Electrostatic Screening and Friedel Oscillations In Nanostructures

A.V. Chaplik
in collaboration with
V.M. Kovalev, L.I. Magarill, R.Z. Vitlina
A.V. Rzhanov Institute of Semiconductor Physics,
Novosibirsk, Russia

Outline

- 1.Introduction.Screening by charged particles
- Basic equations
- Nanotube
- Double quantum well (DQW)
- Multilayer structure (superlattice)
- 2.Screening by neutral partricles (excitons)
- Friedel oscillations in a hybrid system
- Conclusion

Introduction

3D isotropic system with metallic spectrum: $$\frac{1}{r} \to \frac{e^{-\kappa r}}{r} + \sim \cos(2p_F r)/r^3$$

2D plasma: $$\frac{1}{r} \to N_0 - H_0 \to \frac{a_B^2}{r^3} + \sim \sin(2p_F r)/r^2$$

Dielectric spectrum, uniform system $$U^{tot} = \frac{U^{ext}}{\varepsilon}$$

For Fourier components $$U^{tot}(\omega, k) = \frac{U^{ext}(\omega, k)}{\varepsilon}$$

Nonuniform system

$$U_{ij}^{ext}(\omega, \mathbf{q}) = \varepsilon_{ijnm}(\omega, \mathbf{q}) U_{nm}^{tot}(\omega, \mathbf{q})$$

$\varepsilon_{ijnm}(\omega, \mathbf{q})$ - Matrix dielectric function

Basic equations

$$\left(\frac{d^2}{dz^2} - q^2\right) U_{ind}(\mathbf{q}, z) = -\frac{4\pi e^2}{\varepsilon} \sum_{nm} \Pi_{nm} \varphi_n(z) \varphi_m(z) U_{nm}(\mathbf{q})$$

$$\Pi_{nm}(\mathbf{q}) = -\sum_{\mathbf{k}} \frac{f_n(\mathbf{k}) - f_m(\mathbf{q}+\mathbf{k})}{E_n(\mathbf{k}) - E_m(\mathbf{q}+\mathbf{k}) + i\delta},$$

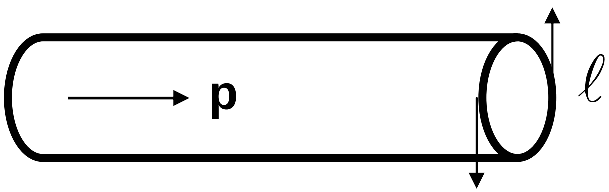
Formal solution: $U_{ind}(z) = \int G(z,z')\, r.h.s.(z')dz' \quad G(z,z') = \frac{1}{2q} e^{-q|z-z'|}$

$$U_{ij}(q) + \frac{2\pi\tilde{e}^2}{q} \sum_{nm} I_{ij,nm}(q) \Pi_{nm}(q) U_{nm} = U^0_{nm}(q), \quad \tilde{e}^2 = e^2/\varepsilon.$$

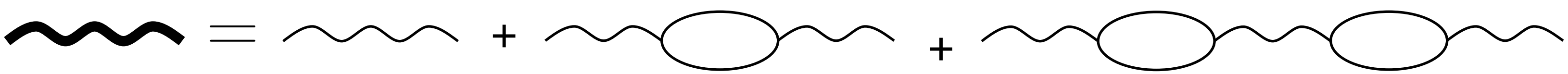
$$I_{ij,nm}(q) = \int \varphi_i(z)\varphi_j(z) e^{-q|z-z'|} \varphi_n(z')\varphi_m(z') dz dz'$$

$$\varepsilon_{ijnm} = \delta_{in}\delta_{jm} + \frac{2\pi\tilde{e}^2}{q} I_{ijnm}(q) \Pi_{nm}(q)$$

Nanotube



$$\varepsilon_{p,l} = \frac{p^2}{2m} + Bl^2; \quad B \equiv \frac{1}{2ma^2}, \qquad l = 0, \pm 1, \pm 2.....$$



$$V(k,n) = \frac{V^{(0)}(k,n)}{1 + V^{(0)}(k,n)\Pi(\omega; k, n)},$$

$$V^{(0)}(k,n) = \tilde{e}^2 \int_{-\infty}^{\infty} \int_0^{2\pi} \frac{e^{-ikz-in\varphi} dz d\varphi}{\sqrt{z^2 + 4a^2 \sin^2(\varphi/2)}} =$$

$$= 4\pi\tilde{e}^2 I_n(|k|a) K_n(|k|a),$$

$$\Pi(\omega;k,n) = \frac{1}{2\pi^2}\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty} dp \frac{f_{p-k,l-n} - f_{p,l}}{\varepsilon_{p,l} - \varepsilon_{p-k,l-n} - \omega - i\delta}$$

$$V(z,\varphi) = \int_{-\infty}^{\infty}\frac{dk}{(2\pi)^2}\exp(ikz)(V(k,0) + 2\sum_{n=1}^{\infty} V(k,n)\cos(n\varphi)).$$

$n = 0,\ V^{(0)}$ *singular at k=0*

$n \neq 0,\ V^{(n)}$ *regular at k=0*

$\Pi \quad regular\ at\ k = 0$

Nanotube

$$V_0(z) \simeq \frac{\tilde{e}^2}{z}\left(\frac{ma_B}{4\pi\kappa_0\Lambda}\right)^2\left(1 - \frac{ma_B/\pi\kappa_0 + 4C}{2\Lambda} + \cdots\right) \sim \frac{1}{z\ln^2(2|z|/a)}$$

$$\kappa_0 \equiv \Pi_0(k \to 0) = m[1/p_0 + 2\sum_{l=1}^{L}(1/p_l)]/\pi^2$$

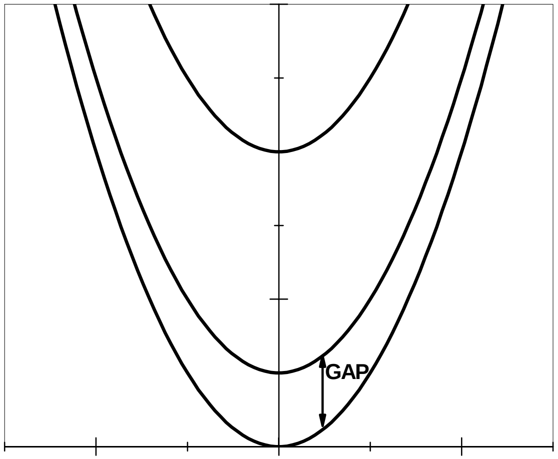
$$V_n^{(0)}(z) = \frac{\tilde{e}^2}{\pi a}Q_{n-1/2}\left(1 + \frac{z^2}{2a^2}\right) \simeq \frac{\Gamma(n+1/2)}{\sqrt{\pi}n!}\frac{\tilde{e}^2}{z}\left(\frac{a}{z}\right)^{2n}$$

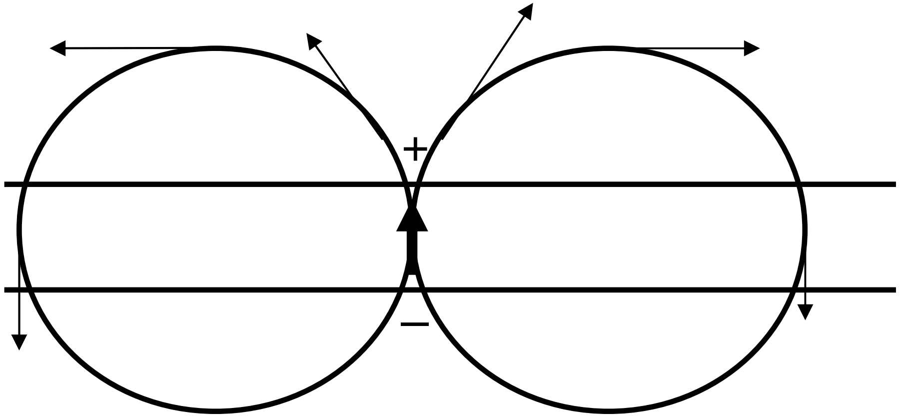
$$V_n(z) \simeq \frac{\Gamma(n+1/2)}{\sqrt{\pi}n!}\frac{\tilde{e}^2}{z}\left(\frac{a}{z}\right)^{2n}\left(1 + \frac{\pi\kappa_n}{ma_Bn}\right)^{-2} \sim \frac{1}{z^{2n+1}}$$

$$\epsilon_n = \left(1 + \frac{\pi\kappa_n}{ma_Bn}\right)^2 \quad \kappa_n = \Pi(\omega = 0; k = 0; n)$$

Effective dielectric constant

Nanotube





Friedel oscillations, zero harmonic

Singularity at $k = 2p_e,\qquad \Pi_0(k \to 2p_e) \to \infty$

rather than $\to 0$ **as in 1D and 2D systems**

$$\widetilde{V}_0(z) = -\frac{Q}{e}\sum_{l=-L}^{l=L}\frac{2\pi^2 p_l}{m}\frac{\cos(2p_l z)}{|z|\ln^2(4p_l|z|)}[1 - \frac{2C}{\ln(4p_l|z|)} + \ldots]$$

$\widetilde{V}_0(z)$ **decreases not slower than** $\overline{V}_0(z)$

$\widetilde{V}_0 / \overline{V}_0 \propto 1/p_F a_B$ **and for metallic limit** $p_F a_B >> 1$

effect of $\widetilde{V}_0(z)$ **is small**

Friedel oscillations, non-zero harmonics

Singularity exists not for all values of *n*.

$$\mathrm{Re}(\Pi(k,n)) = \frac{m}{2\pi^2 k}\sum_{l=-L}^{L} \ln\left|\frac{(k^2a^2+n^2+2kp_l a^2)^2-4n^2l^2}{(k^2a^2+n^2-2kp_l a^2)^2-4n^2l^2}\right|$$

$$L=[p_F a] \qquad |l| \le L$$

$$k_c = p_l \pm \sqrt{p_F^2 - \frac{(n-l)^2}{a^2}} \Rightarrow p_F^2 a^2 > (n-l)^2$$

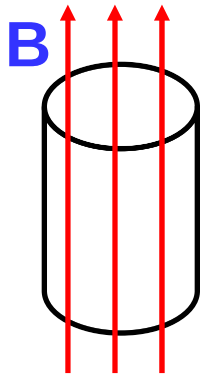
Oscillations exist only for $n \le 2L+1$

Otherwise only monotonous part.

$$\tilde{V}_n(z) = -\frac{Q}{e}\frac{2\pi^2}{m|z|}\sum_l \frac{k_c\cos(k_c z)}{\ln^2(|z|q_l)}\,; \quad \Pi \sim \ln\left|\frac{q_l}{k-k_c}\right|$$

$$\tilde{V}_n(z) >> \bar{V}_n(z) \propto z^{-(2n+1)}$$

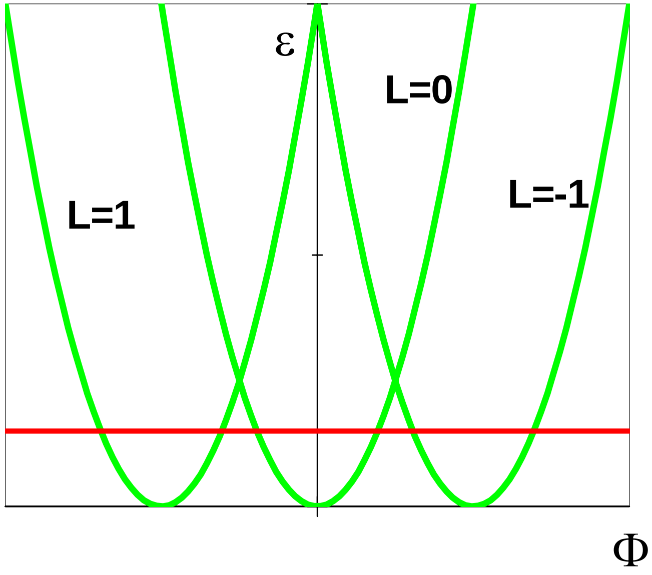
Nanotube in $B_{\parallel}$



$$\varepsilon_{p,\ell}(\Phi) = \frac{p^2}{2m} + B(\ell + \Phi)^2$$

$$\Phi = \frac{\pi a^2 B}{\Phi_0}$$

$$\Pi(\Phi) = \Pi(\Phi + 1)$$



$$\kappa_0 \to \kappa_0(\Phi) = \kappa_0(\Phi + 1)$$

$$\varepsilon_n \to \varepsilon_n(\Phi) = \varepsilon_n(\Phi + 1)$$

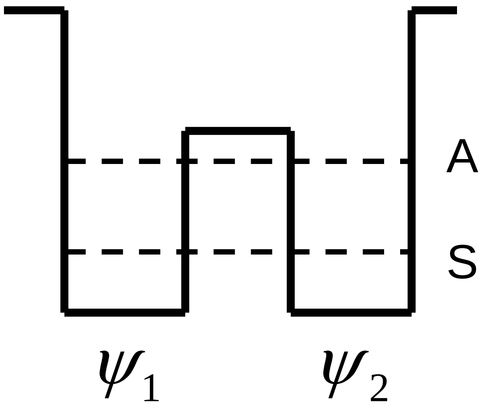
Screening oscillates with changing Φ

Double quantum well

Symmetric structure

$$\varphi_n(-z) = \pm\varphi_n(z)$$

$$I_{11,12} = I_{22,21} = 0$$

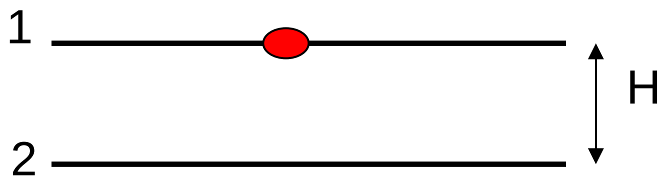


Equation for U_{12} is split off

$$U_{12}(q) = \frac{U^0_{12}(q, z_0)}{1 + \gamma_q[\Pi_{12}(q) + \Pi_{21}(q)]I_4(q)} \qquad I_4(q) = I_{12,12}(q)$$

$$\varphi_1(z) = \frac{\psi_1(z) + \psi_2(z)}{\sqrt{2}}, \varphi_2(z) = \frac{\psi_1(z) - \psi_2(z)}{\sqrt{2}} \qquad \gamma_q = \frac{2\pi e^2}{\varepsilon q}$$

Screened potential in the wells 1 and 2



$$\langle U \rangle_{1,2} = \frac{U_{11} + U_{22}}{2} \pm U_{12},$$

At $\rho \to \infty$

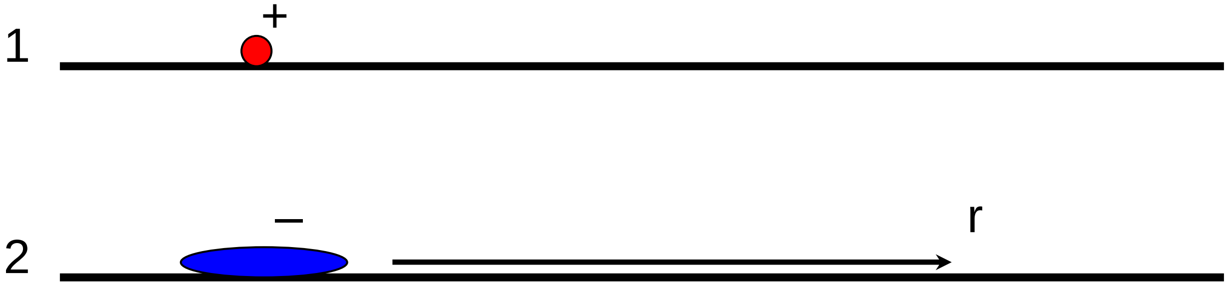
$$U_{11}(\rho) = U_{22}(\rho) \sim \frac{\tilde{e}^2}{(2q_s)^2 \rho^3}, \quad q_s = 2/a_B$$

$$U_{12}(\rho) \sim \frac{\tilde{e}^2 H^2}{2(1 + \pi \tilde{e}^2 H \Pi_0)\rho^3}.$$

$$\Pi_0 = \frac{2(N_1 - N_2)}{E_2 - E_1}$$

Overscreening in the QW 2

$$H > H_C = a_B / 2, \quad \frac{U_{11} + U_{22}}{2} < U_{12}$$



Friedel oscillations in DQW

Singularity stems from

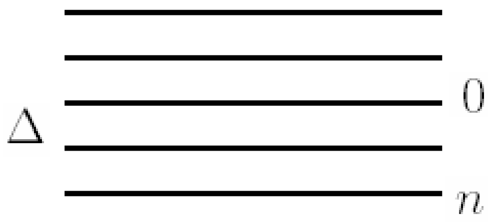
$$q = 2p_1, 2p_2$$

$$\tilde{U}_{11} \propto A\frac{\sin(2p_1\rho)}{(2p_1\rho)^2} + B\frac{\sin(2p_2\rho)}{(2p_2\rho)^2}$$

$$\left\langle U \right\rangle_{1,2} \propto \tilde{U}_{11} \pm C\frac{\sin(p_1 + p_2)\rho}{(p_1 + p_2)^2\rho^2}$$

Combination frequency

Multilayer structure



$$\varphi_n^2(z) = \delta(z - n\Delta)$$

$$I_{nn,mm} = e^{-k\Delta|n-m|}$$

$$U_{nn} + \gamma_q \sum_m \Pi_{mm} e^{-q\Delta|n-m|} U_{mm} = \gamma_q e^{-q\Delta|n_0-n|}$$

$$\Pi_{mm} \equiv \Pi(q)$$

$$U(k,q) = \frac{\gamma_q Q(k,q)}{1 + \gamma_q \Pi(q) Q(k,q)},$$

$$U(k,q) = \sum_n U_{nn}(q) e^{-ik\Delta n},$$

$$-\frac{\pi}{\Delta} < k < \frac{\pi}{\Delta}$$

$$Q(k,q) = \frac{\sinh(q\Delta)}{\cosh(q\Delta) - \cos(k\Delta)}.$$

Multilayer structure

$\rho >> \Delta, n >> 1$ $k\Delta, q\Delta << 1$ $q << p_F$

$$U(\rho, n) = \frac{\tilde{e}^2}{r_n} \exp(-r_n \kappa)$$

$$\frac{1}{\kappa} = \sqrt{\Delta a_B} / 2$$

$$r_n^2 = \rho^2 + (n\Delta)^2$$

$$U(\rho = 0, n >> 1) = \left(1 + \frac{q_s \Delta}{3}\right)^{-1} \frac{\tilde{e}^2}{|z|} \exp(-\kappa |z|),$$

$$U(\rho >> \Delta, n = 0) = \left(1 + \frac{q_s \Delta}{2}\right)^{-1/2} \frac{\tilde{e}^2}{\rho} \exp(-\kappa \rho).$$

Friedel oscillations

$$q \sim 2p_F$$

$$U_n(\rho) = -\tilde{e}^2 q_s \frac{\sinh^2(2p_F\Delta)}{\sinh^2(2p_F\bar{\Delta})} \coth(2p_F\bar{\Delta}) e^{-2p_F\bar{\Delta}|n|} \frac{\sin(2p_F\rho)}{(2p_F\rho)^2},$$

$$\cosh(2p_F\bar{\Delta}) = \cosh(2p_F\Delta) + \frac{q_s}{2p_F}\sinh(2p_F\Delta). \quad q_s = 2/a_B$$

Decay length in z – direction: $(2p_F\bar{\Delta}/\Delta)^{-1} \neq$ period of oscillations in x,y – directions: $(2p_F)^{-1}$

Screening by neutral particles: indirect dipolar excitons

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Trapping Indirect Excitons in a GaAs Quantum-Well Structure with a Diamond-Shaped Electrostatic Trap

A. A. High,[1] A. K. Thomas,[1] G. Grosso,[1] M. Remeika,[1] A. T. Hammack,[1] A. D. Meyertholen,[1] M. M. Fogler,[1] L. V. Butov,[1] M. Hanson,[2] and A. C. Gossard[2]

[1]Department of Physics, University of California at San Diego, La Jolla, California 92093-0319, USA
[2]Materials Department, University of California at Santa Barbara, Santa Barbara, California 93106-5050, USA

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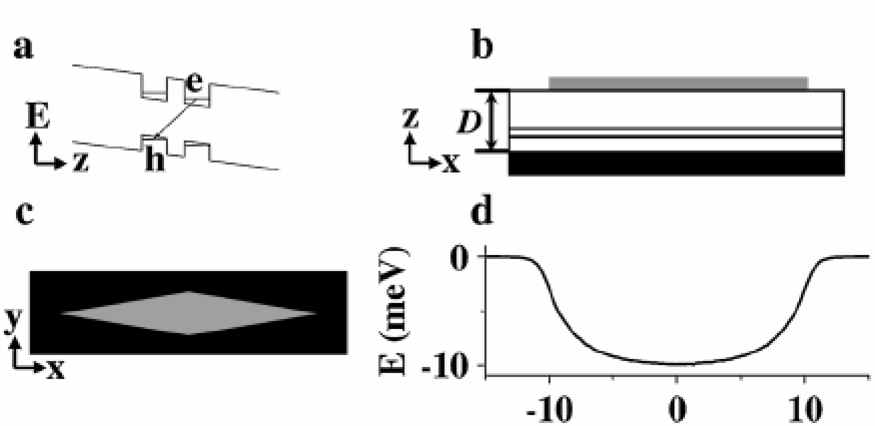
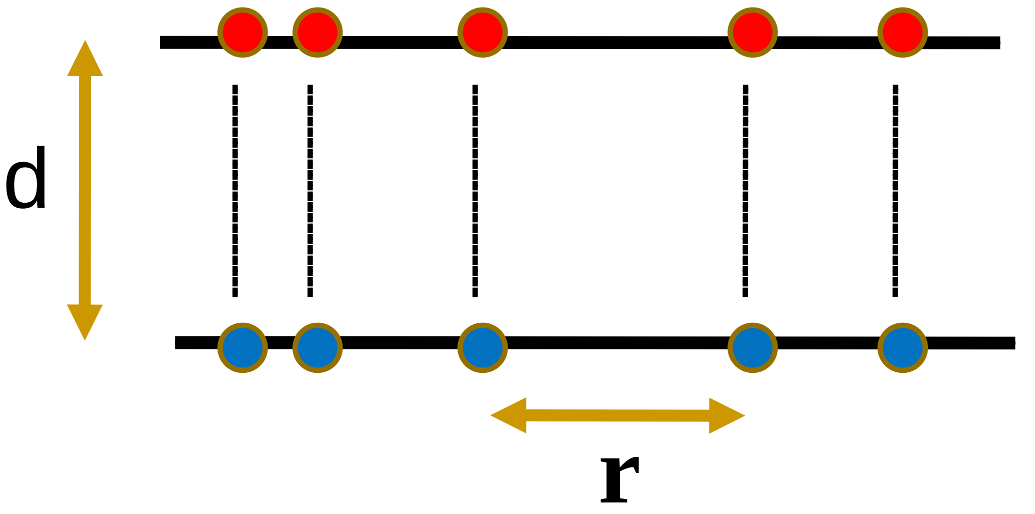


At low densities and temperatures, excitons in the trap are localized by the disorder potential. However, with increasing density, the disorder is screened by exciton-exciton interaction, and the excitons become free to collect to the trap center.

Our question:
How do neutral particles screen defects?

System under study: Excitonic Bose gas with repulsive interaction



$$W^{ex-ex}(\mathbf{r}) = \frac{2e^2}{\varepsilon_0}\left(\frac{1}{|\mathbf{r}|} - \frac{1}{\sqrt{d^2+\mathbf{r}^2}}\right) \qquad W^{ex-ex}(\mathbf{q}) = \frac{4\pi e^2}{q\varepsilon_0}\left(1-e^{-qd}\right)$$

Screening: Basic equations of the linear static response

$$W^{tot} = U + W^{ind} \quad (1)$$

$$W^{ind}(\mathbf{r}) = \int W^{ex-ex}(\mathbf{r} - \mathbf{r}')\delta n(\mathbf{r}')d\mathbf{r}' \quad (2)$$

$$\delta n(\mathbf{q}) = W^{tot}(\mathbf{q}) \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}^{B} - f_{\mathbf{k}+\mathbf{q}}^{B}}{E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}} - i0} \quad (3)$$

$$W^{ind}(\mathbf{q}) = \frac{4\pi e^2}{q\varepsilon_0}\left(1 - e^{-qd}\right)\delta n(\mathbf{q}) \quad (4)$$

Screening: Results

$$W^{tot}(\mathbf{q}) = \frac{U(\mathbf{q})}{1 - W^{ex-ex}(\mathbf{q})\Pi(\mathbf{q})}; \quad \Pi(\mathbf{q}) = \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}^{B} - f_{\mathbf{k}+\mathbf{q}}^{B}}{E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}} - i0}$$

Behavior of the total potential at large distance (r>>d) is given by

$$W^{tot}(\mathbf{r}) = \frac{U(\mathbf{r})}{\varepsilon} \qquad \varepsilon = 1 + \frac{2d}{a_B^*}\left(e^{\frac{2\pi}{mT}n} - 1\right)$$

Screening is of *dielectric* type

Screening: Basic equations of the linear response with Bose-Einstein condensate

$$W^{tot} = U + W^{ind} \quad \text{where} \quad W^{ind}(\mathbf{q}) = \frac{4\pi e^2}{q\varepsilon_0}\left(1 - e^{-qd}\right)\delta n(\mathbf{q})$$

$\delta n(\mathbf{q})$ **is found from the Gross-Pitaevskii equation:**

$$\left(-\frac{\Delta}{2m} + U(\mathbf{r}) + \int d\mathbf{r}' \,|\Psi(\mathbf{r}')|^2\, W^{ex-ex}(\mathbf{r}-\mathbf{r}')\right)\Psi(\mathbf{r}) = \mu\Psi(\mathbf{r})$$

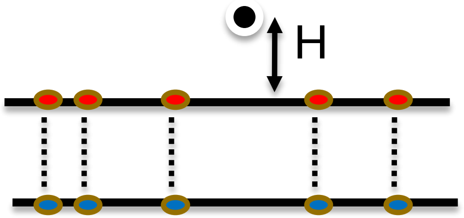
$$\Psi(\mathbf{r}) = \sqrt{n_c} + \varphi(\mathbf{r}); \quad \varphi(\mathbf{r}) << \sqrt{n_c}$$

$$W^{tot}(\mathbf{q}) = \frac{U(\mathbf{q})}{\varepsilon(\mathbf{q})} \qquad \varepsilon(\mathbf{q}) = 1 + \frac{4mn_c W^{ex-ex}(\mathbf{q})}{\mathbf{q}^2}$$

Results of calculations

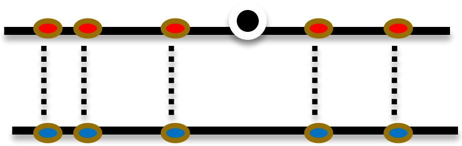
Screening of Coulomb impurity placed at the distance H above exciton layer:

$$W^{tot}(\rho) \propto \frac{3H(2H^2 - 3\rho^2)}{n_c (H^2 + \rho^2)^{7/2}}$$



Screening of Coulomb impurity placed at H=0:

$$W^{tot}(\rho) \propto \frac{1}{n_c^4 \rho^7} + \frac{\alpha}{\rho^5}$$



Contribution of the condensate particles

Contribution of the over condensate particles

Screening of neutral perturbation (like a well width fluctuation):

$$W^{tot}(\rho) \propto -\frac{1}{n_c \rho^5}$$

At T=0 BEC results in steep decrease of the screened potential.

Nonlinear screening: basic equations

$$W^{tot} = U + W^{ind}$$

For large distances (r>>d) we have a local relation:

$$W^{ind}(\mathbf{r}) = \int W^{ex-ex}(\mathbf{r}-\mathbf{r}')\delta n(\mathbf{r}')d\mathbf{r}' \Rightarrow W^{ind}(\mathbf{r}) \approx \frac{4\pi e^2 d}{\varepsilon_0}\delta n(\mathbf{r})$$

In the case of degenerate exciton gas the total potential $W^{tot}(r)$ obeys the nonlinear equation:

$$W^{tot}(\mathbf{r}) = U(\mathbf{r}) - \frac{2d}{a^*}T\ln\left(\frac{1-Qe^{W^{tot}(\mathbf{r})/T}}{1-Q}\right)$$

$$a^* = \varepsilon_0\hbar^2 / me^2 \qquad Q = 1 - e^{-2\pi n/mT}$$

Strong attraction

$|U| >> T$ suppose $|W^{tot}| << |U|$

neglect left-hand-side

Solution: $W^{tot} = \mu + T(1 - e^{\beta\mu})\exp[a_B^* U(r)/2dT]$

Density

$$n(\mathbf{r}) = -\frac{mT}{2\pi}\ln\left(1 - e^{\beta(\mu - W^{tot})}\right) \approx -\frac{mT}{2\pi}\left[\ln(1 - e^{\beta\mu}) + \frac{a_B^* U}{2dT}\right]$$

Strong attraction

Total number of particles:

$$N = \int d\mathbf{r}\, n(\mathbf{r}) = -\frac{mT}{2\pi} S \ln(1 - e^{\beta\mu}) - \frac{m a_B^*}{4\pi d} \int d\mathbf{r}\, U(\mathbf{r})$$

$$n_0 = N/S, \qquad \overline{U} = \frac{1}{S} \int d\mathbf{r}\, U(\mathbf{r})$$

$$W^{tot} = -T e^{-2\pi n_0/mT} e^{-a_B^* \overline{U}/2dT} \left(1 - e^{a_B^* U(\mathbf{r})/2dT}\right), \quad U < 0$$

Coulomb $\overline{U} = 2ze^2/R$

Nonlinear screening: results

Analytic solution of nonlinear equation can be found in limiting cases: *Weak perturbation:*

$$|U(\mathbf{r})| << T$$

$$W^{tot}(\mathbf{r}) = \frac{U(\mathbf{r})}{\varepsilon_{eff}}; \quad \varepsilon_{eff} = 1 + \frac{2d}{a_B^*}\left(e^{\frac{2\pi}{mT}n} - 1\right)$$

Strong perturbation:

$$|U(\mathbf{r})| >> T$$

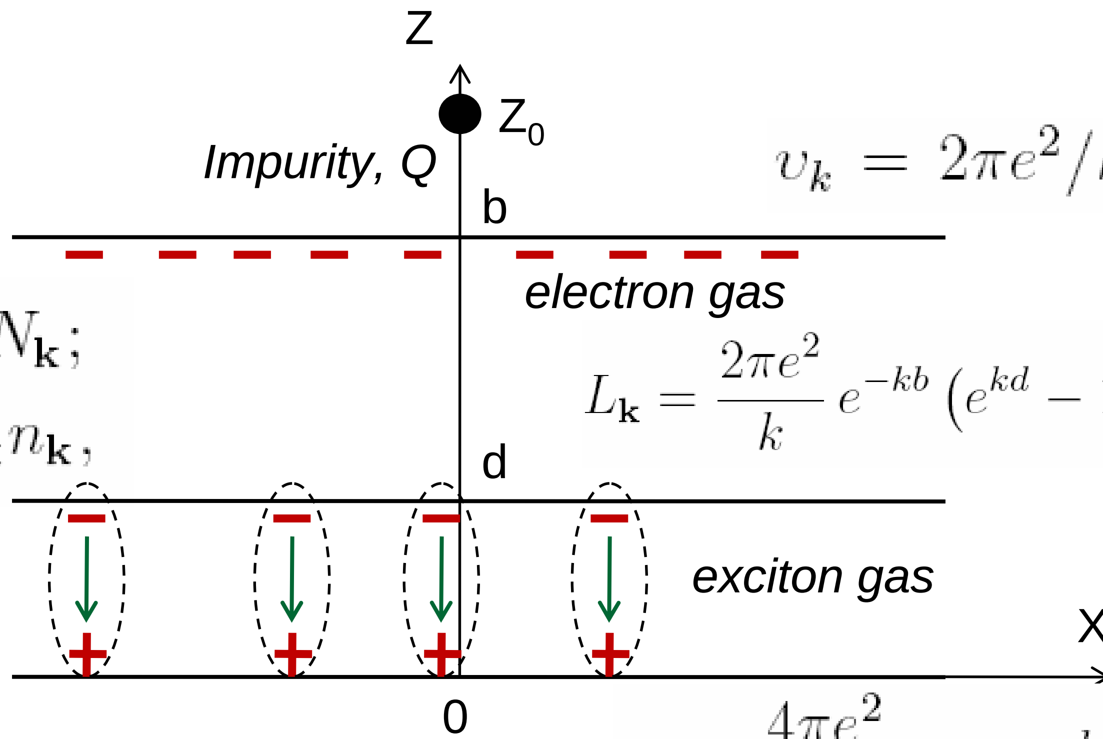
$$W^{tot} = Te^{-\frac{2\pi}{mT}n} << T << |U(\mathbf{r})|$$

In both cases screening becomes very strong with increasing exciton concentration n.

Modulation of exciton density in a hybrid structure

$$n_k = U_k^e \Pi_k^e$$

$$N_k = U_k^{ex} \Pi_k^{ex}$$



$$v_k = 2\pi e^2 / k$$

$$U_{\mathbf{k}}^e = V_{\mathbf{k}}^e + v_{\mathbf{k}} n_{\mathbf{k}} + L_{\mathbf{k}} N_{\mathbf{k}};$$

$$U_{\mathbf{k}}^{ex} = V_{\mathbf{k}}^{ex} + g_{\mathbf{k}} N_{\mathbf{k}} + L_{\mathbf{k}} n_{\mathbf{k}},$$

$$L_{\mathbf{k}} = \frac{2\pi e^2}{k} e^{-kb} \left(e^{kd} - 1\right)$$

$$g_k = \frac{4\pi e^2}{k} (1 - e^{-kd})$$

$$V_{\mathbf{k}}^e = \frac{2\pi e Q}{k} e^{-k|b - z_0|}$$

$$V_{\mathbf{k}}^{ex} = \frac{2\pi e Q}{k} \left(e^{-k|z_0 - d|} - e^{-k|z_0|}\right)$$

Friedel oscillations of excitons

$$N_k = \Pi_k^{ex} \frac{V_k^{ex}(1 - \upsilon_k \Pi_k^e) + V_k^e L_k \Pi_k^e}{(1 - \upsilon_k \Pi_k^e)(1 - g_k \Pi_k^{ex}) - L_k^2 \Pi_k^e \Pi_k^{ex}}.$$

$$\Pi_k^e = -\frac{m}{\pi}\left[1 - \theta\left(1 - \frac{4p_0^2}{k^2}\right)\sqrt{1 - \frac{4p_0^2}{k^2}}\right]$$

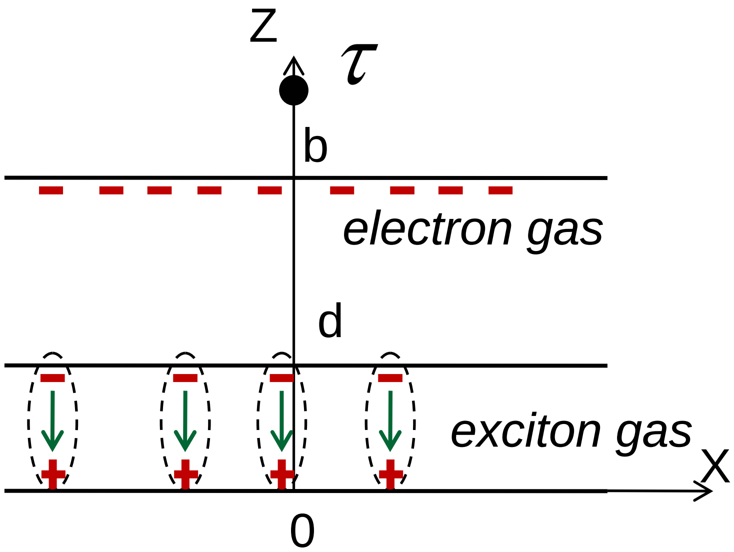
$$N(\rho) = \frac{Qk_0}{4\pi e \rho^3}\left[\frac{\alpha + (1 + k_0 d)\beta}{k_s(1 + k_0 d)^2}\right]$$

$$\tilde{N}(\rho) = -\frac{A}{2\pi\sqrt{2}}\frac{\sin(2p_0\rho)}{\rho^2}.$$

$$N_0 << n_0$$

$$A \approx -\frac{Q}{e}\frac{mMe^4}{p_0^2}\frac{N_0}{n_0} e^{-2p_0(b+|b-z_0|)}\left[e^{2p_0 d} - 1\right]$$

Estimations



$$\tilde{N}(x) = -\frac{A}{2\sqrt{\pi p_0}} \frac{\sin(2p_0 x + \pi/4)}{x^{3/2}}$$

$N_0 << n_0$

$$A \approx -\frac{\tau}{e} \frac{mMe^4}{p_0^2} \frac{N_0}{n_0} e^{-2p_0(b+|b-z_0|)} \left[e^{2p_0 d} - 1\right].$$

$$d = 100A, b = 250A, z_0 = 300A$$

$$N_0 = 10^{10}\, cm^{-2},\ n_0 = 10^{12}\, cm^{-2},\ \tau/e = 10^8 cm^{-1} \quad x = 10^{-4}\, cm$$

$$-\frac{A}{2\sqrt{\pi p_0}\, x^{3/2}} \approx 2.5 \cdot 10^8\, cm^{-2}.$$

Conclusion

- Zero azimuth harmonic of the Coulomb potential in nanotubes is screened rather weakly $1/z(\ln z)^2$.
- All n-th ($n \neq 0$) harmonics are screened in accord with dielectric mechanism and the effective dielectric constant depends on ***n***.
- In DQW radius of screening depends on difference of the populations of the subbands because of contribution of the intersubband transitions (off-diagonal element); in the equilibrium case this radius becomes constant as soon as the second subband starts to be populated.
- Friedel oscillations include contribution with combination period if both subbands of DQW are populated.
- In infinite periodic system of 2D layers screening of the Coulomb potential becomes three-dimensional (Yukawa law); the role of the radius of screening plays a quantity independent of the electron concentration. Anisotropy of the system manifests itself in the dependence of the preexponential factor on direction.
- Amplitude of the Friedel oscillations in the ***n***-th plane of the superlattice exponentially decreases with increasing ***n .***