice.

Solving the model

- Distribute localized fermions (if any) $\rightarrow$ create open boundary regions
- Solve remaining problem for itinerant fermions by mapping into the t-V chain
- To solve the t-V chain problem: Bethe Ansatz or Dias method for strong coupling (R. G. Dias. Phys. Rev. B **62**, 7791–7801 (2000))

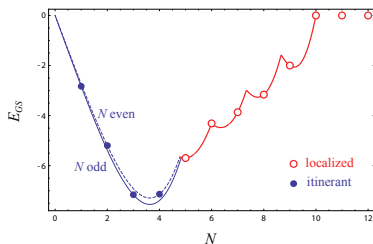
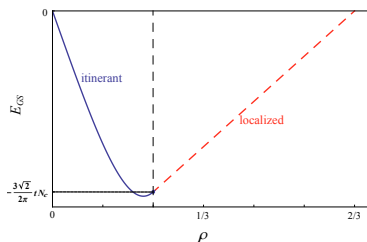
E_{GS} (a) E_{GS} for $N_c = 6$ (numerical and analytical)(b) E_{GS} in thermodynamic limit

Figure 22:

 E_{GS} thermodynamic limit

$$\frac{E_{GS}^{\text{itin}}}{N_c} = -\frac{2\sqrt{2}t}{\pi}(2-3\rho)\sin\left(\frac{\pi\rho}{\frac{2}{3}-\rho}\right) \quad (18)$$

$$\frac{E_{GS}^{\text{loc}}}{N_c} = -\frac{2\sqrt{2}t}{\pi}(2-3\rho), \quad (19)$$

Phase separation

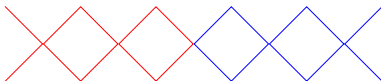


Figure 23: Phase separation - localized states gather together and form a larger area where itinerant electrons can move (and delocalize).

- At $\rho = 2/9$ (reduced chain half-filled) phase separation occurs - larger delocalization zone (reduced kinetic energy)
- Itinerant band as close as possible to half-filling (all negative energy states filled)

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Present work

- Conduction through the flux threaded AB_2 chain
- Geometric frustration in the AB_2 chain and similar lattices

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Summary

- Flat, dispersionless band for any value of ϕ
- Localized energy eigenbasis for any ϕ (flat band)
- Method for finding flat states in arrays of quantum rings
- For V interaction we have obtained an interesting phase diagram
- Exact solution in the strong coupling limit presented
- Phase separation for $\rho > 2/9$ in strong coupling