

Electronic, thermodynamic and transport properties of the diamond chain

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- 1 Diamond chain
- 2 Diamond star
- 3 Connecting the diamond
- 4 Impurities and ABC diamonds
- 5 Interactions
 - On-site Coulomb interaction
 - Nearest neighbors Coulomb interaction
- 6 Conductance
- 7 Summary

Outline

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Diamond chain

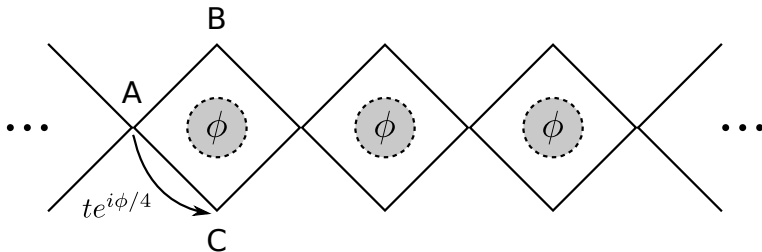


Figure 1: The diamond chain tight binding model (ϕ is a dimensionless reduced flux).

Hamiltonian

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

Experimental systems

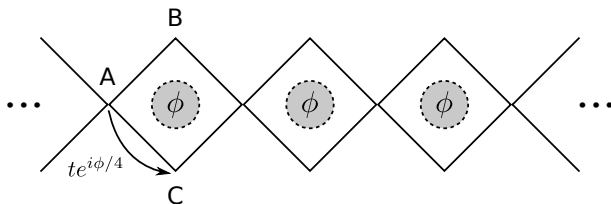


Figure 2: The diamond chain tight binding model (ϕ is a dimensionless reduced flux).

- ML_2
- Azurite
- Organic molecules
- QDs

Properties

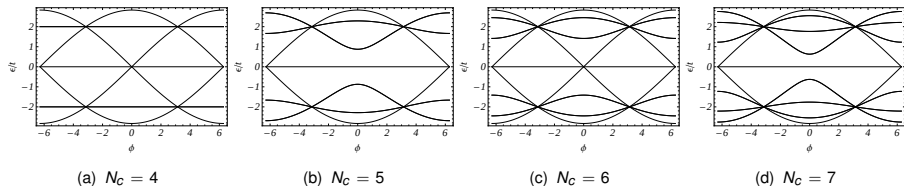


Figure 3: One particle $\epsilon_k(\phi)$ for different number of N_c .

- Flat, ϕ independent band for $\epsilon_k = 0$
- N_c odd and $\phi = 0 \Rightarrow \phi$ dependent eigenvalues don't cross $\epsilon_k = 0$ but they do for an N_c even
- Periodic on ϕ with period $\phi = 2\pi$ when N_c even. Period $\phi = 4\pi$ when N_c odd
- $N_c = 4n$, $n \in \mathbb{Z}$ two flux independent energies appear for $\epsilon_k = \pm 2t$
- $\phi = \pi \Rightarrow$ three levels system $\Rightarrow$ singular DOS

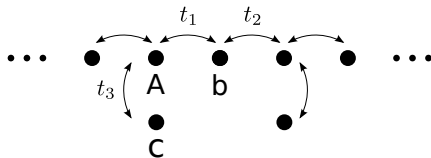
General ϕ 

Figure 4: 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

$$\phi = 0, \pi$$

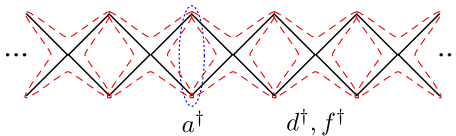


Figure 5: Eigenstates for $\phi = 0$.

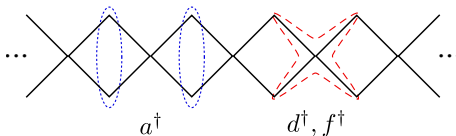


Figure 6: Localized eigenstates for $\phi = \pi$. Note that states $a_j^\dagger |0\rangle$ are only localized on B and C sites.

General ϕ

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

Dispersion relation

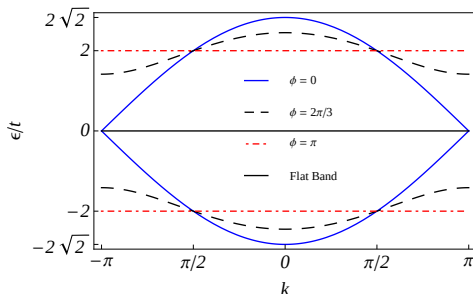


Figure 7: Dispersion relation for several values of ϕ . Gapless for $\phi = 0$ but gapped for finite ϕ achieving maximum gap for $\phi = \pi$. The bandwidth decreases with finite flux, achieving its minimum value for $\phi = \pi$.

Eigenvalues

$$\epsilon_a = 0,$$

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

Gap & bandwidth

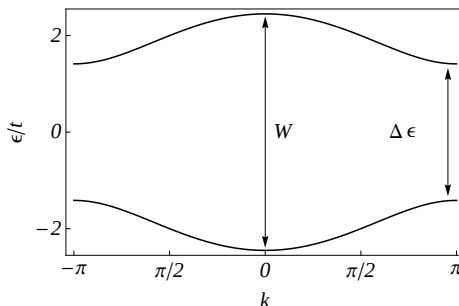


Figure 8: Dispersion relation for $\phi = 2\pi/3$ (we have omitted $\epsilon_k = 0$ since it is not affected by ϕ). Gapless for $\phi = 0$ but gapfull for finite ϕ achieving maximum gap for $\phi = \pi$. The bandwidth decreases with finite flux, achieving its minimum value for $\phi = \pi$.

Gap & bandwidth

$$\Delta\epsilon = 4t\sqrt{1 - \cos(\phi/2)}.$$

$$W = 4t\sqrt{1 + \cos(\phi/2)}.$$

DOS

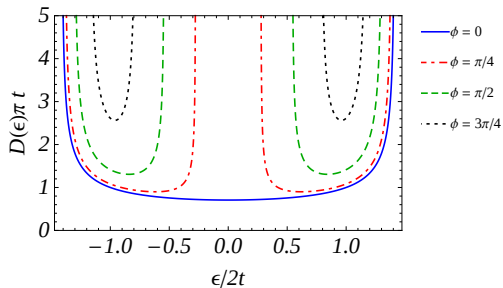


Figure 9: DOS of the diamond chain for several values of flux. Note the absence of a gap for $\phi = 0$

DOS

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

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

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Diamond star

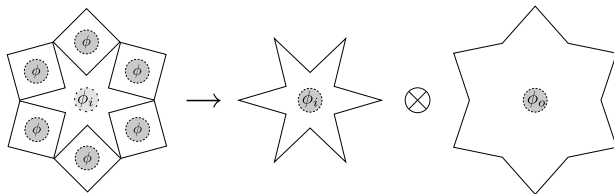


Figure 10: A diamond star: a system of *trully* periodic diamond rings. Each diamond ring is threaded by a flux ϕ . The inner star is threaded by a flux ϕ_i . This system can be factorized into an outer ring with flux ϕ_o and an inner ring with a flux ϕ_i - but these two rings share the A sites!

Inner and outer stars flux

$$\begin{aligned}\phi_o &= \phi' + 2N_c \frac{\phi}{4}, \\ \phi_i &= \phi' - 2N_c \frac{\phi}{4}\end{aligned}$$

Eigenvalues

$$\epsilon_k = 0, \pm 2t \sqrt{1 + \cos(\phi/2) \cos(\phi'/N_c + k)}.$$

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Connecting the diamond

Internal hops

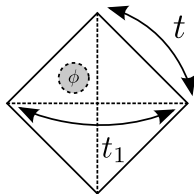
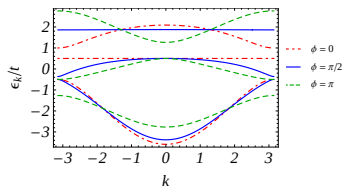


Figure 11: Model.

Figure 12: Dispersion relation by setting $t_1 = t/2$.

Internal & external hops

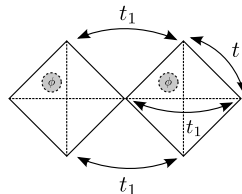
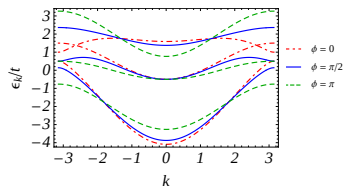


Figure 13: Model.

Figure 14: Dispersion relation by setting $t_1 = t/2$.

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Single impurity

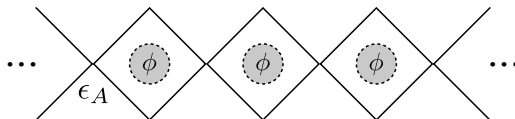


Figure 15: Example of one of the situations studied using a single impurity. In this case we have a different on-site energy on an A site, ϵ_A .

- Gives rise to an impurity level outside the dispersive bands
- Its effect on localized states do not decrease with increasing N_c
- Its effect on extended states decreases with increasing N_c

AB2

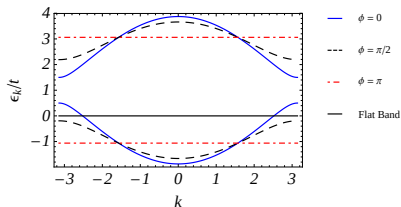


Figure 16: Dispersion relation for $\epsilon_B = \epsilon_C = 0$, $\epsilon_A = t$. Note the gap for $\phi = 0$, absent when $\epsilon_A = 0$ and the band crossing. Note also that the top and bottom band states with $k = \pm\pi/2$ have an energy independent of the flux.

AB2

- Assume $B = C$
- $\epsilon_A \neq 0$, $\epsilon_B = 0$ (for simplicity)

$$\epsilon_k = 0, \pm 2t \sqrt{1 + \cos(k) \cos(\phi/2) + \left(\frac{\epsilon_A}{4t}\right)^2} + \epsilon_A.$$

Regimes

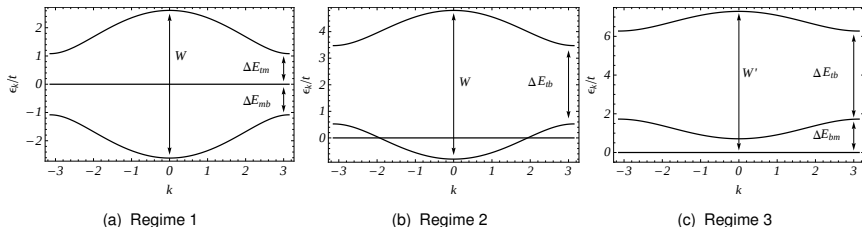


Figure 17: The three regimes of the studied system, here considering $\epsilon_A > 0$. The three regimes are distinguished by the relative position of the energy bands.

Regimes

- ❶ Before the bottom (for $\epsilon_A > 0$)/top (for $\epsilon_A < 0$) band intercepts the middle band.
- ❷ While the bottom/top band is intercepting the bottom band.
- ❸ After the bottom/top band has completely crossed the middle band and exchanged positions.

Gaps and bandwidths

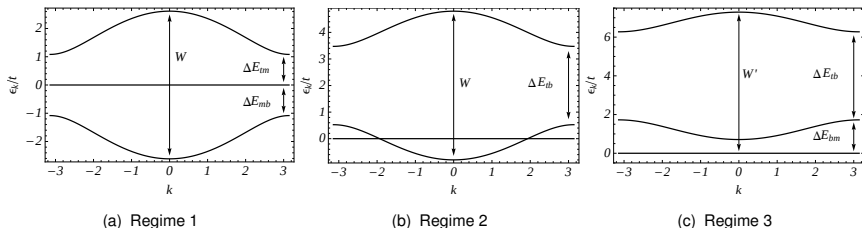


Figure 18: The three regimes of the studied system, here considering $\epsilon_A > 0$. The three regimes are distinguished by the relative position of the energy bands.

Gaps and bandwidths

$$\Delta E_{tm} = 2t\sqrt{2\sin^2(\phi/4) + (\epsilon_A/4t)^2} + \epsilon_A,$$

$$\Delta E_{mb} = 2t\sqrt{2\sin^2(\phi/4) + (\epsilon_A/4t)^2} - \epsilon_A,$$

$$W = 4t\sqrt{2\cos^2(\phi/4) + (\epsilon_A/4t)^2},$$

$$\Delta E_{bm} = 2t\sqrt{2\cos^2(\phi/4) + (\epsilon_A/2t)^2} - \epsilon_A,$$

$$W' = 2t\sqrt{2\sin^2(\phi/4) + (\epsilon_A/4t)^2} + \epsilon_A.$$

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Hubbard interaction

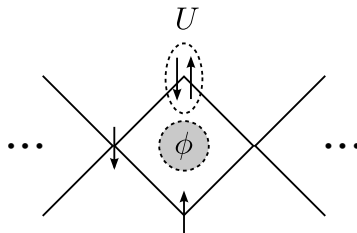


Figure 19: On-site Coulomb interaction (Hubbard interaction) of strength U .

Hamiltonian

$$H = H_0 + U \sum_j^{N_c} n_{j,\uparrow}^A n_{j,\downarrow}^A + n_{j,\uparrow}^B n_{j,\downarrow}^B + n_{j,\uparrow}^C n_{j,\downarrow}^C,$$

MF approximation

Number of particles operator

$$n_{j\sigma} = \bar{n}_{j\sigma} + (n_{j\sigma} - \bar{n}_{j\sigma}).$$

MF approximation

$$n_{j\uparrow}n_{j\downarrow} \approx n_{j\uparrow}\bar{n}_{j\downarrow} + n_{j\downarrow}\bar{n}_{j\uparrow} - \bar{n}_{j\uparrow}\bar{n}_{j\downarrow}.$$

Assumptions

Assume uniform density A and B and C sites

$$\begin{aligned}\bar{n}_\sigma^A &= \bar{n}_{j\sigma}^A, \\ \bar{n}_\sigma^B &= \bar{n}_{j\sigma}^B = \bar{n}_{j\sigma}^C.\end{aligned}$$

This still allow the study of ferromagnetic, antiferromagnetic and ferrimagnetic configurations due to the bipartite nature of the diamond chain.

Ferromagnetism

Assumptions

$$\bar{n}_\sigma = \bar{n}_{j\sigma}^A = \bar{n}_{j\sigma}^B = \bar{n}_{j\sigma}^C.$$

Total density of particles

$$\bar{n} = \bar{n}_\uparrow + \bar{n}_\downarrow = \frac{N_p}{N_s}.$$

Magnetization

$$m = \frac{\bar{n}_\uparrow - \bar{n}_\downarrow}{\bar{n}_\uparrow + \bar{n}_\downarrow} \in [-1, 1].$$

Diamond chain

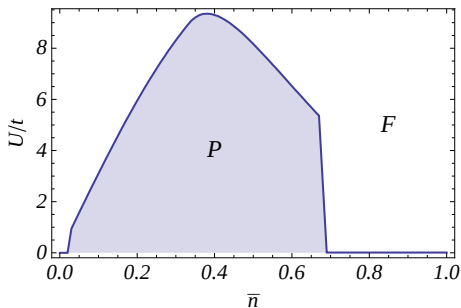


Figure 20: The phase transition between paramagnetic and ferromagnetic order for a system with 300 obtained by studying MF ferromagnetic ordering. We only plot until $\bar{n} = 1$ since the graphic is even around $\bar{n} = 1$.

Stoner's criterion

$$U_c = \frac{1}{D(\epsilon_F)},$$

Antiferromagnetism

Assumptions

$$\begin{aligned}\bar{n}_\sigma^A &= \bar{n}_{j\sigma}^A, \\ \bar{n}_\sigma^B &= \bar{n}_{j\sigma}^B = \bar{n}_{j\sigma}^C, \\ \bar{n}_\sigma^A &= 2\bar{n}_{-\sigma}^B,\end{aligned}$$

The total magnetization of the system is zero as required by an AF configuration.

Total density of particles

$$\bar{n} = \frac{2\bar{n}_A}{3},$$

Staggered magnetization

$$m_S = \frac{\bar{n}_\uparrow^A - \bar{n}_\downarrow^A}{\bar{n}_\uparrow^A + \bar{n}_\downarrow^A},$$

Diamond chain

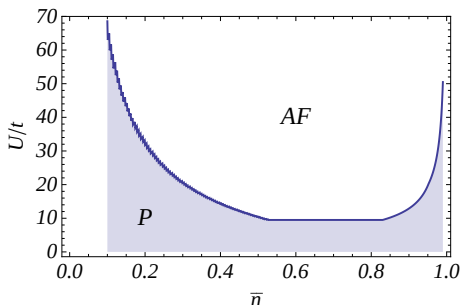


Figure 21: The phase transition between paramagnetic and antiferromagnetic order for a system with 128 cells obtained by studying MF antiferromagnetic ordering. We only plot until $\bar{n} = 1$ since the graphic is even around $\bar{n} = 1$.

- It was observed that AF *always* loses to F or P.
- Agrees with already observed behavior for $\phi = 0$ (Macêdo, et al., 1995)

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Nearest neighbor Coulomb interaction

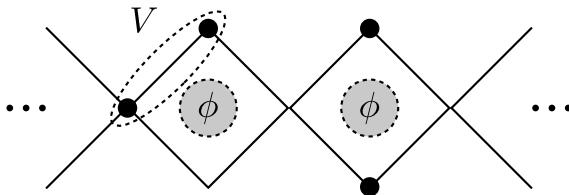


Figure 22: Nearest neighbors Coulomb interaction of strength V .

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 $\phi = 0$:

$$\epsilon_{\sigma}^{\text{flat}} = 2V\bar{n}_A$$

$$\epsilon_{\sigma}^{\pm} = V(\bar{n}_A + 2\bar{n}_B) \pm \sqrt{8t^2 \cos(k/2) + \Delta_V^2},$$

where $\Delta_V = V(\bar{n}_A - 2\bar{n}_B)$.

Order parameter

$$\Delta\bar{n} = \frac{\bar{n}_A - 2\bar{n}_B}{\bar{n}_A + 2\bar{n}_B}.$$

Phase diagram

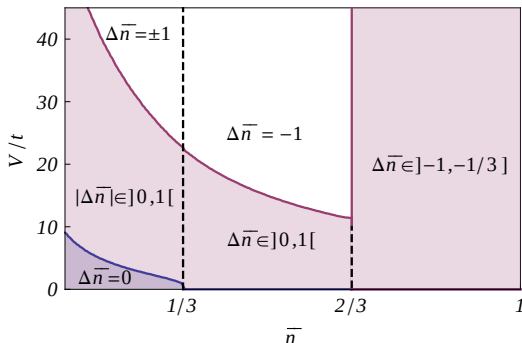
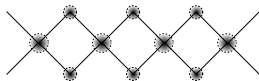
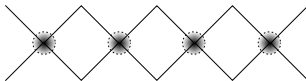


Figure 23: MF phase diagram for the spinless diamond chain considering a nearest neighbors Coulomb interaction and $N_c = 256$.

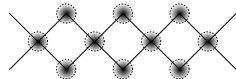
$$\Delta\bar{n} = 0 \Rightarrow \bar{n}_A = 2\bar{n}_B$$



$$\Delta\bar{n} = 1 \Rightarrow \bar{n}_B = 0$$



$$\begin{aligned} \bar{n} = 1 &\Rightarrow \bar{n}_A = \bar{n}_{B,C} = 1 \\ &\Rightarrow \Delta\bar{n} = -1/3 \end{aligned}$$



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Conductance

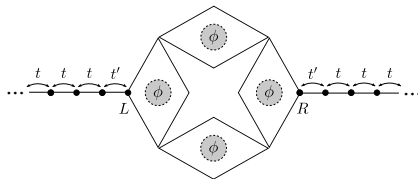


Figure 24: In this chapter we consider the diamond star to be connected, at sites L and R , to semi-infinite tight binding leads via a hopping amplitude t' . The hopping amplitude of the leads is taken to be the same to that of the star, t .

Hamiltonian

$$H_{star} + H_{leads} + H_{hyb}$$

Leads Hamiltonian

$$H_{leads} = -t \sum_{j=1, \sigma}^{\infty} a_{j, \sigma}^{\dagger} a_{j+1, \sigma} + a_{-j-1, \sigma}^{\dagger} a_{-j, \sigma} + \text{H.c.},$$

Hybridization Hamiltonian

$$H_{hyb} = -t' \sum_{\sigma} a_{-1, \sigma}^{\dagger} c_{L, \sigma} + a_{1, \sigma}^{\dagger} c_{R, \sigma} + \text{H.c.}$$

Transmittance

Transmittance

For an incident particle with $\omega = -2t \cos(k)$,

$$T = \frac{4t^2 \sin^2(k) |\tilde{t}(\omega)|^2}{\left| [\omega - \epsilon(\omega) + te^{ik}]^2 - |\tilde{t}(\omega)|^2 \right|}$$

with,

$$\epsilon(\omega) = t'^2 G_{LL}^R(\omega)$$

$$\tilde{t}(\omega) = t'^2 G_{LR}^R(\omega)$$

(Balseiro et al., 1993)

Green's function - momentum space

$$G_{LR}^R(\omega) = \sum_e \frac{\langle g | c_{R\sigma}^\dagger | e \rangle \langle e | c_{L\sigma} | g \rangle}{\omega + E_e - E_g}$$

Numeration

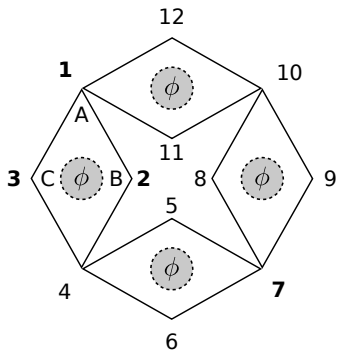


Figure 25: The numeration used for the diamond star.

Conductance peaks

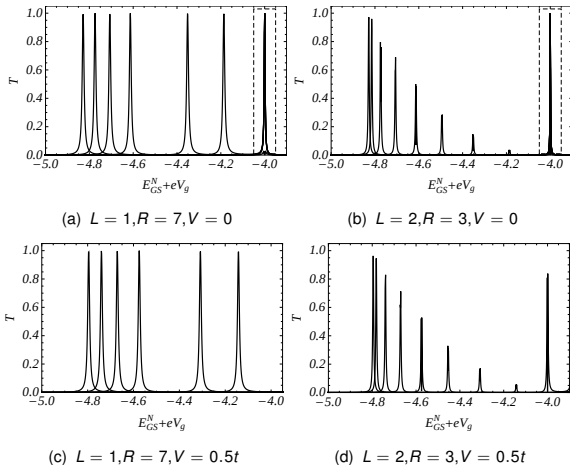


Figure 26: Transmittance peaks for diamond star with $N_c = 4$, $N = 3$, $t' = 0.1t$. The unboxed peaks correspond to the coupling between the ground states of the N and $N - 1$ particles systems for several values of flux. From left to right these are, $\phi = 0, \pi/8, \pi/4, 3\pi/8, \pi/2, 5\pi/8, 3\pi/4, 7\pi/8, \pi$.

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Summary

- Flat, dispersionless band for any value of ϕ
- Periodicity on ϕ is parity(N_c) dependent $\rightarrow$ relevant for molecular systems
- Localized energy eigenbasis for any ϕ (at least for the flat band)
- Addition of hops between next nearest neighbors allow flat band to become dispersive
- Hops can be used to tune m^* (and even its sign)
- Possible to control the number and width of gaps of the system and its bandwidth
- For U interaction we confirmed previous results (for $\phi = 0$) that there is no AF ordering (MF) and extended them to any ϕ
- For V interaction we have obtained an interesting phase diagram
- Very different tunable conductances depending on position of leads (still investigating)