$T_c(p)$ for a disordered superconductor

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We describe a calculation of $T_c(p)$ in a model of a disordered superconductor which is based on the de Gennes–Skal–Shklovskii (dGSS) picture of the large cluster in a percolation system. The calculation is done by carrying out successive decimations on the Landau-Ginzburg Hamiltonian describing the "links" in the model. We calculate $T_c(p)$ by evaluating the renormalized Landau-Ginzburg coupling when the renormalized Landau-Ginzburg length equals the percolation link length in the dGSS picture. The results reduce to a previous scaling theory in an appropriate limit but contain effects of variations in the amplitude of the superconducting order parameter. The results are in good agreement with experiments on Hg_xXe_{1-x} mixtures by Epstein, Goldman, Dahlberg, and Mikkelson.

I. INTRODUCTION

Inhomogeneous superconductors have been modeled in at least two ways.[1,2] In one model,[1] particularly appropriate for granular superconductors, the conducting paths limiting sample conductance include gaps between grains of superconducting material. In a second model,[2] studied previously by one of us and in more detail here, the limiting conducting paths consist of the one-dimensional (1D) "links" which the de Gennes[3] and Skal and Shklovskii[4] picture suggests in the large percolating cluster. In this second model, superconducting material is assumed to be microscopically mixed with insulating material in a random way so that the geometry can be described by a percolation model. Such a geometrical model seems more appropriate for experimental systems which are produced by vapor codeposition of an insulating and a superconducting material. A percolation model for the geometrical morphology of superconducting material does not, of course, mean that the concentration or temperature dependence of the conductance of a sample can immediately be deduced. For this, one needs a scaling theory which takes account of the superconducting nature of the field on the percolation network. Such a scaling hypothesis was formulated by us earlier,[2] based on ideas of Lubensky[5] and others. Among other things, the scaling hypothesis suggested that $T_c(p) \propto p-p_c$ near p_c, in approximate agreement with experiments on Hg_xXe_{1-x} by Epstein, Goldman, Dahlberg, and Mikkelson.[6] Away from $p=p_c$, however, $T_c(p)$ deviated from linearity and saturated to a value near the bulk value. Here, we describe a calculation based on the model of Ref. 2 which accounts for this effect in terms of the average variation of the amplitude of the superconducting order parameter along the links as p changes.

II. DESCRIPTION OF MODEL AND PLAN OF CALCULATION

Beginning with the de Gennes[3] and Skal and Shklovskii[4] picture, we will only need a model of the 1D links of the large cluster. A model of a one-dimensional superconductor was formulated by Scalapino, Sears, and Ferrell,[7]

$$F=\int_0^l dx/\xi_0 \left[a\,|\psi(x)|^2+b\,|\psi(x)|^4+c\left|\frac{d\psi(x)}{dx}\right|^2\right]. \tag{1}$$

Here, $a=(T-T_c)a'$ and a', b, and c are the familiar Landau-Ginzburg parameters[8] for a superconductor (but since the link is one-dimensional, one must take some care in relating a', b, and c to bulk values; see Sec. IV). The partition function of the link is

$$Z_{\rm link}=\int \mathscr{D}(\psi) e^{-\beta F[\psi]}. \tag{2}$$

Following Ref. 7 the functional integral is approximated by defining stepwise constant functions $\psi(x)=\psi_i$ for x in a region (of length Δx and labeled i) of x values along the chain,

$$Z_{\rm link}\simeq \int d^2\psi_1 \cdots \int d^2\psi_l e^{-\beta F[\psi]}, \tag{3}$$

in which

$$F=\sum_{i=1}^{l-1}\left[\frac{a\Delta x}{\xi_0}|\psi_i|^2+\frac{b\Delta x}{\xi_0}|\psi_i|^4+\frac{c\,|\psi_i-\psi_{i+1}|^2}{\Delta x\,\xi_0}\right]$$
$$\equiv \sum_{i=1}^{l-1}(\tilde{a}\,|\psi_i|^2+\tilde{b}\,|\psi_i|^4+\tilde{c}\,|\psi_i-\psi_{i+1}|^2). \tag{4}$$

The plan of the calculation is as follows: We rewrite $Z_{\rm link}$ by decimation (if l is even),

$$Z_{\rm link}=\int\cdots\int d^2\psi_1 d^2\psi_2\cdots d^2\psi_l \exp-\beta F(\tilde{a},\tilde{b},\tilde{c},\psi_1,\psi_2,\ldots,\psi_l)$$
$$=\int\cdots\int d^2\psi_1 d^2\psi_3\cdots d^2\psi_{l-1}\exp-\beta F(\tilde{a}',\tilde{b}',\tilde{c}',\psi_1,\psi_3,\ldots,\psi_{l-1}), \tag{5}$$

thus defining a renormalization-group transformation

$$R(\tilde{a},\tilde{b},\tilde{c})=\tilde{a}'(\tilde{a},\tilde{b},\tilde{c}),\tilde{b}'(\tilde{a},\tilde{b},\tilde{c}),\tilde{c}'(\tilde{a},\tilde{b},\tilde{c}) ,$$

or, by iteration,

$$R(\tilde{a}_n,\tilde{b}_n,\tilde{c}_n)=\tilde{a}_{n+1},\tilde{b}_{n+1},\tilde{c}_{n+1} . \tag{6}$$

We obtain $T_c(p)$ by iterating this transformation, not at (or near) a fixed point, as in the most common application of renormalization-group ideas, but rather until the (unscaled) length of the bond is equal to the length of the de Gennes–Skal–Shklovskii link. More precisely, suppose that the initial bond length is Δx [as assumed in Eq. (4)]. Then, after n decimations the bond length is $2^n\Delta x$. We write the de Gennes–Skal–Shklovskii link length as $l=l_0\,|p-p_c|^{-\varphi}$, so that at the final iteration $2^n\Delta x=l_0\,|p-p_c|^{-\varphi}$, and the required number of iterations is

$$n=\frac{-\varphi\ln|p-p_c|+\ln(l_0/\Delta x)}{\ln 2} . \tag{7}$$

When this number of iterations is reached, $T_c(p)$ is evaluated by assuming that the resulting network of links and nodes orders like the X-Y model: Referring to Eq. (4), the effective node-node coupling is $-2\tilde{c}_n\,|\psi_i|\,|\psi_{i+1}|$. For long links, one expects the fluctuations in the renormalized $|\psi|$'s to become small. Thus, we take $|\psi_i|\simeq|\psi_{i+1}|=-\tilde{a}_n/2\tilde{b}_n$ so that the node-node coupling is $\tilde{c}_n\tilde{a}_n/\tilde{b}_n$. Turning to the X-Y model, one has $k_BT_c=\alpha J$ where J is the node-node coupling and α depends on the coordination number and dimension of the lattice.[9] Thus, finally,

$$k_BT_c=-\alpha\tilde{c}_n\tilde{a}_n/\tilde{b}_n . \tag{8}$$

This equation defines T_c in terms of p through Eqs. (5)–(7), once the renormalization (6) resulting from the definition (5) has been determined. We next turn to an approximate evaluation of this transformation.

III. APPROXIMATE EVALUATION OF RENORMALIZATION-GROUP TRANSFORMATION BY DECIMATION

Here, we find an approximate explicit form for the transformation (6). We choose periodic boundary conditions so that $\psi_{l+1}=\psi_1$. This will not affect the result when l is large. (l must be of the form 2^m where m is greater than the total number of iterations required.) Then from (3) and (4),

$$Z_{\rm link}=\prod_{m=2,4,\ldots,l}^{l}\int d\psi_m\exp\{-\beta[F_2^{(0)}(\psi_{m-1},\psi_m)+F_2^{(0)}(\psi_m,\psi_{m+2})]\} , \tag{9}$$

in which

$$F_2^{(0)}(\psi,\psi')=\tfrac{1}{2}\tilde{a}(|\psi|^2+|\psi'|^2)+\tfrac{1}{2}\tilde{b}(|\psi|^4+|\psi'|^4)+\tilde{c}\,|\psi-\psi'|^2 . \tag{10}$$

We obtain an approximation renormalization transformation by comparing the coefficient of the leading terms in an expansion of $F_2(\psi,\psi')$ about its minimum before and after decimation. Making this expansion in $F_2^{(0)}(\psi,\psi')$, we have

$$F_2^{(0)}(\psi,\psi')=F_m^{(0)}+(\tilde{c}-\tilde{a})[(\Delta|\psi|)^2+(\Delta|\psi'|)^2]-2\tilde{c}\Delta|\psi|\Delta|\psi'|-\frac{\tilde{a}\tilde{c}}{2\tilde{b}}(\phi-\phi')^2+\cdots . \tag{11}$$

Here,

$$\psi=|\psi|e^{i\phi},\quad \psi'=|\psi'|e^{i\phi'},\quad \Delta|\psi|=|\psi|-(-\tilde{a}/2\tilde{b})^{1/2},\quad \Delta|\psi'|=|\psi'|-(-\tilde{a}/2\tilde{b})^{1/2} ,$$

and

$$F_m^{(0)}=-\tilde{a}^2/4\tilde{b} .$$

We write Z after decimation as

$$Z_{\rm link}=\prod_{m=3,7,11,\ldots,l-1}\int d\psi_m\exp\{-\beta[F_2^{(1)}(\psi_{m-2},\psi_m)+F_2^{(1)}(\psi_m,\psi_{m+2})]\} . \tag{12}$$

From Eqs. (9) and (10), $F_2^{(1)}$ is given by

$$\begin{aligned}\exp[-\beta F_2^{(1)}(\psi_{m-1},\psi_{m+1})]=&\exp\{-\beta[\tfrac{1}{2}(\tilde{a}+2\tilde{c})(|\psi_{m-1}|^2+|\psi_{m+1}|^2)+\tfrac{1}{2}\tilde{b}(|\psi_{m-1}|^4+|\psi_{m+1}|^4)]\}\\ &\times\int|\psi_m|\,d|\psi_m|\int d\phi_m\exp(-\beta\{(\tilde{a}+2\tilde{c})|\psi_m|^2+b|\psi_m|^4\\ &-2\tilde{c}|\psi_m|[|\psi_{m-1}|\cos(\phi_m-\phi_{m-1})\\ &+|\psi_{m+1}|\cos(\phi_m-\phi_{m+1})]\}) .\end{aligned} \tag{13}$$

The integration on ϕ_m can be done with the use of

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{z\sin\phi}d\phi = I_0(z) ,$$

where $I_0(z)$ is a Bessel function of imaginary argument. Approximating $I_0(z)$ by its large argument form one approximates the remaining integral on $|\psi_m|$ by the use of the method of steepest descents. The resulting free energy leads (see the Appendix) to the following form for the transformation defined by Eq. (6):

$$\tilde{c}_{n+1}-\tilde{a}_{n+1}=\tilde{c}_n-\tilde{a}_n - \tilde{c}_n\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{|\psi|=|\psi'|=(-\tilde{a}_n/2\tilde{b}_n)^{1/2},\ \phi=\phi'} , \tag{14a}$$

$$\tilde{c}_{n+1}=\tilde{c}_n\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{|\psi|=|\psi'|=(-\tilde{a}_n/2\tilde{b}_n)^{1/2},\ \phi=\phi'} , \tag{14b}$$

$$\tilde{c}_{n+1}\tilde{a}_{n+1}/\tilde{b}_{n+1}=\tilde{c}_n\tilde{a}_n/2\tilde{b}_n . \tag{14c}$$

Here, x_{2m} is the real positive solution to Eq. (A1) which gives the lowest free energy. Solving the cubic equation (A1) explicitly (see Appendix) permits Eqs. (14) to be explicitly evaluated with results shown in Fig. 1. As expected, the stable fixed point is completely decoupled for a one-dimensional system.

IV. RESULTS FOR $T_c(p)$

Comparing (8) and (14) one sees that only Eq. (14c) is needed for finding T_c. Iterating (14c) n times we have

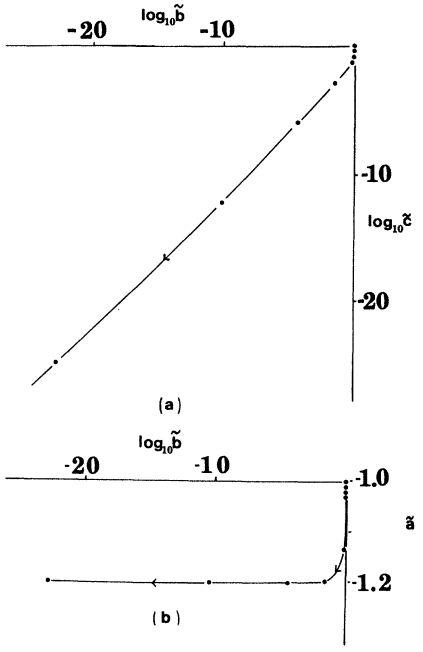

FIG. 1. Results of iteration of Eqs. (14). (a) Shows $\log_{10}\tilde{b}$ vs $\log_{10}\tilde{c}$ for the starting point $(\tilde{a},\tilde{b},\tilde{c})=(-1,1,1)$. (b) Shows $\tilde{a}$ vs $\log_{10}\tilde{b}$ for the starting point $(-1,1,1)$. Solid lines are guides to the eye and show direction of flow.

$$\tilde{c}_n\tilde{a}_n/\tilde{b}_n=2^{-n}\tilde{c}_1\tilde{a}_1/\tilde{b}_1 .$$

Thus,

$$k_BT_c=-\alpha 2^{-n}\tilde{c}_1\tilde{a}_1/\tilde{b}_1 .$$

With the use of (7), taking $\varphi=1$ and supposing that $n\gg\ln(l_0/\Delta x)$, we have $2^{-n}=(\Delta x/l_0)|p-p_c|$, so that

$$k_BT_c=-\alpha\Delta x(p-p_c)\tilde{c}_1\tilde{a}_1/l_0\tilde{b}_1 .$$

By using $\tilde{a}_1=\tilde{a}'(T-T_c^{(0)})$, we find

$$T_c=\frac{\alpha a'c}{k_Bb\xi_0l_0}(p-p_c)(T_c^{(0)}-T_c) ,$$

so that

$$T_c=\frac{K(p-p_c)}{1+K(p-p_c)}T_c^{(0)} , \tag{15}$$

in which

$$K=\alpha a'c/k_Bb\xi_0l_0 . \tag{16}$$

To compare (15) with experiment we require an estimate of the constant K in terms of experimentally accessible parameters. To make the required associations we write the free energy F of a three-dimensional superconductor[8] as

$$F=\frac{\hbar^2}{2m}\int\int\int dx\,dy\,dz\left[\frac{A}{C}|\psi_3|^2+\frac{\hbar^2}{2m}\left[\frac{B}{2C^2}\right]|\psi_B|^4 + |\nabla\psi_3|^2\right] , \tag{17}$$

where the integral is over three dimensions and the quantities A, B, and C are

$$\begin{aligned} A&=N(0)(T-T_c^{(0)})/T_c^{(0)} ,\\ B&=0.098N(0)/(k_BT_c^{(0)})^2 ,\\ C&=0.49\xi_0^2N(0) , \end{aligned} \tag{18}$$

where $N(0)$ is the density of states (per unit volume) at the Fermi level and ξ_0 is the zero-temperature coherence length. $\psi_3(x,y,z)$ is the three-dimensional order parameter. We express (17) in terms of averages across the two directions normal to the chain. (Here, we ignore terms arising from the curvature of the chain. This can only be strictly valid when $\xi_1<l$, that is, on the normal side of the superconducting transition. Corrections arising from curvature of the chain can be studied, but we have not done so here.) Writing $\psi(x)=|\psi(x)|e^{i\phi(x)}$, where x is the distance along the chain, we can determine $|\psi(x)|$, $\phi(x)$, and a normalization area $\mathscr{A}$ through the three equations

$$\begin{aligned} &\int d^2r\,|\psi_3(\vec{r})|^2=|\psi(x)|^2\mathscr{A} ,\\ &\int d^2r\left|\frac{d\psi_3(\vec{r})}{dx}\right|^2=\left|\frac{d\psi(x)}{dx}\right|^2\mathscr{A} ,\\ &\int d^2r\,|\psi_3(\vec{r})|^4=|\psi(x)|^4\mathscr{A} . \end{aligned} \tag{19}$$

$\mathscr{A}$ will be a microscopic area. Because we are studying a chain of metallic atoms surrounded by insulating atoms, it

will be of order (atomic size)^2, and is *not* related to the zero-temperature coherence length. With the use of Eqs. (17)—(19), and omitting a term in

$$\left|\frac{\partial\psi_3}{\partial y}\right|^2+\left|\frac{\partial\psi_3}{\partial z}\right|^2$$

which will not affect the transition, we have

$$F=\frac{\hbar^2\mathscr{A}}{2m}\int\left[\frac{A\xi_0}{C}|\psi(x)|^2+\frac{\hbar^2\xi_0}{2m}\left(\frac{B}{2C^2}\right)|\psi(x)|^4+\left|\frac{d\psi(x)}{dx}\right|^2\xi_0\right]\frac{dx}{\xi_0}\ . \tag{20}$$

Comparing Eq. (20) with Eqs. (1) and (4) gives

$$\tilde{a}=\Delta x\,\mathscr{A}\frac{\hbar^2}{2m}\frac{A}{C}\ ,$$
$$\tilde{b}=\Delta x\,\mathscr{A}\left(\frac{\hbar^2}{2m}\right)^2\frac{B}{2C^2}\ , \tag{21}$$
$$\tilde{c}=\frac{\mathscr{A}}{\Delta x}\left(\frac{\hbar^2}{2m}\right)\ .$$

Combining (16), (18), and (21), one finds

$$K=10.0\left(\frac{\alpha}{l_0}\right)[\mathscr{A}\xi_0^2N(0)k_BT_c^{(0)}]\ .$$

$N(0)$ is estimated from the specific heat[10] [$N(0)=3\gamma/2k_B{}^2\pi^2$; $\gamma=2.2\times10^{-3}$ J/mol(K)^2 for Hg]. For Hg we take $\xi_0=1.3\times10^{-5}$ cm and[8] $T_c^{(0)}=4.15$ K, using $\xi_0=hv_F/\pi\Delta$, $\Delta\simeq2k_BT_c$, and estimating $v_F=k_F^2/hN(0)2\pi^2$. $\mathscr{A}$ is not known. We estimate $\mathscr{A}\approx a^2$ where a is the lattice spacing of 4—5 Å in Hg so that $\mathscr{A}\approx2\times10^{-15}$ cm^2. Thus $K\approx(\alpha/l_0)(2370$ Å).

To compare Eq. (15) with experiment we take p to be the volume fraction of metal (VFM) and make a least-squares fit[11] of Eq. (19) to the data of Epstein *et al.*[6] We find that the following parameters optimize the fit:

$$T_c^{(0)}=(4.34\pm0.12)\text{ K}\ ,$$
$$p_c(\text{VFM})=0.162\pm0.002\ , \tag{22}$$
$$K=157\pm37\ .$$

The quality of the fit is indicated in Fig. 2. The errors are estimated standard deviations in the fit.

V. DISCUSSION AND CONCLUSIONS

The fit of the data to experiment is moderately good. In principle, it would give a measure of l_0 if α were known. Unfortunately, the latter depends on the structure of the large cluster. For cubic ordered three-dimensional lattices one has[9] $\alpha=5.0$ (fcc), 3.25 (bcc), and 2.33 (sc). With these values one finds $l_0\approx(55\pm20)$ Å. The uncertainties are large but the magnitude is plausible. An interesting question is whether this kind of analysis can distinguish between the present model of the large cluster and another proposed by Coniglio.[12] In this latter model, a length $L(p)$ appears such that, at T_c, $\xi_1(T_c)=L(p)$, as in the de Gennes picture. The difference is that $L(p)$ has a different geometrical definition, and $L(p)\propto|\Delta p|^{-\varphi}$, where Coniglio estimates $\varphi=1.12$ in three dimensions. In a model consistent with Coniglio's one may again consider decimation of a chain of length $L(p)$ as done here. The calculation proceeds as before, except that $\varphi\neq1$, and the equation for T_c becomes

$$T_c=\frac{K|p-p_c|^{\varphi}}{1+K|p-p_c|^{\varphi}}T_c^{(0)}\ .$$

With $\varphi=1.12$, this expression fits the data similarly well.

We note that we have found a variation in $T_c(p)$ arising from changes with p in the average amplitude of the order parameter along a link and not from critical fluctuation in the amplitude of the order parameter. The use of a renormalization-group transformation works here because the decimation on one-dimensional links is exact within the de Gennes—Skal—Shklovskii model, and can thus be used to calculate effects involving variables, such as the amplitude of the superconducting order parameter, which are "irrelevant" for calculating the effects of fluctuations at critical points.

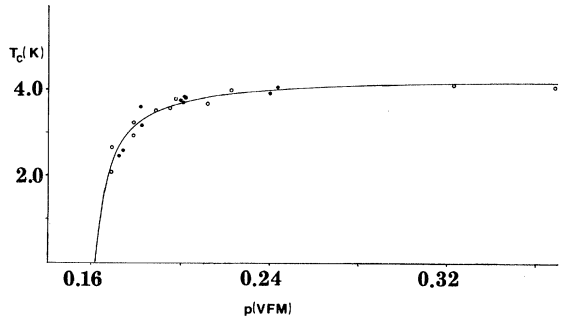

FIG. 2. $T_c(p)$ vs p(VFM). The solid line is Eq. (15) with the values given in Eq. (22). The circles show the data of Epstein *et al.* (Ref. 6). All of the experimental T_c's are defined at the point at which the resistance is 0.5 times normal resistance. Data are included for which p was determined from both partial pressures (open circles) and resistivity (solid circles).

APPENDIX: DERIVATION OF THE RECURSION RELATION

After integrating the ϕ variable one finds that the integrand in Eq. (13) is maximized when

$$|\psi_m|=x_{2m}(|\psi_{m-1}|,|\psi_{m+1}|,\phi_{m-1}-\phi_{m+1})\ ,$$

where x_{2m} satisfies

$$2(\tilde{a}+2\tilde{c})x_{2m}+4\tilde{b}x_{2m}^3-w(|\psi_{m-1}|,|\psi_{m+1}|,\phi_{m-1}-\phi_{m+1})=0\ . \tag{A1}$$

Here,

$$w(x,y,\phi)=2\tilde{c}(x^2+y^2+2xy\cos\phi)^{1/2}\ . \tag{A2}$$

Thus, using the method of steepest descents, the free energy is

$$F_2^{(1)}(\psi_{m-1},\psi_{m+1})=\tfrac{1}{2}(\tilde{a}+2\tilde{c})(|\psi_{m-1}|^2+|\psi_{m+1}|^2)+\tfrac{1}{2}\tilde{b}(|\psi_{m-1}|^4+|\psi_{m+1}|^4)$$
$$+(\tilde{a}+2\tilde{c})x_{2m}^2+\tilde{b}x_{2m}^4-x_{2m}w(|\psi_{m-1}|,|\psi_{m+1}|,\phi_{m-1}-\phi_{m+1})\ . \tag{A3}$$

Here, x_{2m} is the positive real solution to Eq. (A2) which minimizes $F_2^{(1)}(\psi_{m-1},\psi_{m+1})$.

The position x_0,x_0,ϕ_0 of the minimum of $F_2^{(1)}$ with respect to $|\psi_{m-1}|,|\psi_{m+1}|,\phi_{m-2}-\phi_{m+1}$ is given by the equations

$$\left.\frac{\partial F_2^{(1)}}{\partial|\psi_{m\pm1}|}\right|_{|\psi_{m-1}|=|\psi_{m+1}|=x_0,\ \phi_{m-1}-\phi_{m+1}=\phi_0}=0\ , \tag{A4}$$

$$\left.\frac{\partial F_2^{(1)}}{\partial(\phi_{m-1}-\phi_{m+1})}\right|_{|\psi_{m-1}|=|\psi_{m+1}|=x_0,\ \phi_{m-1}-\phi_{m+1}=\phi_0}=0\ . \tag{A5}$$

With the use of (A3), (A4) becomes

$$(\tilde{a}+2\tilde{c})x_0+2bx_0^3-x_{2m}\left.\frac{\partial w}{\partial x}\right|_{x_0,x_0,\phi_0}=0\ , \tag{A6}$$

where Eq. (A1) has been used. (A5) is similarly

$$-x_{2m}\left.\frac{\partial w}{\partial\phi}\right|_{x_0,x_0,\phi_0}=0\ . \tag{A7}$$

If $x_{2m}(x_0,x_0,\phi_0)\neq0$ (as we will assume here and show to be self-consistent), then, from (A7),

$$\left.\frac{\partial w}{\partial\phi}\right|_{x_0,x_0,\phi_0}=0\ .$$

Thus, using (A2),

$$\frac{x_0\sin\phi_0}{\sqrt{2}(1+\cos\phi_0)^{1/2}}=0\ , \tag{A8}$$

which has the physically reasonable solution of $\phi_0=0$. With the use of this solution and Eq. (A2), we obtain

$$\left.\frac{\partial w}{\partial x}\right|_{x_0,x_0,\phi_0}=2\tilde{c}\ .$$

Thus (A6) becomes

$$(\tilde{a}+2\tilde{c})x_0+2\tilde{b}x_0^3-2x_{2m}(x_0,x_0,\phi_0)\tilde{c}=0\ . \tag{A9}$$

On the other hand, from (A2), $w(x_0,x_0,\phi_0)=4\tilde{c}x_0$, so that (A1) can be written as

$$(\tilde{a}+2\tilde{c})x_{2m}(x_0,x_0,\phi_0)+2\tilde{b}x_{2m}^3(x_0,x_0,\phi_0)-2\tilde{c}x_0=0\ . \tag{A10}$$

(A9) and (A10) have the solution

$$x_0=x_{2m}(x_0,x_0,\phi_0)=\left[\frac{-\tilde{a}}{2\tilde{b}}\right]^{1/2}\ . \tag{A11}$$

We have explicitly confirmed numerically that the solution (A11) (with $\phi_0=0$) gives a minimum for $F_2^{(1)}$. Expanding (A3) to second order in $\Delta|\psi_{m\pm1}|=|\psi_{m\pm1}|-x_0$ and $\phi_{m+1}-\phi_{m-1}$ then gives

$$F_2^{(1)}(\psi,\psi')=F_2^{(1)}\left(\left[\frac{-\tilde{a}}{2\tilde{b}}\right]^{1/2},\left[\frac{-\tilde{a}}{2\tilde{b}}\right]^{1/2}\right)+\left[\tilde{c}-\tilde{a}-\tilde{c}\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{|\psi|=|\psi'|=(-\tilde{a}/2\tilde{b})^{1/2},\ \phi=\phi'}\right][(\Delta|\psi|)^2+(\Delta|\psi'|)^2]$$
$$-2\tilde{c}\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{|\psi|=|\psi'|=(-\tilde{a}/2\tilde{b})^{1/2},\ \phi=\phi'}\Delta|\psi|\Delta|\psi'|-\frac{\tilde{a}\tilde{c}}{4\tilde{b}}(\phi-\phi')^2+\cdots\ . \tag{A12}$$

Comparing (A12) and (10) we obtain the transformation defined by Eq. (6) in this approximation, as given in Eqs. (14). To evaluate the transformation (14) explicitly requires the analytical solution of the cubic equation (A1). As is well known, the nature of the solution depends on the sign of a discriminant which in this case takes the form

$$D_n=\frac{w^2}{64b_n^2}+\frac{1}{27}\left[\frac{a_n+2c_n}{2b_n}\right]^3\ .$$

When $D_n>0$ there is only one real solution for x_{2m} and the evalution of

$$\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{x_0,x_0,0}$$

is unambiguous. When $D_n<0$ there are three real solution and

$$\left.\frac{\partial x_{2m}}{\partial|\psi|}\right|_{x_0,x_0,0}$$

must be evaluated for the solution with lowest free energy. Results of implementing this program are shown in Fig. 1.

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