能隙方程的计算

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我们在这里处理能隙方程，这是一个典型的非线性方程，即自洽方程，其中问题的难点并不是解方程本身，而是其中的无量纲化问题.

1 BCS 能隙方程

$$\frac{1}{N(0)V}=\int_0^{\hbar\omega_D}\frac{\tanh\frac{\beta\sqrt{\xi^2+\Delta^2}}{2}}{\beta\sqrt{\xi^2+\Delta^2}}d\xi, \tag{1}$$

其中 $N(0)$ 是能态密度，V 是相互吸引作用强度，ω_D 是德拜频率，Δ 是能隙函数.

下面开始做准备工作. 令

$$\delta=\frac{\Delta(T)}{\Delta(0)}, \tag{2}$$

$$\tau=\frac{T}{T_c}, \tag{3}$$

$$\eta=\frac{1}{N(0)V}. \tag{4}$$

1.1 求 T_c

$$\begin{aligned}\eta&=\int_0^{\hbar\omega_D}\tanh\frac{\xi}{2k_BT_c}\frac{d\xi}{\xi}\\&=\int_0^{\kappa}\frac{\tanh z}{z}dz\qquad\left(\kappa=\frac{\hbar\omega_D}{2k_BT_c}\right)\\&=\ln z\tanh z\Big|_0^{\kappa}-\int_0^{\kappa}\frac{\ln z}{\cosh^2 z}dz\\&\approx\ln\kappa+\ln\frac{4e^{\gamma}}{\pi}\\&=\ln\frac{4e^{\gamma}\kappa}{\pi},\end{aligned} \tag{5}$$

其中用到了欧拉积分公式

$$\int_0^{\infty}\frac{\ln x}{\cosh^2 x}dx=-\ln\frac{4e^{\gamma}}{\pi} \tag{6}$$

其中 γ 为欧拉常数，并有条件 $\hbar\omega_D\gg k_BT_c$. 因此，

$$\frac{\hbar\omega_D}{k_BT_c}=\frac{2e^{\gamma}}{\pi}e^{-\eta}\approx 1.134e^{-\eta}. \tag{7}$$

1.2 求零温能隙

$$\eta=\int_0^{\hbar\omega_D}\frac{d\xi}{\sqrt{\xi^2+\Delta_0^2}}, \tag{8}$$

得出

$$\frac{\hbar\omega_D}{\Delta_0}=\sinh\eta, \tag{9}$$

化简后有

$$\Delta_0 = 2\pi k_B T_c e^{-\gamma} \approx 1.76 k_B T_c, \tag{10}$$

其中用到了 $\hbar\omega_D \gg k_B T_c$.

1.3 无量纲化能隙方程

$$\begin{aligned}
\eta &= \int_0^{\delta^{-1}\sinh\eta} \tanh\left(\frac{\Delta\sqrt{1+z^2}}{2k_BT}\right)\frac{dz}{\sqrt{1+z^2}} \qquad \left(z=\frac{\xi}{\Delta(T)}\right) \\
&= \int_0^{\delta^{-1}\sinh\eta} \tanh\left(\frac{\Delta}{\Delta_0}\frac{\Delta_0}{2k_BT}\sqrt{1+z^2}\right)\frac{dz}{\sqrt{1+z^2}} \\
&= \int_0^{\delta^{-1}\sinh\eta} \tanh\left(\delta\frac{1.76k_BT_c}{2k_BT}\sqrt{1+z^2}\right)\frac{dz}{\sqrt{1+z^2}} \\
&= \int_0^{\delta^{-1}\sinh\eta} \tanh\left(\frac{\delta}{\tau}0.882\sqrt{1+z^2}\right)\frac{dz}{\sqrt{1+z^2}}.
\end{aligned} \tag{11}$$

1.4 Matlab 代码

```
n = 0.35;
D = zeros(40,1);
t = 0;
for n = 1:40

d0 = [rand];

F = @(d)[

n-integral(@(z) tanh(0.882*d.*sqrt(1+z.^2)./t)./...
sqrt(1+z.^2),0,sinh(n)./d)

];
d = fsolve(F,d0);
t = t + 0.025;
T(n,:) = [t];
D(n,:) = [d];
end
plot(T,D,'p')
```

1.5 一些说明

在解物理中的方程时，无量纲化是很重要的，有时候忘了无量纲化，你选择的参数范围可能是非物理的，所画出来的图自然也是非物理的，即没有任何规律可言.

2 Slave-boson mean-field self-consistent equations

这其实是求解非线性方程组，其中的非线性方程组是从 salve-boson 平均场方法通过求解 t-J 模型得到的，下面的方程取自 Physical Review B **70**,054504(2004):

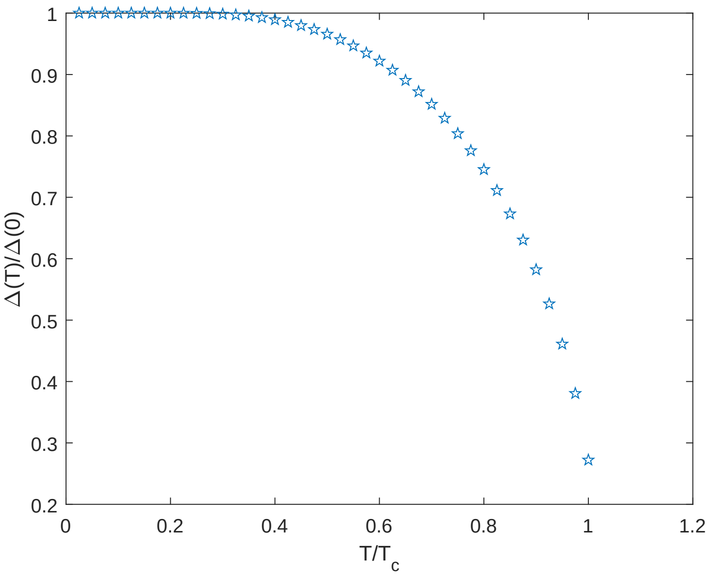

Figure 1: 能隙随温度的变化

$$\frac{1}{J} = \frac{3}{8}\int \frac{d^2k}{(2\pi)^2}\frac{\left(\cos k_x - \cos k_y\right)^2}{E_{\boldsymbol{k}}}, \tag{12}$$

$$\chi = -\frac{1}{4}\int \frac{d^2k}{(2\pi)^2}\left(\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)\left(\cos k_x + \cos k_y\right), \tag{13}$$

$$x = \int \frac{d^2k}{(2\pi)^2}\left(\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right), \tag{14}$$

其中 x 为掺杂浓度.

$$\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$$

$$E_{\boldsymbol{k}} = \sqrt{\xi_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}$$

$$\epsilon_{\boldsymbol{k}} = -2\left(xt + \frac{3J\chi}{4}\right)\left(\cos k_x + \cos k_y\right) + 4xt'\cos k_x \cos k_y, t' = t/4$$

$$\Delta_{\boldsymbol{k}} = \frac{\Delta^{sb}\left(\cos k_x - \cos k_y\right)}{2} = \frac{3J|\Delta|\left(\cos k_x - \cos k_y\right)}{2}$$

2.1 以 J 标度使方程无量纲化

$$\tilde{\epsilon_{\boldsymbol{k}}} = \frac{\epsilon_{\boldsymbol{k}}}{J} = -2\left(x\frac{t}{J} + \frac{3\chi}{4}\right)\left(\cos k_x + \cos k_y\right) + x\frac{t}{J}\cos k_x \cos k_y$$

$$\tilde{\mu} = \frac{\mu}{J}$$

$$\tilde{\Delta_{\boldsymbol{k}}} = \frac{\Delta_{\boldsymbol{k}}}{J} = 1.5|\Delta|\left(\cos k_x - \cos k_y\right)$$

$$\tilde{\xi_{\boldsymbol{k}}} = \frac{\epsilon_{\boldsymbol{k}}}{J} = -2\left(x\frac{t}{J} + \frac{3\chi}{4}\right)\left(\cos k_x + \cos k_y\right) + x\frac{t}{J}\cos k_x \cos k_y - \tilde{\mu}$$

$$\tilde{E_{\boldsymbol{k}}} = \sqrt{\left\{2\left(x\frac{t}{J} + \frac{3\chi}{4}\right)\left(\cos k_x + \cos k_y\right) - x\frac{t}{J}\cos k_x \cos k_y + \tilde{\mu}\right\}^2 + 2.25|\Delta|^2\left(\cos k_x - \cos k_y\right)^2}$$

因此当 $t/J = 3$ 时，我们有下面这一组无量纲化的方程：

$$0 = 1 - \frac{3}{8}\int \frac{d^2k}{(2\pi)^2}\frac{\left(\cos k_x - \cos k_y\right)^2}{\sqrt{\left\{\left(6x + \frac{3\chi}{2}\right)\left(\cos k_x + \cos k_y\right) - 3x\cos k_x \cos k_y + \tilde{\mu}\right\}^2 + 2.25|\Delta|^2\left(\cos k_x - \cos k_y\right)^2}}, \tag{15}$$

$$0 = \chi - \frac{1}{4}\int \frac{d^2k}{(2\pi)^2}\left(\frac{\left(6x+\frac{3\chi}{2}\right)(\cos k_x+\cos k_y)-3x\cos k_x\cos k_y+\tilde{\mu}}{\sqrt{\left\{\left(6x+\frac{3\chi}{2}\right)(\cos k_x+\cos k_y)-3x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+2.25|\Delta|^2(\cos k_x-\cos k_y)^2}}\right)(\cos k_x+\cos k_y)\,, \tag{16}$$

$$0 = x + \int \frac{d^2k}{(2\pi)^2}\frac{\left(6x+\frac{3\chi}{2}\right)(\cos k_x+\cos k_y)-3x\cos k_x\cos k_y+\tilde{\mu}}{\sqrt{\left\{\left(6x+\frac{3\chi}{2}\right)(\cos k_x+\cos k_y)-3x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+2.25|\Delta|^2(\cos k_x-\cos k_y)^2}}. \tag{17}$$

2.1.1 以 t 标度使方程无量纲化

$$\tilde{\epsilon_{\boldsymbol{k}}} = \frac{\epsilon_{\boldsymbol{k}}}{t} = -2\left(x+\frac{3J\chi}{4t}\right)(\cos k_x+\cos k_y)+x\cos k_x\cos k_y$$

$$\tilde{\mu} = \frac{\mu}{t}$$

$$\tilde{\Delta_{\boldsymbol{k}}} = \frac{\Delta_{\boldsymbol{k}}}{t} = \frac{3J|\Delta|(\cos k_x-\cos k_y)}{2t}$$

$$\tilde{E_{\boldsymbol{k}}} = \sqrt{\left\{2\left(x+\frac{3J\chi}{4t}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+2.25\left(\frac{J}{t}\right)^2|\Delta|^2(\cos k_x-\cos k_y)^2}$$

因此当 $t/J = 3$ 时，我们有下面这一组无量纲化的方程：

$$0 = 1 - \frac{1}{8}\int \frac{d^2k}{(2\pi)^2}\frac{(\cos k_x-\cos k_y)^2}{\sqrt{\left\{\left(2x+\frac{\chi}{2}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+0.25|\Delta|^2(\cos k_x-\cos k_y)^2}}, \tag{18}$$

$$0 = \chi - \frac{1}{4}\int \frac{d^2k}{(2\pi)^2}\left(\frac{\left(2x+\frac{\chi}{2}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}}{\sqrt{\left\{\left(2x+\frac{\chi}{2}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+0.25|\Delta|^2(\cos k_x-\cos k_y)^2}}\right)(\cos k_x+\cos k_y)\,, \tag{19}$$

$$0 = x + \int \frac{d^2k}{(2\pi)^2}\frac{\left(2x+\frac{\chi}{2}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}}{\sqrt{\left\{\left(2x+\frac{\chi}{2}\right)(\cos k_x+\cos k_y)-x\cos k_x\cos k_y+\tilde{\mu}\right\}^2+0.25|\Delta|^2(\cos k_x-\cos k_y)^2}}. \tag{20}$$

2.2 Matlab 代码

```
P = zeros(20,3);
d = 0.01;
p0 = [-0.01;rand;1];

for n =  1:20

F=@(p)[

1-((1/8)*(1/(4*pi*pi))*(integral2(@(x,y)  (cos(x)-cos(y)).^2./...
sqrt(((2*d+0.5*p(2)).*(cos(x)+cos(y))-d*cos(x).*cos(y)+p(1)).^2+...
0.25*abs(p(3)).^2.*(cos(x)-cos(y)).^2),-pi,pi,-pi,pi)));

p(2)-((1/4)*(1/(4*pi*pi))*(integral2(@(x,y)  ...
((2*d+0.5*p(2)).*(cos(x)+cos(y))-d*cos(x).*cos(y)+p(1)).*...
(cos(x)+cos(y))./...
sqrt(((2*d+0.5*p(2)).*(cos(x)+cos(y))-d*cos(x).*cos(y)+p(1)).^2+...
0.25*abs(p(3)).^2.*(cos(x)-cos(y)).^2),-pi,pi,-pi,pi)));

d+((1/(4*pi*pi))*(integral2(@(x,y)  ...
```

```
((2*d+0.5*p(2)).*(cos(x)+cos(y))-d*cos(x).*cos(y)+p(1))./...
sqrt(((2*d+0.5*p(2)).*(cos(x)+cos(y))-d*cos(x).*cos(y)+p(1)).^2+...
0.25*abs(p(3)).^2.*(cos(x)-cos(y)).^2),-pi,pi,-pi,pi)))
];

p = fsolve(F,p0);

d = d+0.02;

P(n,:) = [p(1),p(2),p(3)];

p0 = P(n,:);
end

m = 0.01:0.02:0.4;
plot(m,P(:,3),'p')
hold on
plot(m,P(:,2),'*')
```

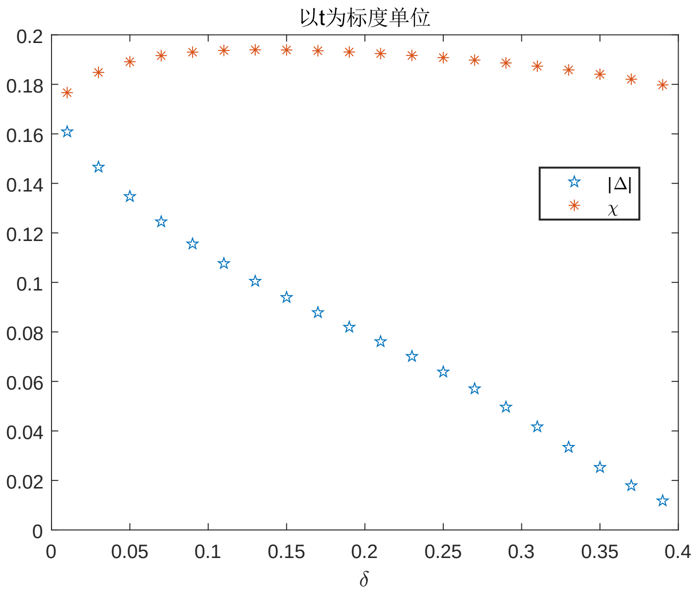

Figure 2: 能隙随掺杂的变化