Interplay of spin and charge channels in zero-dimensional systems: non-perturbative approach to tunneling density of states

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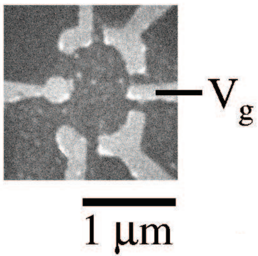
Landau Days Conference, June 22 - 24, 2009

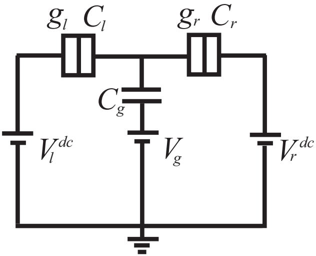
Many thanks to

Igor Kolokolov

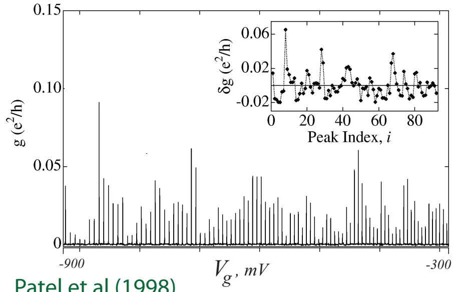
Motivation

- Experiments on transport through quantum dots (QDs) indicating a role of spin degrees of freedom
  - Patel, Stewar, Marcus, Gökçedağ, Alhassid, Stone, Duruöz, Harris, PRL81, 5900 (1998)
  - Lüscher, Heinzel, Ensslin, Wegscheider, Bichler, PRL86, 2118 (2001)





Motivation



Patel et al (1998)

$T = 45\ mK$

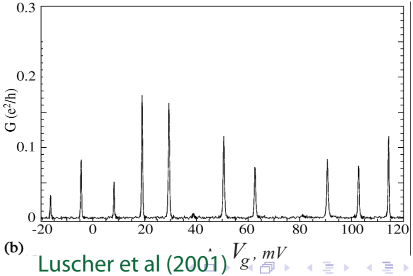
$\delta = 400\ mK$

$E_c = 5\ K$

$T = 120\ mK$

$\delta = 2.3\ K$

$E_c = 14.5\ K$



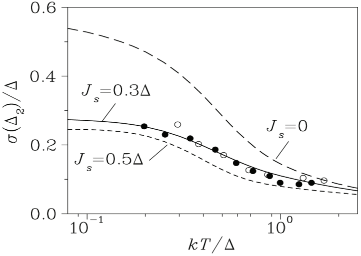
Luscher et al (2001)

Motivation

- Theory on transport through QDs (conductance) at low temperatures $g_{l,r}\delta \ll T \ll \delta$
  - Alhassid, Rupp, PRL91, 056801 (2003)
  - Usaj, Baranger PRB67, 121308 (2003)
- Theory on tunneling density of states (DOS) at high temperatures $\delta \ll T$ (strongly anisotropic exchange $J_z \gg J_\perp$)
  - Kiselev, Gefen PRL96, 066805 (2006)

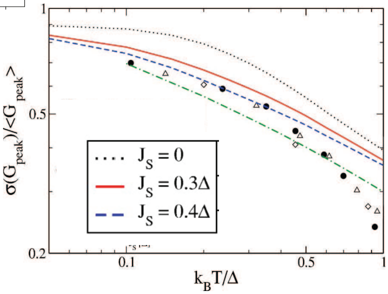
Motivation

Variation of conductance-peak spacing



Alhassid, Rupp (2003)

Variation of conductance-peak height



Usaj, Baranger (2003)

Question to answer

Can we find some signatures of the exchange interaction in physical observables, e.g. conductance, tunneling DOS, at $T \gg \delta$?

Parameters of QDs

E_{Th}	-	Thouless energy
E_c	-	charging energy
T	-	temperature
δ	-	mean level spacing
J	-	exchange energy
N_0	-	external charge

Condition assumed

Thouless conductance $\quad g_T = \dfrac{E_{Th}}{\delta} \gg 1$

Transport via QD

Current through the QD ($g_{l,r}\delta \ll T$)

$$I = e\frac{g_l g_r}{g_l + g_r}\int_{-\infty}^{\infty} d\varepsilon\Big[f(\varepsilon-\mu) - f(\varepsilon-\mu+eV)\Big]\frac{\nu(\varepsilon)}{\nu_0}$$

where $g_{l,r}$ are the tunneling conductances of the left/right junctions and $\nu(\varepsilon)$ stands for the tunneling DOS of the isolated QD.

Tunneling DOS of the isolated QD is the simplest quantity to study!

Universal Hamiltonian

Kurland, Aleiner, Altshuler (2000)

$$\mathcal{H} = \sum_{\alpha,\sigma} \varepsilon_\alpha a^\dagger_{\alpha,\sigma} a_{\alpha,\sigma} + E_c \left(\hat{n} - N_0\right)^2 - J\hat{\boldsymbol{s}}^2$$

$\hat{n} = \sum_{\alpha,\sigma} a^\dagger_{\alpha,\sigma} a_{\alpha,\sigma}$ - particle number operator

$\hat{\boldsymbol{s}}_{\sigma\sigma'} = \frac{1}{2} \sum_{\alpha,\sigma} a^\dagger_{\alpha,\sigma} \vec{\sigma}_{\sigma\sigma'} a_{\alpha,\sigma'}$ - spin operator

Tunneling DOS

$$\nu(\varepsilon) = -\frac{1}{\pi} \operatorname{Im} \sum_{\alpha,\sigma} \mathcal{G}^R_{\alpha\sigma;\alpha\sigma}(\varepsilon),$$

$$\mathcal{G}^R_{\alpha_1\sigma_1;\alpha_2\sigma_2}(t_1, t_2) = -i\theta(t_1 - t_2) \left\langle \left\{ a_{\alpha_1\sigma_1}(t_1), a^\dagger_{\alpha_2\sigma_2}(t_2) \right\} \right\rangle$$

Exact result

$$\nu(\varepsilon) = \frac{1+e^{-\beta\varepsilon}}{\mathcal{Z}} \sum_{n,m} \sum_{\alpha} \delta\Big(\varepsilon - \varepsilon_\alpha - E_c(2n - 2N_0 + 1) - J(m + \frac{1}{4})\Big)$$

$$\times \Big[2m \Big(\mathcal{Z}_{\frac{n}{2}+m}(\varepsilon_\alpha)\mathcal{Z}_{\frac{n}{2}-m}(\varepsilon_\alpha) - \mathcal{Z}_{\frac{n}{2}+m+1}(\varepsilon_\alpha)\mathcal{Z}_{\frac{n}{2}-m-1}(\varepsilon_\alpha)\Big)$$

$$+(2m+1)\Big(\mathcal{Z}_{\frac{n}{2}+m}\mathcal{Z}_{\frac{n}{2}-m}(\varepsilon_\alpha) - \mathcal{Z}_{\frac{n}{2}+m}(\varepsilon_\alpha)\mathcal{Z}_{\frac{n}{2}-m}\Big)\Big] e^{-\beta E_c(n-N_0)^2+\beta J m(m+1)}$$

where

$$\mathcal{Z}_n = \oint \frac{dz}{2\pi i} \frac{\prod_\gamma \left(1 + z e^{-\beta\varepsilon_\gamma}\right)}{z^{n+1}}, \qquad \mathcal{Z}_n(\varepsilon_\alpha) = \oint \frac{dz}{2\pi i} \frac{\prod_{\gamma\neq\alpha} \left(1 + z e^{-\beta\varepsilon_\gamma}\right)}{z^{n+1}}$$

N.B.: In general, there is no periodicity in N_0!

Reasons to believe that our result is right

Grand partition function

$$\mathcal{Z} = \sum_{n,m} (2m+1) \mathcal{Z}_{\frac{n}{2}+m} \mathcal{Z}_{\frac{n}{2}-m} e^{-\beta E_c (n-N_0)^2 + \beta J m(m+1)}$$

is the same as found by Alhassid, Rupp, PRL91, 056801 (2003).

Our result satisfies sum rule:

$$\int_{-\infty}^{\infty} \frac{d\varepsilon \, \nu(\varepsilon)}{1+e^{\beta\varepsilon}} = N_0 + \frac{T}{2E_c} \frac{\partial}{\partial N_0} \ln \mathcal{Z}.$$

At $J=0$ our result coincides with the result of Sedlmayr, Yurkevich, Lerner, EPL76, 109 (2006).

Two remarks

- Emergence of new energy scale: renormalized exchange energy

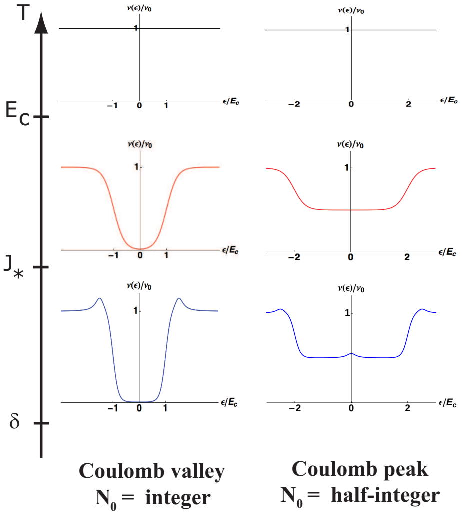
$$J_\star = \frac{J}{1 - J/\delta}$$

Stoner instability at $J = \delta$ similar to Fermi-liquid ($\delta = 1/(\nu V)$)

- For $T \gg \delta$ we shall compute the average tunneling DOS

$$\bar{\nu}(\varepsilon) = \langle \nu(\varepsilon) \rangle_{\{\varepsilon_\alpha\}}$$

TDOS in the case $E_c \gg J_\star \gg \delta > J$



High temperatures: $T \gg J_\star$

$T \gg E_c$: (Coulomb blockade is absent)

$$\overline{\nu}(\varepsilon) = \nu_0 = \text{const}$$

$E_c \gg T \gg J_\star$: (Coulomb blockade)

$$\frac{\overline{\nu}_{J=0}(\varepsilon)}{\nu_0} = \begin{cases} 1 - f(\varepsilon - E_c) + f(\varepsilon + E_c), & N_0 = \text{integer} \\ \frac{1}{2}\Big[2 - f(\varepsilon - 2E_c) + f(\varepsilon + 2E_c)\Big], & N_0 = \text{half}-\text{integer} \end{cases}$$

where $f(E) = 1/[1 + exp(E/T)]$.

Sedlmayr, Yurkevich, Lerner (2006)

No signature of exchange J!
Periodic in N_0

Intermediate temperatures: $J_\star \gg T \gg \delta$

N_0 = integer (Coulomb valley)

$$\overline{\nu}(\varepsilon) = \nu_{J=0}(\varepsilon) + \delta\nu(\varepsilon - E_c) + \delta\nu(-\varepsilon - E_c)$$

where

$$\delta\nu(E) = \frac{\nu_0}{2}\frac{J}{J_\star}\left[1 - f(E) - \mathcal{F}\left(\frac{E}{J_\star}, \frac{J_\star}{T}\right)\right]$$

$$\mathcal{F}(x,y) = \frac{1}{2}\,\mathrm{sgn}\left(\cos\frac{\pi x}{2}\right) e^{-\frac{y(x-1)^2}{4} + \frac{y}{\pi^2}\cos^2\left(\frac{\pi x}{2}\right)}\left[1 - \Phi\left(\frac{\sqrt{y}}{\pi}\left|\cos\frac{\pi x}{2}\right|\right)\right]$$
$$-e^{y(x-|x|)/2}\sum_{m\geqslant 0}(-1)^{m+1}e^{-y|x|m+ym(m+1)}\theta(|x|-(2m+1))$$

and $\Phi(z) = (2/\sqrt{\pi})\int_0^z dt\, exp(-t^2)$

Oscillatory dependence with characteristic energy scale $2J_\star$!

Unfortunately, oscillations are exponentially damped... Periodic in N_0

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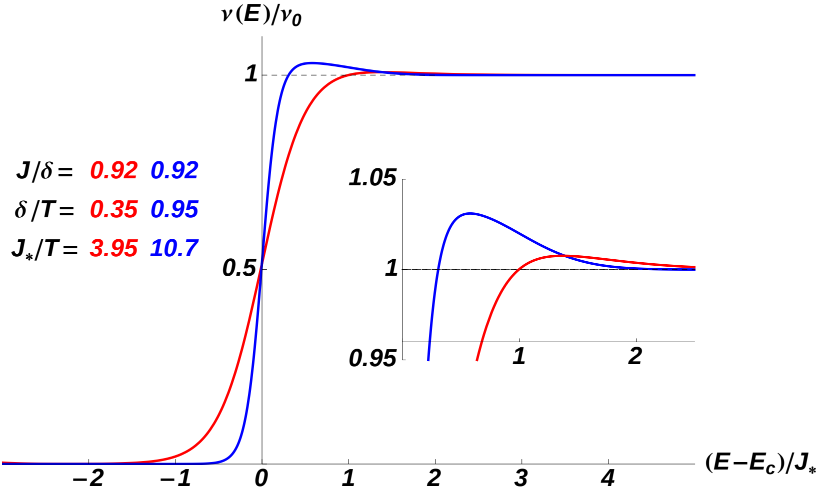

Intermediate temperatures: $J_\star \gg T \gg \delta$

N_0 = half-integer (Coulomb peak)

$$\overline{\nu}(\varepsilon) = \nu_{J=0}(\varepsilon) + \delta\nu(\varepsilon) + \delta\nu(-\varepsilon) + \delta\nu(\varepsilon - 2E_c) + \delta\nu(-\varepsilon - 2E_c)$$

where

$$\delta\nu(E) = \frac{\nu_0 J}{4J_\star}\left[1 - f(E) - \mathcal{F}\left(\frac{E}{J_\star}, \frac{J_\star}{T}\right)\right]$$

$$\mathcal{F}(x,y) = \frac{1}{2}\,\mathrm{sgn}\left(\cos\frac{\pi x}{2}\right) e^{-\frac{y(x-1)^2}{4} + \frac{y}{\pi^2}\cos^2\left(\frac{\pi x}{2}\right)} \left[1 - \Phi\left(\frac{\sqrt{y}}{\pi}\left|\cos\frac{\pi x}{2}\right|\right)\right]$$
$$- e^{y(x-|x|)/2} \sum_{m \geqslant 0} (-1)^{m+1} e^{-y|x|m + ym(m+1)} \theta(|x| - (2m+1))$$

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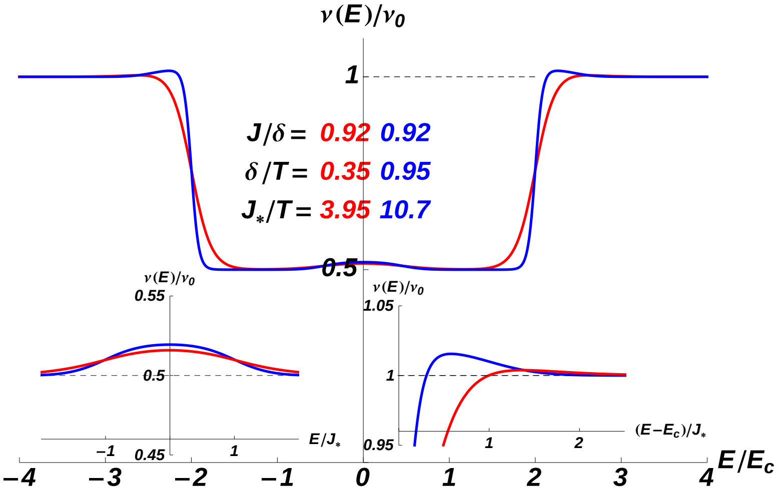

Low temperatures: $\delta \gg T$

- Importance of level statistics
- Signatures of mesoscopic Stoner instability

Numerics in progress ...

Charge and spin separation

$$\mathcal{H} = \sum_{\alpha,\sigma} \varepsilon_\alpha a^\dagger_{\alpha,\sigma} a_{\alpha,\sigma} + E_c \left(\hat{n} - N_0\right)^2 - J\hat{\mathbf{s}}^2$$

$$\hat{n} = \sum_{\alpha,\sigma} a^\dagger_{\alpha,\sigma} a_{\alpha,\sigma}$$ - particle number operator

$$\hat{\mathbf{s}}_{\sigma\sigma'} = \frac{1}{2}\sum_{\alpha,\sigma} a^\dagger_{\alpha,\sigma} \vec{\sigma}_{\sigma\sigma'} a_{\alpha,\sigma'}$$ - spin operator

- Imaginary (Matsubara) time
- Decoupling Coulomb interaction by the Hubbard-Stratonovich field ϕ

Charge and spin separation

$$\mathcal{G}_{\alpha\sigma_1;\alpha\sigma_2}(\tau_1,\tau_2) = \int_{-\pi T}^{\pi T} d\phi_0\, \frac{\tilde{Z}[\phi_0]}{Z} \mathcal{G}_{\alpha\sigma_1\sigma_2}(\tau_1,\tau_2|\phi_0)\mathcal{D}(\tau_1,\tau_2|\phi_0), \qquad Z = \int_{-\pi T}^{\pi T} d\phi_0\, \mathcal{D}(\tau_1,\tau_1|\phi_0)\tilde{Z}[\phi_0]$$

Charge problem:

$$\mathcal{D}(\tau_1,\tau_2|\phi_0) = \sum_{m\in\mathbb{Z}} \int \mathcal{D}[\tilde{\phi}] e^{-\frac{1}{4E_c}\int_0^\beta d\tau\, \tilde{\phi}^2(\tau) - i\int_{\tau_1}^{\tau_2} d\tau\, \tilde{\phi}(\tau) - \frac{\pi^2 T}{E_c}(m+\frac{\beta\phi_0}{2\pi})^2 + 2\pi i N_0 (m+\frac{\beta\phi_0}{2\pi}) - i2\pi m T(\tau_1-\tau_2)}$$

Spin problem:

$$\mathcal{G}_{\alpha\sigma_1\sigma_2}(\tau_1 > \tau_2|\phi_0) = -\frac{\mathrm{Tr}\, e^{-\tau_{12}\mathcal{H}_J} a^\dagger_{\alpha,\sigma_1} e^{(\tau_{12}-\beta)\mathcal{H}_J} a_{\alpha,\sigma_2}}{\mathrm{Tr}\, e^{-\beta\mathcal{H}_J}} = -\frac{K_{\alpha,\sigma_1,\sigma_2}(-i\tau_{12}, -i(\tau_{12}-\beta))}{\tilde{Z}[\phi_0]}$$

$$\mathcal{G}_{\alpha\sigma_1\sigma_2}(\tau_1 < \tau_2|\phi_0) = \frac{\mathrm{Tr}\, e^{-(\tau_{12}+\beta)\mathcal{H}_J} a^\dagger_{\alpha,\sigma_1} e^{(\tau_{12})\mathcal{H}_J} a_{\alpha,\sigma_2}}{\mathrm{Tr}\, e^{-\beta\mathcal{H}_J}} = \frac{K_{\alpha,\sigma_1,\sigma_2}(-i(\tau_{12}+\beta), -i\tau_{12})}{\tilde{Z}[\phi_0]}$$

where

$$\mathcal{H}_J = \sum_{\alpha,\sigma} \tilde{\varepsilon}_\alpha a^\dagger_{\alpha,\sigma} a_{\alpha,\sigma} - J\hat{\mathbf{s}}^2 \qquad \tilde{\varepsilon}_\alpha = \varepsilon_\alpha - i\phi_0$$

N.B.: Charge and spin are entangled due to integration over ϕ_0!

Spin problem

The Hubbard-Stratonovich transformation:

$$e^{\mp itJ\hat{\mathbf{s}}^2} = \lim_{N\to\infty} \prod_{\alpha} \prod_{n=1}^{N} \int d\boldsymbol{\theta}_n \, e^{\pm \frac{i}{4J} t\boldsymbol{\theta}_n^2/N} e^{it\boldsymbol{\theta}_n \hat{\mathbf{s}}_\alpha/N} = \prod_{\alpha} \int \mathcal{D}[\boldsymbol{\theta}] \, e^{\pm \frac{i}{4J} \int_0^t dt' \, \boldsymbol{\theta}^2} \mathcal{T} e^{i \int_0^t dt' \, \boldsymbol{\theta} \hat{\mathbf{s}}_\alpha}$$

Time-ordering $\mathcal{T}$ due to noncommutativity of the spin operators!

We use the method developed in

Kolokolov, Ann. Phys. (1990); Chertkov, Kolokolov JETP (1994), Phys Rev B (1995)

$$\mathcal{T} e^{i \int_0^t dt' \, \boldsymbol{\theta} \hat{\mathbf{S}}} = e^{\pm \hat{S}_\mp \psi_\pm(t)} e^{i\hat{S}_z \int_0^t dt' \rho(t')} \exp\left[i\hat{S}_\pm \int_0^t dt' \, \psi_\mp(t') e^{\mp i \int_0^{t'} d\tau \rho(\tau)} dt' \right] e^{\mp \hat{S}_\mp \psi_\pm(0)}$$

$$\theta_z = \rho - 2\psi_+\psi_-, \quad \frac{\theta_x \mp i\theta_y}{2} = \psi_\mp, \quad \frac{\theta_x \pm i\theta_y}{2} = \mp i\dot{\psi}_\pm + \rho\psi_\pm - \psi_\mp\psi_\pm^2, \quad \boldsymbol{\theta}^2 = \rho^2 \mp 4i\psi_\mp\dot{\psi}_\pm$$

N.B.: The Jacobian of transformation from $\boldsymbol{\theta}$ to $\rho, \psi_\pm$ is $\mathcal{J} = \exp\left[\frac{i}{2} \int_0^t dt' \rho(t')\right]$
Initially, $\theta_{x,y,z}$ are real variables, but now $(\theta_x - i\theta_y)^* \neq \theta_x + i\theta_y$
We impose constraints $\psi_+ = \psi_-^*$ and $\rho = -\rho^*$

From spin problem to quantum mechanics

- Two sets of variables: $\boldsymbol{\theta_{1,2}}$ $\Longrightarrow$ two sets of new variables $\rho_{1,2}$ and $\psi^{\pm}_{1,2}$
- We choose initial condition $\psi^{+}_{1}(0) = \psi^{-}_{2}(0) = 0$
- Exact integration over $\psi^{\pm}_{1,2}$
- New variables: $\rho_{1,2}(t) = \mp i\dot{\xi}_{1,2}$, $\xi_1(0) = \xi_2(0)$, $\xi_1(t_1) + \xi_2(t_2) = 0$,

$$\tilde{Z}[\phi_0] = \prod_{\gamma} \left(- \oint_{|z|=1} \frac{dz_\gamma}{2\pi i z_\gamma^2} e^{-z_\gamma [1+e^{-2\beta\tilde{\varepsilon}_\gamma}]} \right) \int_0^\infty \frac{dy}{4yd} e^{-y} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \delta(\xi_1 + \xi_2 + 2\ln 4yd)$$

$$\times e^{-2d\cosh\frac{\xi_1-\xi_2}{2}} \langle \xi_1 | e^{-i\mathcal{H}_0 t_1} e^{-\xi} e^{i\mathcal{H}_0(t_1+i\beta)} | \xi_2 \rangle, \quad d = \sum_\gamma z_\gamma e^{-\beta\tilde{\varepsilon}_\gamma},$$

$$K_{\alpha\uparrow\uparrow}(t_1, t_2) = e^{-i\tilde{\varepsilon}_\alpha t_1} \prod_{\gamma\neq\alpha} \left(- \oint_{|z|=1} \frac{dz_\gamma}{2\pi i z_\gamma^2} e^{-z_\gamma [1+e^{-2\beta\tilde{\varepsilon}_\gamma}]} \right) \int_0^\infty \frac{dy}{4yd_\alpha} e^{-y} \int_{-\infty}^{\infty} d\xi_1 d\xi_2$$

$$\times \delta(\xi_1 + \xi_2 + 2\ln 4yd_\alpha) e^{-2d_\alpha \cosh\frac{\xi_1-\xi_2}{2}} \left[e^{\xi_1/2} + e^{-\beta\tilde{\varepsilon}_\alpha} e^{\xi_2/2} \right] \langle \xi_1 | e^{-i\mathcal{H}_0 t_1} e^{-3\xi/2} e^{i\mathcal{H}_0 t_2} | \xi_2 \rangle,$$

$$d_\alpha = \sum_{\gamma\neq\alpha} z_\gamma e^{-\beta\tilde{\varepsilon}_\gamma}, \quad \mathcal{H}_0 = -J\frac{\partial^2}{\partial\xi^2} + \frac{J}{4}e^{-\xi}, \quad E_\nu = J\nu^2 \Psi_\nu(\xi), \quad \Psi_\nu(\xi) = \frac{2}{\pi}\sqrt{\nu \sinh 2\pi\nu} K_{2i\nu}(\eta)$$

The final step

$$\tilde{Z}[\phi_0] = \int_{-\infty}^{\infty} dh\, h \sinh(\beta h) e^{-\beta h^2/J} \prod_{\gamma} \left(1 + e^{-\beta(\tilde{\varepsilon}_\gamma + h)}\right) \left(1 + e^{-\beta(\tilde{\varepsilon}_\gamma - h)}\right)$$

$$K_{\alpha\uparrow\uparrow}(\tau) = \frac{1}{2} e^{\frac{J}{4}\tau - \frac{JT}{4}\tau^2} \int_{-\infty}^{\infty} dh \sinh(\beta h) e^{-\beta h^2/J} e^{-\tilde{\varepsilon}_\alpha \tau} \prod_{\gamma \neq \alpha} \left(1 + e^{-\beta(\tilde{\varepsilon}_\gamma - h)}\right) \left(1 + e^{-\beta(\tilde{\varepsilon}_\gamma + h)}\right)$$
$$\times \left[e^{-h\tau}(2\beta h + J\tau - J\beta) + e^{-\beta\tilde{\varepsilon}_\alpha} e^{h(\tau-\beta)}(2\beta h - J\tau) \right]$$

$$\nu(\varepsilon) = -\frac{2}{\pi} \cosh \frac{\varepsilon}{2T} \int_{-\infty}^{\infty} dt\, e^{i\varepsilon t} \sum_{\alpha} \mathcal{G}_{\alpha\uparrow,\alpha\uparrow}\left(it + \frac{1}{2T}\right)$$

Conclusions

- Exact computation of tunneling DOS in quantum dot with direct Coulomb and exchange interaction
- Distinct signatures of exchange in tunneling DOS at intermediate temperatures $J < \delta \ll T \ll J_\star$

- Future work:
  - Tunneling DOS in the presence of magnetic field (Zeeman splitting)
  - Dynamic spin susceptibility

Mesoscopic Stoner instablity ($T \ll \delta$)

Kurland, Aleiner, Altshuler (2000)

$$\mathcal{Z}_N = e^{-\beta E_N^{(0)}} \left(1 + O(e^{-\beta\delta})\right)$$

Equidistant spectrum: $\varepsilon_n = \delta n, \; n = 0, 1, \ldots$

$$\mathcal{Z} \approx \mathcal{Z}^2_{\frac{N_0}{2}} \sum_{S=0}^{\infty} (2S+1) \exp\left[\beta[JS(S+1) - \delta S^2\right]$$

At $T = 0$ transition from $S = s$ to $S = s + 1$ at $J = \delta \dfrac{2s+1}{2s+2}$.

$$S_g = s, \qquad \frac{2s-1}{2s} < J/\delta < \frac{2s+1}{2s+2}, \qquad \begin{cases} s = 0, 1, 2, \ldots & N_0 \gg 1 \quad \text{even} \\ s = 1/2, 3/2, \ldots & N_0 \gg 1 \quad \text{odd} \end{cases}$$