Quasi-Particle Propagation through Interfaces of Weakly and Strongly Correlated Systems

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1 Introduction

- Understanding strongly correlated systems is grand challenge of theoretical physics
- Strongly and weakly interacting particles usually described by different methods
- How to describe a heterostructure thereof while keeping spatial resolution?
- Hierarchy of correlations is a way to solve for the one-site, two-site etc. density operator [1]
- Here: discrete lattice model of solids that provides a mathematical description of systems with a well-defined amount of electronic correlations

2 Hierarchy of correlations [1]

- Systematic expansion in inverse powers of coordination number $1/Z$
- Correlations from reduced density matrices $\hat\rho_{\mu\nu} = \mathrm{tr}_{\mu\nu}(\hat\rho)$, i.e., $\hat\rho_{\mu\nu} = \hat\rho^{\mathrm{corr}}_{\mu\nu} + \hat\rho_\mu\hat\rho_\nu$
- Von-Neumann equation and split up of correlations

$$i\partial_t\hat\rho_\mu = F_1\left(\hat\rho_\mu, \hat\rho^{\mathrm{corr}}_{\mu\nu}\right) \quad i\partial_t\hat\rho^{\mathrm{corr}}_{\mu\nu} = F_2\left(\hat\rho_\mu, \hat\rho^{\mathrm{corr}}_{\mu\nu}, \hat\rho^{\mathrm{corr}}_{\mu\nu\lambda}\right) \quad i\partial_t\hat\rho^{\mathrm{corr}}_{\mu\nu\lambda} = F_3\left(\hat\rho_\mu, \hat\rho^{\mathrm{corr}}_{\mu\nu}, \hat\rho^{\mathrm{corr}}_{\mu\nu\lambda}, \hat\rho^{\mathrm{corr}}_{\mu\nu\lambda\kappa}\right)$$

- Mean-field state $\hat\rho^0_\mu$ without correlations provides the hierarchy

$$\hat\rho_\mu = \mathcal{O}\left(Z^0\right), \quad \hat\rho^{\mathrm{corr}}_{\mu\nu} = \mathcal{O}(1/Z), \quad \hat\rho^{\mathrm{corr}}_{\mu\nu\kappa} = \mathcal{O}\left(1/Z^2\right), \quad \hat\rho^{\mathrm{corr}}_{\mu\nu\kappa\lambda} = \mathcal{O}\left(1/Z^3\right)$$

- Linearization around mean-field to first order yields dynamics of quasi-particles

$$i\partial_t\hat\rho^{\mathrm{corr}}_{\mu\nu} = F_2\left(\hat\rho^0_\mu, \hat\rho^{\mathrm{corr}}_{\mu\nu}\right)$$

3 Fermi-Hubbard model & system

- Mott-insulator (strongly correlated) &semiconductor (weakly correlated)
- Fermi-Hubbard Hamiltonian: Hopping $T_{\mu\nu}$, Coulomb repulsion U_μ and on-site potential V_μ

$$\hat H = -\frac{1}{Z}\sum_{\mu\nu\sigma} T_{\mu\nu}\hat c^\dagger_{\mu\sigma}\hat c_{\nu\sigma} + \sum_\mu U_\mu \hat n_{\mu\uparrow}\hat n_{\mu\downarrow} + \sum_{\mu a} V_\mu \hat n_{\mu\sigma}$$

- U, V used to distinguish Mott and semiconductor
- Mott insulator at half-filling

$$\hat\rho^0_\mu = \left(|\uparrow\rangle_\mu\langle\uparrow| + |\downarrow\rangle_\mu\langle\downarrow|\right)/2$$

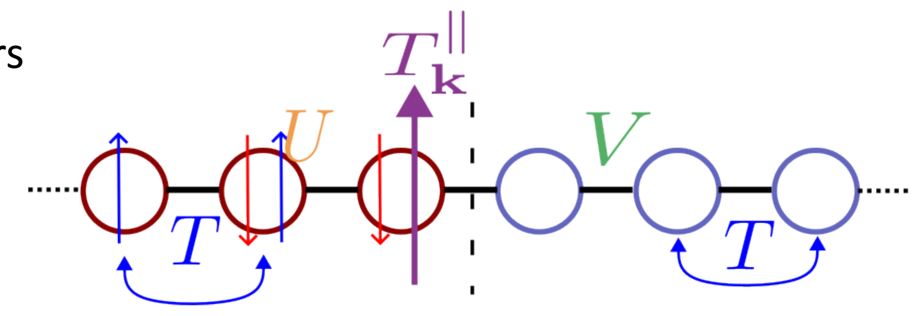
$$U^1_\mu = U, U^0_\mu = 0, V_\mu = 0$$

semiconductor valence (conduction) band

$$\hat\rho^0_\mu = |\uparrow\downarrow\rangle_\mu\langle\uparrow\downarrow| \quad \left(|0\rangle_\mu\langle 0|\right)$$

$$U^i = 0, V_\mu = V$$

- Effective particle $\hat C^1_{\mu\sigma}$ and hole $\hat C^0_{\mu\sigma}$ operators
- Assume hypercubic lattice $T_{\mu\nu} = T\delta_{\mu\nu\pm1}$
- Factorization $\langle\hat C^{\dagger I}_{\mu s}\hat C^J_{\nu s}\rangle^{\mathrm{corr}} = p^*_{\mu s I}p_{\nu s J}$
- Fourier transform parallel to interface
- Effective equations describing quasi-particle modes



$$\left(E - U^I_\mu - V_\mu\right)p^I_\mu + \langle\hat n^I_\mu\rangle^0 \sum_J T^{\parallel}_{\mathbf{k}} p^J_\mu = -T\frac{\langle\hat n^I_\mu\rangle^0}{Z}\sum_J\left(p^J_{\mu-1} + p^J_{\mu+1}\right)$$

4 Mott insulator & semiconductor

- Plane wave ansatz $p^I_\mu = \alpha^I e^{i\kappa\mu} + \beta^I e^{-i\kappa\mu}$ in regions of constant U, V

<u>Mott</u>

- $\cos\kappa_{\mathrm{Mott}} = \frac{Z}{2T}\left[\frac{E(U-E)}{E-U/2} - T^{\parallel}_{\mathbf{k}}\right]$
- $E = \frac{1}{2}\left(U - T_{\mathbf{k}} \pm \sqrt{U^2 + T^2_{\mathbf{k}}}\right)$
- $|\kappa|$ finite for $U \to \infty$
- $\kappa \to \infty$ for $E = U/2$

<u>Semiconductor</u>

- $\cos\kappa_{\mathrm{semi}} = \frac{Z}{2T}\left[V - E - T^{\parallel}_{\mathbf{k}}\right]$
- $E = V - T_{\mathbf{k}}$
- $|\kappa| \propto \ln(V)$

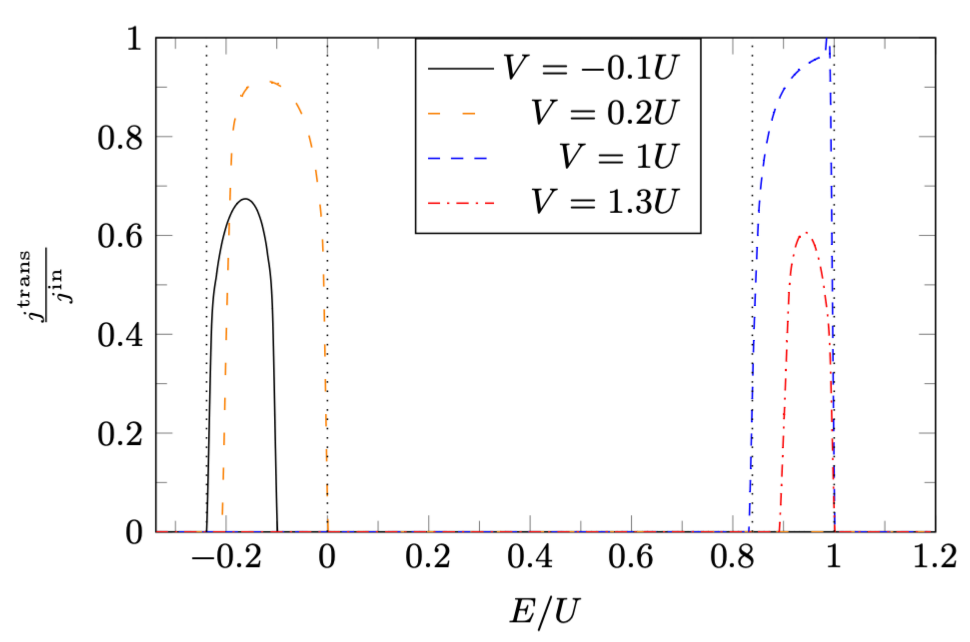
- Divergence in the middle of the Mott gap suggest strong suppression of tunnelling

5 Single interface - Reflection and Transmission

- Incoming wave from Mott $\begin{pmatrix}p^0_\mu\\p^1_\mu\end{pmatrix} = \frac{1}{\sqrt{E^2+(E-U)^2}}\begin{pmatrix}E\\E-U\end{pmatrix}\left[e^{i\kappa_{\mathrm{Mott}}\mu} + Re^{-i\kappa_{\mathrm{Mott}}\mu}\right]$
- $E \approx 0$ hole contributions dominate, $E \approx U$ particle contributions dominate

$$R = -\frac{1-\exp\{-i(\kappa_{\mathrm{Mott}} - \kappa_{\mathrm{semi}})\}}{1-\exp\{i(\kappa_{\mathrm{Mott}} + \kappa_{\mathrm{semi}})\}} \qquad T = \mathcal{N}(2E-U)(1+R)$$

- Analogous to impedance mismatch: $R = 0$ for $\kappa_{\mathrm{Mott}} = \kappa_{\mathrm{semi}}$

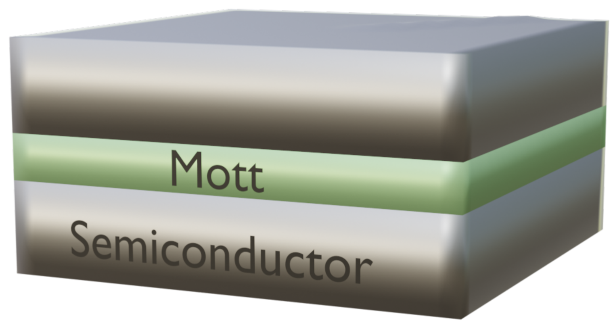


Transmission probability for different semiconductor potentials V over the energy of the incoming wave E/U

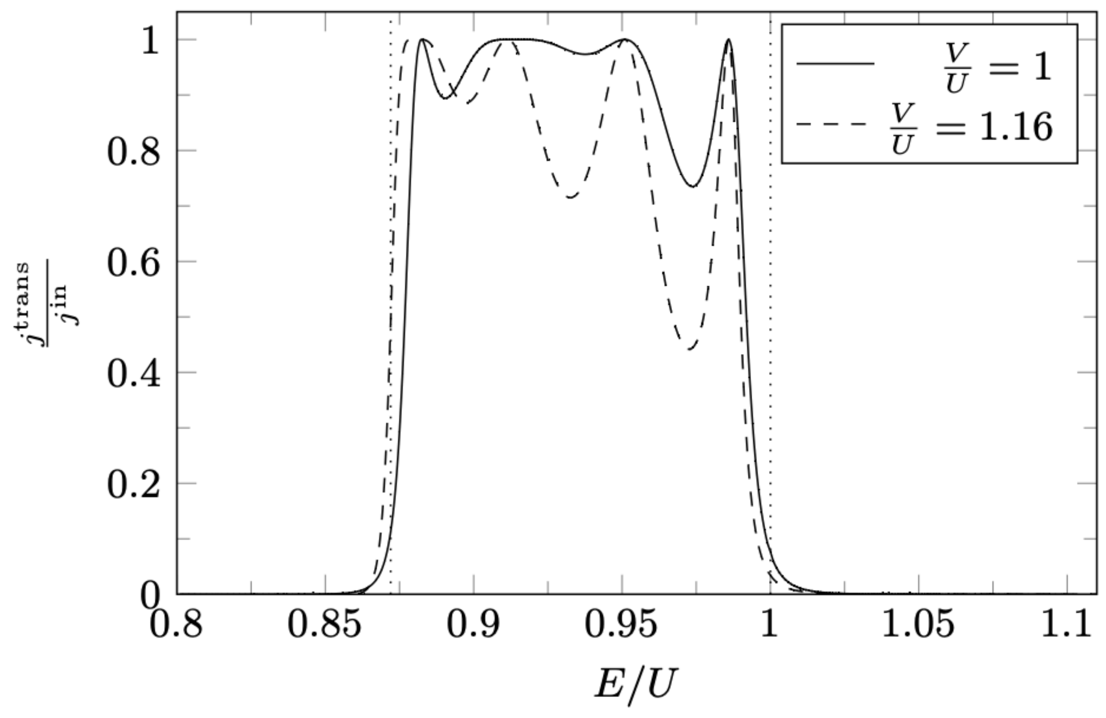
- Semiconductor band edge needs to fall inside the Mott bands (dashed lines)

6 Double interface

- Mott insulator between two semiconducting leads
- Transmission given by



$$\frac{j^{\mathrm{trans}}_n}{j^{\mathrm{in}}_n} = \left|\frac{e^{id\kappa}e^{-i\kappa_{\mathrm{semi}}d}(1-e^{i2\kappa})(1-e^{i2\kappa_{\mathrm{semi}}})}{(1-e^{i\kappa}e^{i\kappa_{\mathrm{semi}}})^2 - e^{i2d\kappa}(e^{i\kappa}-e^{i\kappa_{\mathrm{semi}}})^2}\right|^2$$



Transmission probability through the upper Hubbard band (dotted lines) over the energy of the incoming wave E/U

- Inside Mott bands transmission channels
- Tunnelling inbetween
- Resonances $\kappa_{\mathrm{Mott}} \cdot \pi = zd$

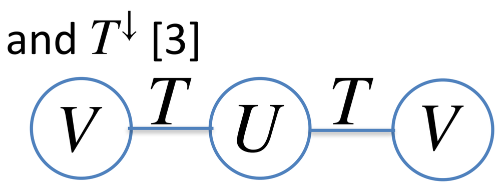
- Tunnelling probability approximated by

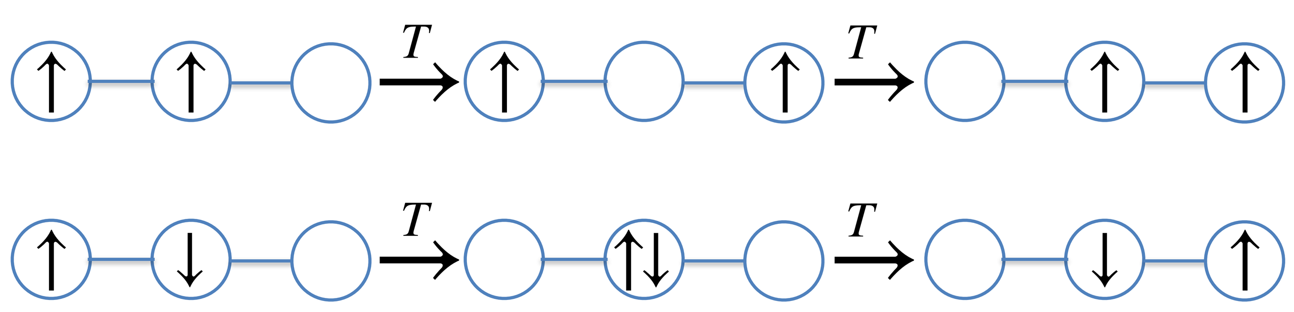
$$\frac{j^{\mathrm{trans}}_n}{j^{\mathrm{in}}_n} \approx 4e^{-2d\kappa_{\mathrm{Mott}}}(1-e^{-2\kappa_{\mathrm{Mott}}})^2(1-\cos(\kappa_{\mathrm{semi}}))^2 \qquad e^{-\kappa_{\mathrm{Mott}}} \approx \frac{4T(E-U/2)}{ZU^2}$$

- Current vanishes in the middle of Mott gap $E = U/2$. Why?

7 Understanding vanishing tunnelling current

- Three-site toy model with second order process amplitude $T^\uparrow$ and $T^\downarrow$ [3]
- Up spin $\uparrow$ needs to pass either $\uparrow$ or $\downarrow$





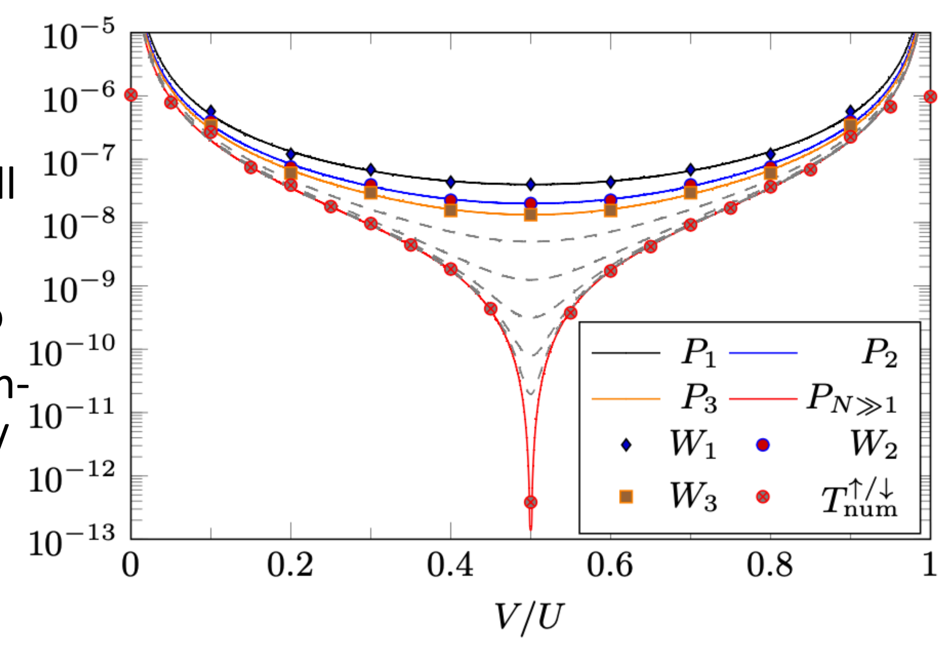
$T^\uparrow = T^2/V$

$T^\downarrow = -T^2/(U-V)$

- Coherent sum of these two possibilites: $T^\uparrow + T^\downarrow = 0$ for $V = U/2$
- The mean-field background $\hat\rho^0_\mu$ of the Mott is a sum over N rows

$$P_N = \frac{N+1}{4N}\left(|T^\uparrow|^2 + |T^\downarrow|^2\right) + \frac{N-1}{2N}\mathrm{Re}(T^\uparrow T^{\downarrow *})$$

- Probability falls as $P_N(V = U/2) \propto 1/N$ and $P_{N\gg1} = |T^\uparrow + T^\downarrow|^2/4$
- Destructive interference of particle and hole channel in the middle of the Mott gap
  - P_N give the analytical formula with perturbation theory amplitudes
  - W_N show numerically obtained transmission probabilty using the full Hamiltonian
  - $T^{\uparrow/\downarrow}_{\mathrm{num}}$ uses amplitudes from the Zeno limit by analytical solution of the von-Neumann equations of the creation/annihilation operators with the full Hamiltonian



➡ Destructive interference of particle and hole current [2]

8 Conclusions & Outlook

- Hierarchy of correlations facilitates iterative scheme to solve von-Neumann equation
- Linearization around mean-field background gives effective dynamics of quasi-particles
- Single Mott-semiconductor interface reflection like electrodynamics impedance mismatch
- Transmission through Mott layer through bands and tunnelling current inbetween
- Destructive interference of particle and hole channel results in vanishing current at $E = U/2$ in the middle of the Mott band gap

Outlook

➡ Include higher order correlations

➡ Do different structures to build, e.g., energy filters

➡ Different mean-field backgrounds give different dispersion relations and hence different

[1] F. Queisser et al. Physical Review A 89.3, 033616 (2014)

[2] J. Verlage et al. arXiv:2303.13507

[3] J. Splettstoesser et.al. Physical Review B86, 035432 (2012)