Superfluid Density and the Drude Weight of the Hubbard Model

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106-9530

S. R. White
Department of Physics, University of California, Irvine, California 92717

S. C. Zhang
IBM Research Division, Almaden Research Center, San Jose, California 95120
(Received 24 February 1992)

We study the superfluid density and the Drude weight of the Hubbard model by investigating two different limiting behaviors of the current-current correlation function. These quantities provide criteria which allow one to distinguish between superconducting, metallic, and insulating ground states of an interacting many-body system. Monte Carlo calculations are performed to study these quantities.

PACS numbers: 74.65.+n

It is well known that the signature of the superconducting phase is the onset of the Meissner effect. That is, a sufficiently weak magnetic field is expelled from a bulk superconductor except for a thin penetration depth λ. The inverse square of λ is a measure of the superfluid density [1]. Here for lattice models we introduce a superfluid weight D_s proportional to λ^{-2} and contrast it with the Drude weight D [2,3]. We then examine D_s and D for the two-dimensional (2D) Hubbard model and discuss how these weights can be used to provide information on whether a given model Hamiltonian has an insulating, metallic, or superconducting phase. For the superconducting case, this avoids the problem of having to choose a particular superconducting order parameter and represents a new approach for studying less well-explored models.

The lattice models we will consider have an electron kinetic energy

$$K=-t\sum_{\langle ij\rangle s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is}). \tag{1}$$

Here $c_{is}^{\dagger}$ creates an electron with spin s in an orbital at site i, and the sum is over near-neighbor sites. The interaction can be, for example, an on-site $Un_{i\uparrow}n_{i\downarrow}$ or extended Vn_in_j Hubbard form or a Holstein electron-phonon coupling gn_ix_i in which the site energy depends on the lattice displacement x_i.

In the following, we will examine the current response to a vector potential of wave vector $\mathbf{q}$ and frequency ω,

$$A_x(l,t)=A_x(\mathbf{q})e^{i\mathbf{q}\cdot l-i\omega t}. \tag{2}$$

In the presence of the vector potential, Eq. (1) is modified by the usual Peierls phase factors $e^{ieA_x(l)}$ for $c_{l+xs}^{\dagger}c_{ls}$ and $e^{-ieA_x(l)}$ for $c_{ls}^{\dagger}c_{l+xs}$. Here we will work with units such that $\hbar=c=1$ and also set the lattice spacing equal to 1. Expanding the phase factors to order A^2 in Eq. (1) gives

$$K_A=K-\sum_l[ej_x^p(l)A_x(l)+\tfrac{1}{2}e^2k_x(l)A_x^2(l)]. \tag{3}$$

Here $ej_x^p(l)$ is the x component of the paramagnetic current density with

$$j_x^p(l)=it\sum_s(c_{l+xs}^{\dagger}c_{ls}-c_{ls}^{\dagger}c_{l+xs}), \tag{4}$$

and $k_x(l)$ is the local kinetic energy associated with the x-oriented links,

$$k_x(l)=-t\sum_s(c_{l+xs}^{\dagger}c_{ls}+c_{ls}^{\dagger}c_{l+xs}). \tag{5}$$

The total current density consists of the usual paramagnetic and diamagnetic terms,

$$j_x(l)=-\frac{\delta K_A}{\delta A_x(l)}=ej_x^p(l)+e^2k_x(l)A_x(l). \tag{6}$$

The linear current response produced by the vector potential in Eq. (2) is given by

$$\langle j_x(\mathbf{q},\omega)\rangle=-[e^2(\langle -k_x\rangle-\Lambda_{xx}(\mathbf{q},\omega))A_x(\mathbf{q},\omega)], \tag{7}$$

where $\Lambda_{xx}(\mathbf{q},\omega)$ is obtained from

$$\Lambda_{xx}(\mathbf{q},i\omega_m)=\frac{1}{N}\int_0^{\beta}d\tau\, e^{i\omega_m\tau}\langle j_x^p(\mathbf{q},\tau)j_x^p(-\mathbf{q},0)\rangle, \tag{8}$$

with $\omega_m=2\pi mT$, by the usual analytic continuation $i\omega_m\to\omega+i\delta$, and

$$j_x^p(\mathbf{q})=it\sum_l e^{-\mathbf{q}\cdot l}(c_{l+xs}^{\dagger}c_{ls}-c_{ls}^{\dagger}c_{l+xs}). \tag{9}$$

Here $\langle k_x\rangle$ is the kinetic energy per site divided by the number of lattice dimensions.

The frequency-dependent, uniform, i.e., $\mathbf{q}=0$, electric conductivity $\sigma_{xx}(\omega)$ is given by the current response to an electric field, $E_x(\mathbf{q}=0,\omega)=i\omega A_x(\mathbf{q}=0,\omega)$. From Eq. (7), we have

$$\sigma_{xx}(\omega)=-e^2\frac{\langle -k_x\rangle-\Lambda_{xx}(\mathbf{q}=0,\omega)}{i(\omega+i\delta)}. \tag{10}$$

If the numerator approaches a finite limit as $\omega\to 0$, the real part of $\sigma_{xx}(\omega)$ will contain a delta function contribution $D\delta(\omega)$ with the "Drude weight" given by

$$\frac{D}{\pi e^2}=\langle -k_x\rangle-\Lambda_{xx}(\mathbf{q}=0,i\omega_m\to 0)\equiv\left(\frac{n}{m}\right)^*. \tag{11}$$

This implies a zero resistance state. On the other hand, the Meissner effect is the current response to a static, i.e., $\omega=0$ and transverse gauge potential, $\mathbf{q}\cdot\mathbf{A}(q,\omega=0)=0$. In the small $\mathbf{q}$ limit,

$$\langle j_\alpha(\mathbf{q})\rangle = f(q)(\delta_{\alpha\beta}-q_\alpha q_\beta/\mathbf{q}^2)A_\beta(\mathbf{q})\,. \tag{12}$$

For a superfluid, $f(\mathbf{q}\to 0)=-1/4\pi\lambda^2\equiv -D_s/\pi$ is finite. From Eq. (7), one obtains

$$D_s/\pi e^2 = \langle -k_x\rangle - \Lambda_{xx}(q_x=0,q_y\to 0,i\omega_m=0) \equiv (n_s/m)^*\,, \tag{13}$$

while $\langle -k_x\rangle - \Lambda_{xx}(q_x\to 0,q_y=0,i\omega_m=0)=0$ as required by gauge invariance. D measures the ratio of the density of the mobile charge carriers to their mass $(n/m)^*$, whereas D_s measures the ratio of the superfluid density to mass $(n_s/m)^*$. From Eqs. (12) and (13) we see that the crucial difference between D and D_s is the order in which q_y and $i\omega_m$ approach zero [1,4]. At *zero temperature* without disorder [5], the character of the ground state is determined by the values that D and D_s approach as the size of the system increases to the bulk limit [6]. In this limit we expect that both D and D_s are finite for a superconductor, $D_s=0$ but D is finite for a metal, and $D=D_s=0$ for an insulator [2]. In the presence of disorder or at finite temperatures, the δ function in $\sigma_{xx}(\omega)$ is smeared out to a Lorentzian, so that $D=0$ but $\sigma_{xx}(\omega=0)$ remains finite.

In order to see how these limits behave, consider the noninteracting case in which

$$\Lambda_{xx}(q_y,\omega_m) = \frac{8}{N}\sum_p \sin^2 p_x \frac{f(\varepsilon_{p+q_y})-f(\varepsilon_p)}{i\omega_m-(\varepsilon_{p+q_y}-\varepsilon_p)}\,. \tag{14}$$

For ω_m finite, $\Lambda_{xx}(q_y,\omega_m)$ vanishes when q_y is set to zero, leading to a Drude weight $D/\pi e^2$ equal to $-\langle k_x\rangle$, and we conclude that this system is a metal. Alternatively, if ω_m is set to zero, the $q_y\to 0$ limit of Λ_{xx} is

$$\Lambda_{xx}(q_y\to 0,\omega_m=0) = -\frac{8}{N}\sum_p \sin^2 p_x \frac{\partial f(\varepsilon_p)}{\partial \varepsilon_p}\,. \tag{15}$$

A partial integration shows that this is equal to $\langle -k_x\rangle$ so that D_s vanishes and there is no superfluid density, as expected.

A BCS mean-field calculation gives

$$\Lambda_{xx}(q_y\to 0,0) = \frac{8}{N}\sum_p \sin^2 p_x \frac{\partial f}{\partial E_p}\,, \tag{16}$$

with $E_p=(\varepsilon_p^2+\Delta^2)^{1/2}$, which vanishes as $T/T_c\to 0$. Here Δ is the BCS gap. In the limit when q_y is first set to zero, $\Lambda_{xx}(0,\omega_m)$ also vanishes. Thus the superconducting mean-field ground state is characterized by $D_s/\pi e^2 = D/\pi e^2 = -\langle k_x\rangle$ [7]. The BCS mean-field solution incorrectly gives $\Lambda_{xx}(q_x\to 0,q_y=0,i\omega_m=0)=0$, violating gauge invariance. However, it is well known [1] that vertex corrections remove this difficulty and one obtains $\Lambda_{xx}(q_x\to 0,q_y=0,i\omega_m=0)=\langle -k_x\rangle$, restoring gauge invariance.

Another example is the half-filled repulsive-U Hubbard model. In mean-field theory, the low-temperature state has a spin-density-wave gap $\Delta_{\rm SDW}$. In this case $\Lambda_{xx}(q_y\to 0,\omega_m=0)=-\langle k_x\rangle$, so the superfluid density vanishes. Alternatively, when $q_y=0$ and ω_m goes to zero,

$$\Lambda_{xx}(q_y=0,\omega_m\to 0) = \frac{4}{N}\sum_p \sin^2 p_x \frac{\Delta_{\rm SDW}^2}{E_p^3}[1-2f(E_p)]\,, \tag{17}$$

which is equal to $-\langle k_x\rangle$ when T goes to zero. Thus in the mean-field ground state of the half-filled repulsive-U Hubbard model both D_s and D vanish, consistent with an insulating ground state.

Using Monte Carlo techniques, we have calculated $\Lambda_{xx}(\mathbf{q},\omega_m)$ and $\langle k_x\rangle$ for both the repulsive and the attractive 2D Hubbard models. Results for $\Lambda_{xx}(\mathbf{q},\omega_m)$ for a half-filled band ($\langle n\rangle=1$) with $U=4$ on an 8×8 lattice at $\beta=10$ are shown in Fig. 1. The error bars in this figure and the following figures represent the stochastic Monte

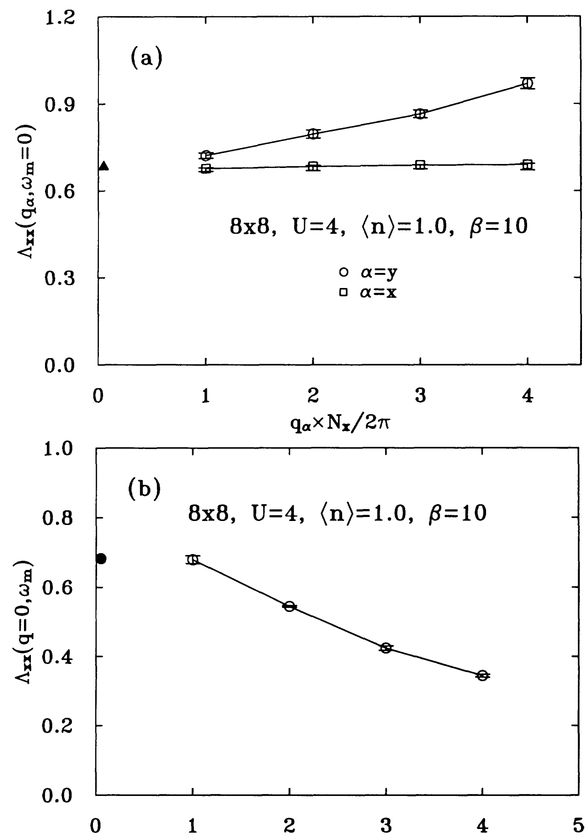

FIG. 1. Monte Carlo results showing (a) $\Lambda_{xx}(q_y,\omega_m=0)$ vs q_y and $\Lambda_{xx}(q_x,\omega_m=0)$ vs q_x; and (b) $\Lambda_{xx}(\mathbf{q}=0,\omega_m)$ vs ω_m for $U=4$, $\langle n\rangle=1$, and $\beta=10$ on an 8×8 lattice. Minus half the kinetic energy per site $\langle -k_x\rangle$ is shown by the solid symbols. The lines are guides to the eye.

Carlo error. Spot checks using different imaginary time slice spacings indicated that any systematic errors from that source were less than 5%. Minus half the kinetic energy per site $\langle -k_x \rangle$ is shown by the solid triangle. In Fig. 1(a), we show $\Lambda_{xx}(q_y,\omega_m=0)$ and $\Lambda_{xx}(q_x,\omega_m=0)$ vs q_y and q_x, respectively. It appears that these both extrapolate towards $\langle -k_x \rangle$ as the momentum transfer goes to zero, leading to $D_s=0$. Figure 1(b) shows $\Lambda_{xx}(\mathbf{q}=0,\omega_m)$ vs ω_m, which appears to extrapolate to a slightly larger value than $\langle -k_x \rangle$ as the temperature goes to zero, leading to a small negative Drude weight for an 8×8 lattice. The half-filled 4×4 lattice has also been found to have a negative Drude weight [8]. As the lattice size increases, we expected this to vanish like $\exp(-N_x/\xi_{\rm SDW})$ as the linear dimension N_x of the lattice increases. Monte Carlo simulations on $4\times 4, 6\times 6, \ldots, 10\times 10$ lattices support this behavior [9]. Thus D and D_s vanish and the half-filled 2D Hubbard model is an insulator.

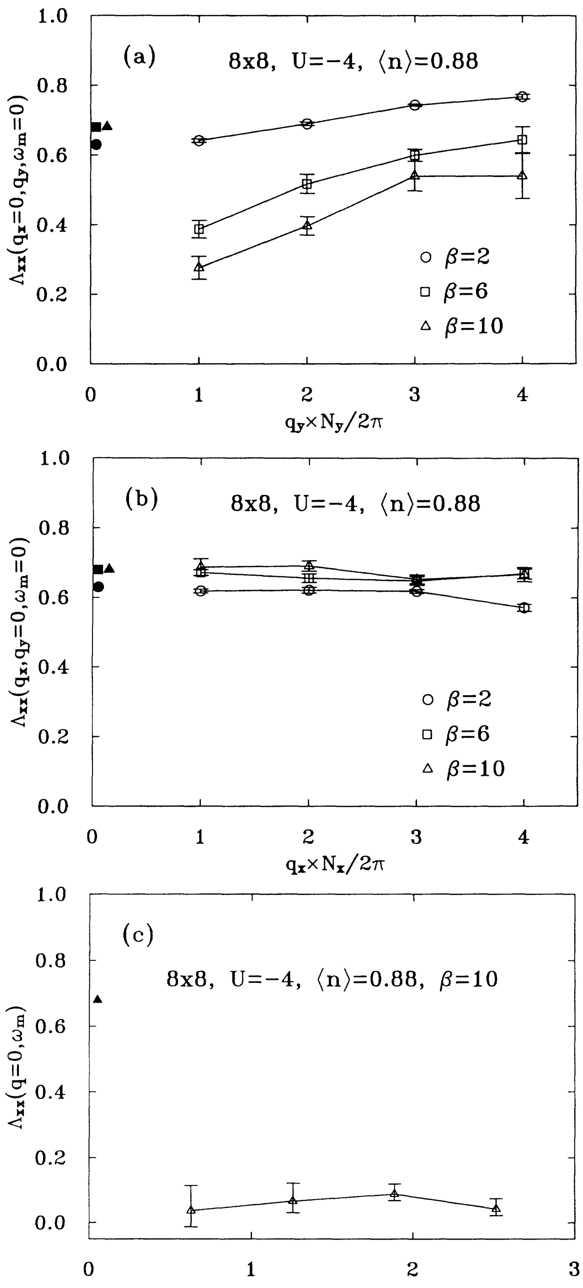

FIG. 2. Monte Carlo results for the attractive Hubbard model. (a) $\Lambda_{xx}(q_y,\omega_m=0)$ vs q_y; (b) $\Lambda_{xx}(q_x,\omega_m=0)$ vs q_x for $U=-4$, $\langle n \rangle \cong 0.875$, and $\beta=2$, 6, and 10. Minus half the kinetic energy, $\langle -k_x \rangle$, is indicated by the solid symbols. (c) Monte Carlo results for $\Lambda_{xx}(\mathbf{q}=0,\omega_m)$ vs ω_m for $U=-4$, $\langle n \rangle \cong 0.875$, and $\beta=10$.

Next consider the attractive Hubbard model with $U=-4$ and a band filling of $\langle n \rangle=0.875$. Results on an 8×8 lattice for $\Lambda_{xx}(q_y,\omega_m=0)$ vs q_y and $\Lambda_{xx}(q_x,\omega_m=0)$ vs q_x are shown in Figs. 2(a) and 2(b) for various temperatures. Again, the kinetic energy $\langle -k_x \rangle$ at a given temperature is shown as the solid symbols. It appears at high temperatures, $\beta=2$, that $\Lambda_{xx}(q_y,\omega_m=0)$ extrapolates towards $\langle -k_x \rangle$ as q_y decreases, implying a zero superfluid density. However, as the system is cooled, the extrapolated value of $\Lambda_{xx}(q_y,\omega_m=0)$ decreases below $\langle -k_x \rangle$ at $\beta=6$ and 10, implying a nonvanishing value for D_s. As $\beta\to\infty$, $\Lambda_{xx}(q_y\to 0,\omega_m=0)$ goes to a finite value less than $\langle -k_x \rangle$ so that n_s/m is finite. Note that $\Lambda_{xx}(q_x\to 0,\omega_m=0)$ continues to approach $\langle -k_x \rangle$, as required from gauge invariance. The behavior of $\Lambda_{xx}(\mathbf{q}=0,\omega_m)$ vs ω_m at $\beta=10$, shown in Fig. 2(c), also leads to a nonvanishing Drude weight. We believe that in the superconducting state $D=D_s$. In two dimensions we expect the negative-U Hubbard model to undergo a Kosterlitz-Thouless [10] transition at a finite temperature [11,12] where both D_s and D would have a step discontinuity on an infinite lattice.

Last we consider the repulsive-U Hubbard model doped away from half filling. In this case, Monte Carlo calculations are hindered by the fermion sign problem [13], which makes it difficult to carry out low-temperature simulations near half filling. Some results for an 8×8 lattice with $U=4$, $\langle n \rangle=0.5$, and $\beta=8$ are shown in Fig. 3. It appears from Fig. 3(a) that both $\Lambda_{xx}(q_x=0,q_y,i\omega_m=0)$ and $\Lambda_{xx}(q_x,q_y=0,i\omega_m=0)$ extrapolate to $\langle -k_x \rangle$, and therefore D_s vanishes. As shown in Fig. 3(b), $\Lambda_{xx}(\mathbf{q}=0,i\omega_m)$ extrapolates to a small value. However, this extrapolation is uncertain because even for $\beta=8$, the Matsubara frequencies $2\pi m/\beta$ at $m=2,3,\ldots$ are at significant energies. An alternative approach, shown in the inset in Fig. 3(b), examines the T going to zero limit using the lowest Matsubara frequency $\omega_1=2\pi T$,

$$D/\pi e^2 = \lim_{T\to 0}\left[-\langle k_x \rangle - \Lambda_{xx}(\mathbf{q}=0,2\pi T)\right]. \qquad (18)$$

Results for $\beta=8$, 6, and 4 are shown in the inset in Fig. 3(b). Both the $\omega_m\to 0$ and the $T\to 0$ extrapolations imply a finite Drude weight $D/\pi e^2$, which is of order 90% of $\langle -k_x \rangle$. Thus it appears that the 2D Hubbard model with

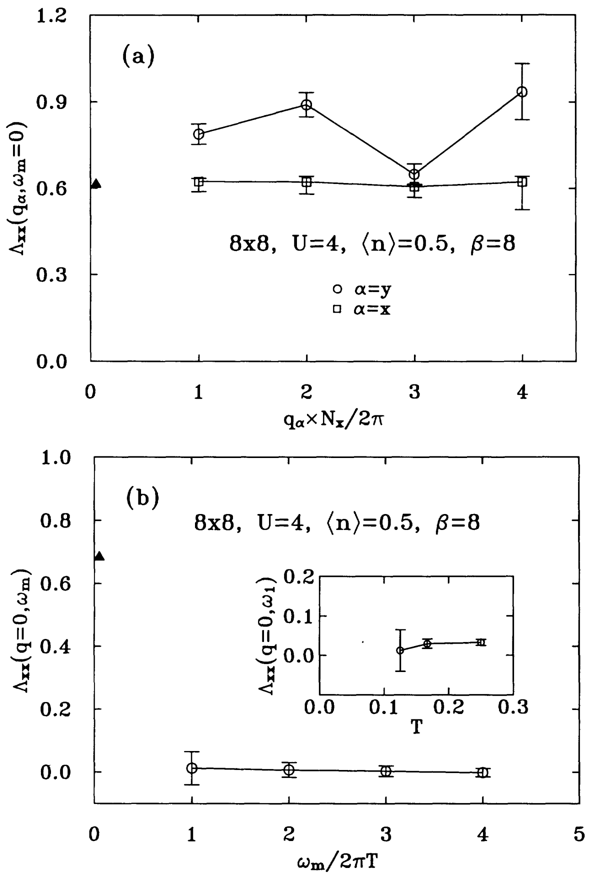

FIG. 3. Monte Carlo results for an 8×8 lattice with $U=4$, $\langle n\rangle=0.5$, and $\beta=8$. (a) $\Lambda_{xx}(q_y,\omega_m=0)$ vs q_y and $\Lambda_{xx}(q_x,\omega_m=0)$ vs q_x; (b) $\Lambda_{xx}(\mathbf{q}=0,\omega_m)$ vs ω_m. $\langle -k_x\rangle$ is plotted as a solid triangle. Inset in (b): $\Lambda_{xx}(\mathbf{q}=0,2\pi T)$ vs T.

$U=4$ and $\langle n\rangle=0.5$ is a metal [14]. Preliminary calculations for values of $\langle n\rangle$ ranging from 0.5 to 0.9 at $\beta=5$ give $D_s\simeq 0$ and finite D.

We thank E. Dagotto, R. T. Scalettar, and J. R. Schrieffer for useful discussions. D.J.S. would like to thank IBM Research and the Almaden Laboratory for their support and hospitality, the Department of Energy for its support under Grant No. DE-FG03-85ER45197, and the Electric Power Research Institute for its support under Grant No. RP8009-18. S.R.W. would like to thank the Office of Naval Research for its support under Grant No. N00014-91-J-1143. This research was also supported in part by the University of California through an allocation of computer time (S.R.W.) and by NERSC (D.J.S.).

[1] J. R. Schrieffer, *Theory of Superconductivity* (Addison-Wesley, Reading, MA, 1964).
[2] W. Kohn, Phys. Rev. **133**, A171 (1964).
[3] B. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[4] D. Pines and P. Nozieres, *The Theory of Quantum Liquids I* (Addison-Wesley, Reading, MA, 1966).
[5] The role of disorder in interacting Bose systems has been recently studied using quantum Monte Carlo techniques by R. T. Scalettar, G. G. Batrouni, and G. T. Zimanyi, Phys. Rev. Lett. **66**, 3144 (1991). The role of disorder in the fermion Hubbard model is being explored by E. Dagotto.
[6] For example, in the insulating spin-density-wave (SDW) state, D and D_s approach zero exponentially [2] with a length scale set by the SDW coherence length, $\xi_{\rm SDW}=v_F/\pi\Delta_{\rm SDW}$.
[7] In this case $(n_s/m)^*=\langle -k_x\rangle$ which varies as t in weak coupling and $t^2/|U|$ in strong coupling [J. E. Hirsch and F. Marsiglio (to be published)].
[8] R. M. Fye *et al.*, Phys. Rev. B **44**, 6909 (1991); E. Dagotto *et al.*, NSF Report No. NSF-ITP-91-58 (to be published).
[9] D. J. Scalapino, S. White, and S. C. Zhang (to be published).
[10] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[11] R. T. Scalettar *et al.*, Phys. Rev. Lett. **62**, 1407 (1989).
[12] A. Moreo and D. J. Scalapino, Phys. Rev. Lett. **66**, 946 (1991).
[13] E. Y. Loh *et al.*, Phys. Rev. B **41**, 9301 (1990).
[14] A nonzero D arises on a finite lattice at temperatures below the threshold for quasi-particle-hole excitation, which is finite on a finite-sized lattice. However, as the lattice size increases this threshold temperature scales to zero so that for a normal metal with an infinite lattice, $D=0$ unless $T=0$.